# A Lambda-Calculus Foundation for Universal Probabilistic Programming\*

Johannes Borgström<sup>†</sup> Ugo Dal Lago<sup>‡</sup> Andrew D. Gordon<sup>§</sup>
Marcin Szymczak<sup>¶</sup>

January 24, 2017

#### Abstract

We develop the operational semantics of an untyped probabilistic  $\lambda$ -calculus with continuous distributions, and both hard and soft constraints, as a foundation for universal probabilistic programming languages such as Church, Anglican, and Venture. Our first contribution is to adapt the classic operational semantics of  $\lambda$ -calculus to a continuous setting via creating a measure space on terms and defining step-indexed approximations. We prove equivalence of big-step and small-step formulations of this distribution-based semantics. To move closer to inference techniques, we also define the sampling-based semantics of a term as a function from a trace of random samples to a value. We show that the distribution induced by integration over the space of traces equals the distribution-based semantics. Our second contribution is to formalize the implementation technique of trace Markov chain Monte Carlo (MCMC) for our calculus and to show its correctness. A key step is defining sufficient conditions for the distribution induced by trace MCMC to converge to the distribution-based semantics. To the best of our knowledge, this is the first rigorous correctness proof for trace MCMC for a higher-order functional language, or for a language with soft constraints.

<sup>\*</sup>The first author is supported by the Swedish Research Council grant 2013-4853. The second author is partially supported by the ANR project 12IS02001 PACE and the ANR project 14CE250005 ELICA. The fourth author was supported by Microsoft Research through its PhD Scholarship Programme.

<sup>&</sup>lt;sup>†</sup>Uppsala University

<sup>&</sup>lt;sup>‡</sup>University of Bologna & INRIA

<sup>§</sup>Microsoft Research and University of Edinburgh

<sup>¶</sup>University of Edinburgh

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### 1 Introduction

In computer science, probability theory can be used for models that enable system abstraction, and also as a way to compute in a setting where having access to a source of randomness is essential to achieve correctness, as in randomised computation or cryptography [11]. Domains in which probabilistic models play a key role include robotics [37], linguistics [24], and especially machine learning [31]. The wealth of applications has stimulated the development of concrete and abstract programming languages, that most often are extensions of their deterministic ancestors. Among the many ways probabilistic choice can be captured in programming, a simple one consists in endowing the language of programs with an operator modelling the sampling from (one or many) distributions. This renders program evaluation a probabilistic process, and under mild assumptions the language becomes universal for probabilistic computation. Particularly fruitful in this sense has been the line of work in the functional paradigm.

In *probabilistic programming*, programs become a way to specify probabilistic models for observed data, on top of which one can later do inference. This has been a source of inspiration for AI researchers, and has recently been gathering interest in the programming language community (see Goodman [12], Gordon et al. [16], and Russell [33]).

### 1.1 Universal Probabilistic Programming in Church

Church [15] introduced universal probabilistic programming, the idea of writing probabilistic models for machine learning in a Turing-complete functional programming language. Church, and its descendants Venture [25], Anglican [39], and Web Church [14] are dialects of Scheme. Another example of universal probabilistic programming is Webpel [13], a probabilistic interpretation of JavaScript.

A probabilistic query in Church has the form:

```
(query (define x_1 e_1)...(define x_n e_n) e_q e_c)
```

The query denotes the distribution given by the probabilistic expression  $e_q$ , given variables  $x_i$  defined by potentially probabilistic expressions  $e_i$ , constrained so that the boolean predicate  $e_c$  is true.

Consider a coin with bias p, that is, p is the probability of heads. Recall that the *geometric distribution* of the coin is the distribution over the number of flips in a row before it comes up heads. An example of a Church query is as follows: it denotes the geometric distribution for a fair coin, constrained to be greater than one.

```
(query
  (define flip (lambda (p) (< (rnd) p)))
  (define geometric (lambda (p)
        (if (flip p) 0 (+ 1 (geometric p))))
  (define n (geometric .5))
  n
  (> n 1))
```

The query defines three variables: (1) flip is a function that flips a coin with bias p, by calling (rnd) to sample a probability from the uniform distribution on the unit interval; (2) geometric is a function that samples from the geometric distribution of a coin with bias p; and (3) n denotes the geometric distribution with bias 0.5. Here are samples from this query:

```
(5 5 5 4 2 2 2 2 2 3 3 2 2 7 2 2 3 4 2 3)
```

This example is a discrete distribution with unbounded support (any integer greater than one may be sampled with some non-zero probability), defined in terms of a continuous distribution (the uniform distribution on the unit interval). Queries may also define continuous distributions, such as regression parameters.

 $<sup>^{1}\</sup>mathrm{See}\ \mathrm{http://forestdb.org/models/geometric.html.}$ 

### 1.2 Problem 1: Semantics of Church Queries

The first problem we address in this work is to provide a formal semantics for universal probabilistic programming languages with constraints. Our example illustrates the common situation in machine learning that models are based on continuous distributions (such as (rnd)) and use constraints, but previous works on formal semantics for untyped probabilistic  $\lambda$ -calculi do not rigorously treat the combination of these features.

To address the problem we introduce a call-by-value  $\lambda$ -calculus with primitives for random draws from various continuous distributions, and primitives for both hard and soft constraints. We present an encoding of Church into our calculus, and some nontrivial examples of probabilistic models.

We consider two styles of operational semantics for our  $\lambda$ -calculus, in which a term is interpreted in two ways, the first closer to inference techniques, the second more extensional:

Sampling-Based: A function from a trace to a value and weight.

Distribution-Based: A distribution over terms of our calculus.

To obtain a thorough understanding of the semantics of the calculus, for each of these styles we present two inductive definitions of operational semantics, in small-step and big-step style.

First, we consider the *sampling-based semantics*: the two inductive definitions have the forms shown below, where M is a closed term, s is a finite *trace* of random real numbers, w > 0 is a *weight* (to impose soft constraints), and G is a *generalized value* (either a value (constant or  $\lambda$ -abstraction) or the exception fail, used to model a failing hard constraint).

- Figure 4 defines small-step relation  $(M, w, s) \to (M', w', s')$ .
- Figure 1 defines the big-step relation  $M \downarrow_w^s G$ .

For example, if M is the  $\lambda$ -term for our geometric distribution example and we have  $M \Downarrow_w^s G$  then there is  $n \geq 0$  such that:

- the trace has the form  $s = [q_1, \ldots, q_{n+1}]$  where each  $q_i$  is a probability, and  $q_i < 0.5$  if and only if i = n + 1. (A sample  $q_i \ge 0.5$  is tails; a sample  $q_i < 0.5$  is heads.)
- the result takes the form G = n if n > 1, and otherwise G = fail (the failure of a hard constraint leads to fail);
- and the weight is w = 1 (the density of the uniform distribution on the unit interval).

Our first result, Theorem 1, shows equivalence: that the big-step and small-semantics of a term consume the same traces to produce the same results with the same weights.

To interpret these semantics probabilistically, we describe a metric space of  $\lambda$ -terms and let  $\mathscr{D}$  range over *distributions*, that is, sub-probability Borel measures on terms of the  $\lambda$ -calculus. We define  $[\![M]\!]_{\mathbb{S}}$  to be the distribution induced by the sampling-based semantics of M, by integrating the weight over the space of traces.

Second, we consider the distribution-based semantics, that directly associate distributions with terms, without needing to integrate out traces. The two inductive definitions have the forms shown below, where n is a step-index:

- Figure 6 defines a family of small-step relations  $M \Rightarrow_n \mathscr{D}$ .
- Figure 7 defines a family of big-step relations  $M \downarrow_n \mathscr{D}$ .

These step-indexed families are approximations to their suprema, distributions written as  $[\![M]\!]_{\Rightarrow}$  and  $[\![M]\!]_{\Downarrow}$ . By Theorem 2 we have  $[\![M]\!]_{\Rightarrow} = [\![M]\!]_{\Downarrow}$ . The proof of the theorem needs certain properties (Lemmas 30, 34, and 36) that build on compositionality results for sub-probability kernels [28] from the measure theory literature. We apply the distribution-based semantics in Section 4.7 to show an equation between hard and soft constraints.

Finally, we reconcile the two rather different styles of semantics: Theorem 3 establishes that  $[\![M]\!]_{\mathbb{S}} = [\![M]\!]_{\Rightarrow}$ .

#### 1.3 Problem 2: Correctness of Trace MCMC

The second problem we address is implementation correctness. As recent work shows [19, 22], subtle errors in inference algorithms for probabilistic languages are a motivation for correctness

proofs for probabilistic inference.

Markov chain Monte Carlo (MCMC) is an important class of inference methods, exemplified by the Metropolis-Hastings (MH) algorithm [26, 17], that accumulates samples from a target distribution by exploring a Markov chain. The original work on Church introduced the implementation technique called  $trace\ MCMC$  [15]. Given a closed term M, trace MCMC generates a Markov chain of traces,  $s_0, s_1, s_2, \ldots$  The MH algorithm is parametric in a  $proposal\ kernel\ Q$ : a function that maps a trace s of M to a probability distribution over traces, used to sample the next trace in the Markov chain.

Our final result, Theorem 4, asserts that the Markov chain generated by trace MCMC converges to a stationary distribution, and that the induced distribution on values is equal to the semantics  $[\![M]\!]$  conditional on success, that is, that the computation terminates and yields a value (not fail). We formalize the algorithm rigorously, defining our proposal kernel as a Lebesgue integral of a corresponding density function, that we show to be measurable with respect to the  $\sigma$ -algebra on program traces. We show that the resulting Markov chain satisfies standard criteria: aperiodicity and irreducibility. Hence, Theorem 4 follows from a classic result of Tierney [38] together with Theorem 3.

### 1.4 Contributions of the Paper

We make the following original contributions:

- 1. Definition of an untyped  $\lambda$ -calculus with continuous distributions capable of encoding the core of Church.
- 2. Development of both sampling-based and distribution-based semantics, shown equivalent (Theorems 1, 2, and 3).
- 3. First proof of correctness of trace MCMC for a  $\lambda$ -calculus (Theorem 4).

The only previous work on formal semantics of  $\lambda$ -calculi with constraints and continuous distributions is recent work by Staton et al. [35]. Their main contribution is an elegant denotational semantics for a simply typed  $\lambda$ -calculus with continuous distributions and both hard and soft constraints, but without recursion. They do not consider MCMC inference. Their work does not apply to the recursive functions (such as the geometric distribution in Section 1.1) or data structures (such as lists) typically found in Church programs. For our purpose of conferring formal semantics on Church-family languages, we consider it advantageous to rely on untyped techniques.

The only previous work on correctness of trace MCMC, and an important influence on our work, is a recent paper by Hur et al. [19] which proves correct an algorithm for computing an MH Markov chain. Key differences are that we work with higher-order languages and soft constraints, and that we additionally give a proof that our Markov chain always converges, via the correctness criteria of Tierney [38].

### 1.5 Structure of the Paper

The rest of the paper is organized as follows.

Section 2 defines the syntax of our probabilistic  $\lambda$ -calculus with draws from continuous distributions, and defines a deterministic sampling-based operational semantics for our calculus. The semantics is based on the explicit consumption of a program trace s of random draws and production of an explicit weight w for each outcome.

Section 3 is concerned with a more in-depth treatment of sampling-based semantics, given in two standard styles: big-step semantics,  $M \Downarrow_w^s G$ , and small-step semantics,  $(M, w, s) \rightarrow (M', w', s')$ , which are equivalent by Theorem 1. We define a distribution  $[\![M]\!]$  on outcomes of M by integrating the weights with respect to a measure on traces and applying a measure transformation.

Section 4 defines our step-indexed distribution-based operational semantics, in both small-step  $(M \Rightarrow_n \mathscr{D})$  and big-step  $(M \Downarrow_n \mathscr{D})$  styles, which by Theorem 2 are equivalent, and define the

meaning  $\llbracket M \rrbracket$  of a term M to be the supremum of the step-indexed semantics. We end by linking the semantics of this section with those of Section 3: Theorem 3 establishes that  $\llbracket M \rrbracket_{\mathbb{S}} = \llbracket M \rrbracket$ 

Section 5 formalizes trace MCMC for our calculus, in the spirit of Hur et al. [19]. Theorem 4 shows equivalence between the distribution computed by the algorithm and the semantics of the previous sections. Hence, Theorem 4 is the first correctness theorem for trace MCMC for a  $\lambda$ -calculus.

Section 6 describes related work and Section 7 concludes.

Appendix A collects various proofs of measurability.

### 2 A Foundational Calculus for Church

In this section, we describe the syntax of our calculus and equip it with an intuitive semantics relating program outcomes to the sequences of random choices made during evaluation. By translating Church constructs to this calculus, we show that it serves as a foundation for Turing-complete probabilistic languages.

To simplify the presentation, we do not include primitives for discrete distributions in the calculus, as they can be encoded using the uniform distribution on the unit interval and inverse mass functions. However, it would be easy to extend the calculus with primitive discrete random distributions, represented by their probability mass functions rather than densities. In Section 3.3, we explain how the semantics could be adapted in this case.

### 2.1 Syntax of the Calculus

We represent scalar data as real numbers  $c \in \mathbb{R}$ . We use 0 and 1 to represent false and true, respectively. Let  $\mathcal{I}$  be a countable set of distribution identifiers (or simply distributions). Metavariables for distributions are D, E. Each distribution identifier D has an integer  $arity |D| \geq 0$ , and defines a density function  $\mathrm{pdf}_{D}: \mathbb{R}^{|D|+1} \to [0,\infty)$  of a sub-probability kernel. For example, a draw (rnd()) from the uniform distribution on the unit interval has density  $\mathrm{pdf}_{\mathsf{rnd}}(c) = 1$  if  $c \in [0,1]$  and otherwise 0, while a draw (Gaussian(m,v)) from the Gaussian distribution with mean m and variance v has density  $\mathrm{pdf}_{\mathsf{Gaussian}}(m,v,c) = 1/(e^{\frac{(c-m)^2}{2v}}\sqrt{2v\pi})$  if v>0 and otherwise 0.

Let g be a metavariable ranging over a countable set of function identifiers each with an integer  $arity \ |g| > 0$  and with an interpretation as a total measurable function  $\sigma_g : \mathbb{R}^{|g|} \to \mathbb{R}$ . Examples of function identifiers include addition +, comparison >, and equality =; they are often written in infix notation. We define the values V and  $terms\ M$  as follows, where x ranges over a denumerable set of variables  $\mathcal{X}$ .

The term fail acts as an exception and models a failed hard constraint. The term score(c) models a soft constraint, and is parametrized on a positive probability  $c \in (0,1]$ . As usual, free occurrences of x inside M are bound by  $\lambda x.M$ . Terms are taken modulo renaming of bound variables. Substitution of all free occurrences of x by a value V in M is defined as usual, and denoted  $M\{V/x\}$ . This can be easily generalized to  $M\{\vec{V}/\vec{x}\}$ , where  $\vec{x}$  is a sequence of variables and  $\vec{V}$  is a sequence of values (of the same length). Let  $\Lambda$  denote the set of all terms, and  $C\Lambda$  the set of closed terms. The set of all closed values is V, and we write  $V_{\lambda}$  for  $V \setminus \mathbb{R}$ . Generalized values G, H are elements of the set  $\mathcal{GV} = \mathcal{V} \cup \{\text{fail}\}$ , i.e., generalized values are either values or fail. Finally, erroneous redexes, ranged over by metavariables like T, R, are closed terms in one of the following five forms:

• c M.

```
\frac{G \in \mathcal{GV}}{G \Downarrow_{1}^{\square} G} \text{ (EVAL VAL)} \qquad \frac{w = \operatorname{pdf}_{\mathsf{D}}(\vec{c},c) \qquad w > 0}{\mathsf{D}(\vec{c}) \Downarrow_{w}^{[c]} c} \text{ (EVAL RANDOM)}
\frac{\operatorname{pdf}_{\mathsf{D}}(\vec{c},c) = 0}{\mathsf{D}(\vec{c}) \Downarrow_{0}^{[c]} \operatorname{fail}} \text{ (EVAL RANDOM FAIL)} \qquad \overline{g(\vec{c}) \Downarrow_{1}^{\square} \sigma_{g}(\vec{c})} \text{ (EVAL PRIM)}
\frac{M \Downarrow_{w_{1}}^{s_{1}} \lambda x. P \qquad N \Downarrow_{w_{2}}^{s_{2}} V \qquad P[V/x] \Downarrow_{w_{3}}^{s_{3}} G}{M N \Downarrow_{w_{1}}^{s_{1}} \mathbb{O}(w_{2}) \mathbb{O}(w_{3})} \text{ (EVAL APPL)}
\frac{M \Downarrow_{w}^{s} \operatorname{fail}}{M N \Downarrow_{w}^{s} \operatorname{fail}} \text{ (EVAL APPL RAISE1)} \qquad \frac{M \Downarrow_{w}^{s} c}{M N \Downarrow_{w}^{s} \operatorname{fail}} \text{ (EVAL APPL RAISE2)}
\frac{M \Downarrow_{w_{1}}^{s_{1}} \lambda x. P \qquad N \Downarrow_{w_{2}}^{s_{2}} \operatorname{fail}}{M N \Downarrow_{w_{1}}^{s_{2}} \mathbb{O}(w_{2}) \mathbb{O}(w_{2})} \text{ (EVAL APPL RAISE3)}
\frac{M \Downarrow_{w}^{s} G}{\operatorname{if true then } M \operatorname{else } N \Downarrow_{w}^{s} G} \text{ (EVAL IF TRUE)}
\frac{N \Downarrow_{w}^{s} G}{\operatorname{if false then } M \operatorname{else } N \Downarrow_{w}^{s} G} \text{ (EVAL IF FALSE)}
\frac{c \in (0,1]}{\operatorname{score}(c) \Downarrow_{c}^{c} \operatorname{true}} \text{ (EVAL SCORE)} \qquad \frac{T \operatorname{is an erroneous redex}}{T \Downarrow_{1}^{\square} \operatorname{fail}} \text{ (EVAL FAIL)}
```

Figure 1: Sampling-Based Big Step Semantics

- $D(V_1, \ldots, V_{|D|})$  where at least one of the  $V_i$  is a  $\lambda$ -abstraction.
- $g(V_1, \ldots, V_{|q|})$  where at least one of the  $V_i$  is a  $\lambda$ -abstraction.
- if V then M else N, where V is neither true nor false.
- score(V), where  $V \notin (0,1]$ .

### 2.2 Big-step Sampling-based Semantics

In defining the first semantics of the calculus, we use the classical observation [23] that a probabilistic program can be interpreted as a deterministic program parametrized by the sequence of random draws made during the evaluation. We write  $M \downarrow_w^s V$  to mean that evaluating M with the outcomes of random draws as listed in the sequence s yields the value V, together with the weight w that expresses how likely this sequence of random draws would be if the program was just evaluated randomly. Because our language has continuous distributions, w is a probability density rather than a probability mass. Similarly,  $M \downarrow_w^s$  fail means that evaluation of M with the random sequence s fails. In either case, the finite trace s consists of exactly the random choices made during evaluation, with no unused choices permitted.

Formally, we define program traces s, t to be finite sequences  $[c_1, \ldots, c_n]$  of reals of arbitrary length. We let  $M \Downarrow_w^s G$  be the least relation closed under the rules in Figure 1. The (EVAL RANDOM) rule replaces a random draw from a distribution D parametrized by a vector  $\vec{c}$  with the first (and only) element c of the trace, presumed to be the outcome of the random draw, and sets the weight to the value of the density of  $D(\vec{c})$  at c. (EVAL RANDOM FAIL) throws an exception if c is outside the support of the corresponding distribution. Meanwhile, (EVAL SCORE), applied to score(c), sets the weight to c and returns a dummy value. The applications of soft constraints using score are described in Section 2.5.

All the other rules are standard for a call-by-value lambda-calculus, except that they allow the traces to be split between subcomputations and they multiply the weights yielded by subcompu-

```
\langle c \rangle_e = c
\langle x \rangle_e = x
\langle g \ e_1, \dots, e_n \rangle_e =
        let x_1 = e_1 in ...let x_n = e_n in g(x_1, \ldots, x_n)
         where x_1, \ldots, x_n \notin fv(e_1) \cup \cdots \cup fv(e_n)
\langle \mathsf{D} \ e_1, \dots e_n \rangle_e =
         let x_1 = e_1 in ...let x_n = e_n in \mathsf{D}(x_1,\ldots,x_n)
where x_1,\ldots,x_n\notin fv(e_1)\cup\cdots\cup fv(e_n) (lambda () e\rangle_e=\lambda x.\langle e\rangle_e where x\notin fv(e)
\langle \text{lambda } x \ e \rangle_e = \lambda x. \langle e \rangle_e
\langle \text{lambda}(x_1 \ldots x_n) | e \rangle_e = \lambda x_1 . \langle \text{lambda}(x_2 \ldots x_n) | e \rangle_e
\langle e_1 \ e_2 \rangle_e = \langle e_1 \rangle_e \ \langle e_2 \rangle_e
\langle e_1 \ e_2 \ \dots \ e_n \rangle_e = \langle (e_1 \ e_2) \ \dots \ e_n \rangle_e
\langle \text{if } e_1 \ e_2 \ e_3 \rangle_e = \text{let } x = e_1 \ \text{in } (\text{if } x \ \text{then } \langle e_2 \rangle_e \ \text{else } \langle e_3 \rangle_e)
         where x \notin fv(e_2) \cup fv(e_3)
\langle \text{query (define } x_1 \ e_1 \rangle \dots (\text{define } x_n \ e_n) \ e_{out} \ e_{cond} \rangle =
        let x_1 = (fix \ x_1 . \langle e_1 \rangle_e) in
         let x_n = (\operatorname{fix} x_n.\langle e_n \rangle_e) in
         \mathtt{let}\ b = e_{cond}\ \mathtt{in}
         if b then e_{out} else fail
```

Figure 2: Translation of Church

tations to obtain the overall weight.

### 2.3 Encoding Church

We now demonstrate the usefulness and expressive power of the calculus via a translation of Church, an untyped higher-order functional probabilistic language.

The syntax of Church's expressions, definitions and queries is described as follows:

To make the translation more intuitive, it is convenient to add to the target language a letexpression of the form let x = M in N, that can be interpreted as syntactic sugar for  $(\lambda x.N)$  M, and sequencing M; N that stands for  $\lambda \star .N$  M where  $\star$  as usual stands for a variable that does not appear free in any of the terms under consideration.

The rules for translating Church expressions to the calculus are shown in Figure 2, where fv(e) denotes the set of free variables in expression e and fix x.M is a call-by-value fixpoint combinator  $\lambda y.N_{fix}N_{fix}(\lambda x.M)y$  where  $N_{fix}$  is  $\lambda z.\lambda w.w(\lambda y.((zz)w)y)$ . Observe that (fix x.M)V evaluates to  $M\{(fix x.M)/x\}V$  deterministically. We assume that for each distribution identifier D of arity k, there is a deterministic function  $pdf_D$  of arity k+1 that calculates the corresponding density at the given point.

In addition to expressions presented here, Church also supports stochastic memoization [15] by means of a mem function, which, applied to any given function, produces a version of it that always returns the same value when applied to the same arguments. This feature allows for functions of integers to be treated as infinite lazy lists of random values, and is useful in defining some nonparametric models, such as the Dirichlet Process.

It would be straightforward to add support for memoization in our encoding by changing the translation to state-passing style, but we omit this standard extension for the sake of brevity.

### 2.4 Example: Geometric Distribution

To illustrate the sampling-based semantics, recall the geometric distribution example from Section 1. It translates to the following program in the core calculus:

```
\begin{split} \text{let } flip &= \lambda x.(\text{rnd}() < x) \text{ in} \\ \text{let } geometric &= \\ & (fix \ g. \\ & \lambda p. \ (\text{let } y = \text{rnd}() < p \text{ in} \\ & \text{if } y \text{ then } 0 \text{ else } 1 + (g \ p))) \text{ in} \\ \text{let } n &= fix \ n'.geometric \ 0.5 \text{ in} \\ \text{let } b &= n > 1 \text{ in} \\ \text{if } b \text{ then } n \text{ else fail} \end{split}
```

Suppose we want to evaluate this program on the random trace s = [0.7, 0.8, 0.3]. By (EVAL APPL), we can substitute the definitions of *flip* and *geometric* in the remainder of the program, without consuming any elements of the trace nor changing the weight of the sample. Then we need to evaluate *geometric* 0.5.

It can be shown (by repeatedly applying (EVAL APPL)) that for any lambda-abstraction  $\lambda x.M$ ,  $M\{(fix\ x.M)/x\}\ V\ \psi_w^s\ G$  if and only if  $(fix\ x.M)\ V\ \psi_w^s\ G$ , which allows us to unfold the recursion. Applying the unfolded definition of geometric to the argument 0.5 yields an expression of the form

```
let y = \text{rnd}() < 0.5 in if y then 0 else 1 + (...).
```

For the first random draw, we have  $\operatorname{rnd}() \ \psi_1^{[0.7]} \ 0.7$  by (EVAL RANDOM) (because the density of rnd is 1 on the interval [0,1]) and so (EVAL PRIM) gives  $\operatorname{rnd}() < 0.5 \ \psi_1^{[0.7]}$  false. After unfolding the recursion two more times, evaluating the subsequent "flips" yields  $\operatorname{rnd}() < 0.5 \ \psi_1^{[0.8]}$  false and  $\operatorname{rnd}() < 0.5 \ \psi_1^{[0.3]}$  true. By (EVAL IF TRUE), the last if-statement evaluates to 0, terminating the recursion. Combining the results by (EVAL APPL), (EVAL IF FALSE) and (EVAL PRIM), we arrive at  $\operatorname{geometric} 0.5 \ \psi_1^{[0.7,0.8,0.3]}$  2.

At this point, it is straightforward to see that the condition in the if-statement on the final line is satisfied, and hence the program reduces with the given trace to the value 2 with weight 1.

This program actually yields weight 1 for every trace that returns an integer value. This may seem counter-intuitive, because clearly not all outcomes have the same probability. However, the probability of a given outcome is given by an integral over the space of traces, as described in Section 3.4.

### 2.5 Soft Constraints and score

The geometric distribution example in Section 2.4 uses a hard constraint: program execution fails and the value of n is discarded whenever the Boolean predicate n > 1 is not satisfied. In many machine learning applications we want to use a different kind of constraint that models noisy data. For instance, if c is the known output of a sensor that shows an approximate value of some unknown quantity c that is computed by the program, we want to assign higher probabilities to values of c that are closer to c. This is sometimes known as a soft constraint.

One naive way to implement a soft constraint is to use a hard constraint with a success probability based on |x-c|, for instance,

condition 
$$x \in M := \inf flip(exp(-(x-c)^2))$$
 then  $M$  else fail.

Then condition  $x \ c \ M$  has the effect of continuing as M with probability  $exp(-(x-c)^2)$ , and otherwise terminating execution. In the context of a sampling-based semantics, it has the effect of

adding a uniform sample from  $[0, exp(-(x-c)^2))$  to any successful trace, in addition to introducing more failing traces.

Instead, our calculus includes a primitive score, that avoids both adding dummy samples and introducing more failing traces. It also admits the possibility of using efficient gradient-based methods of inference (e.g., Homan and Gelman [18]). Using score, the above conditioning operator can be redefined as

$$score\text{-}condition \ x \ c \ M := score(exp(-(x-c)^2)); M$$

## 2.6 Example: Linear Regression

For an example of soft constraints, consider the ubiquitous linear regression model  $y = m \cdot x + b + noise$ , where x is often a known feature and y an observable outcome variable. We can model the noise as drawn from a Gaussian distribution with mean 0 and variance 1/2 by letting the success probability be given by the function squash below.

The following query<sup>2</sup> predicts the y-coordinate for x = 4, given observations of four points: (0,0), (1,1), (2,4), and (3,6). (We use the abbreviation (define  $(f x_1 \ldots x_n) e$ ) for (define f (lambda  $(x_1 \ldots x_n) e$ ), and use and for multiadic conjunction.)

The model described above puts independent Gaussian priors on m and b. The condition of the query states that all observed ys are (soft) equal to  $k \cdot x + m$ . Assuming that softeq is used only to define constraints (i.e., positively), we can avoid the nuisance parameter that arises from each flip by redefining softeq as follows (given a score primitive in Church, mapped to score(-) in our  $\lambda$ -calculus):

```
(define (softeq x y) (score (squash x y)))
```

## 3 Sampling-Based Operational Semantics

In this section, we further investigate sampling-based semantics for our calculus. First, we introduce small-step sampling-based semantics and prove it equivalent to its big-step sibling as introduced in Section 2.2. Then, we associate to any closed term M two sub-probability distributions: one on the set of random traces, and the other on the set of return values. This requires some measure theory, recalled in Section 3.2.

### 3.1 Small-step Sampling-based Semantics

We define small-step call-by-value evaluation. Evaluation contexts are defined as follows:

$$E ::= [\cdot] \mid EM \mid (\lambda x.M)E$$

 $<sup>^2\</sup>mathrm{Cf.}\ \mathrm{http://forestdb.org/models/linear-regression.html.}$ 

$$E[g(\vec{c})] \xrightarrow{\det} E[\sigma_g(\vec{c})]$$

$$E[(\lambda x.M) \ V] \xrightarrow{\det} E[M\{V/x\}]$$

$$E[\text{if } 1 \text{ then } M_2 \text{ else } M_3] \xrightarrow{\det} E[M_2]$$

$$E[\text{if } 0 \text{ then } M_2 \text{ else } M_3] \xrightarrow{\det} E[M_3]$$

$$E[T] \xrightarrow{\det} E[\text{fail}]$$

$$E[\text{fail}] \xrightarrow{\det} \text{ fail } \text{ if } E \text{ is not } [\cdot]$$

Figure 3: Deterministic Reduction.

We let  $\mathcal{C}$  be the set of all closed evaluation contexts, i.e., where every occurrence of a variable x is as a subterm of  $\lambda x.M$ . The term obtained by replacing the only occurrence of  $[\cdot]$  in E by M is indicated as E[M]. Redexes are generated by the following grammar:

$$R \, ::= (\lambda x.M) V \, \, \Big| \, \, \mathsf{D}(\vec{c}) \, \, \Big| \, \, g(\vec{c}) \, \, \Big| \, \, \mathsf{score}(c)$$
 
$$\Big| \, \, \mathsf{fail} \, \, \Big| \, \, \mathsf{if true then} \, M \, \mathsf{else} \, N$$
 
$$\Big| \, \, \mathsf{if false then} \, M \, \mathsf{else} \, N \, \, \Big| \, \, T$$

Reducible terms are those closed terms M that can be written as E[R].

**Lemma 1** For every closed term M, either M is a generalized value or there are unique E, R such that M = E[R]. Moreover, if M is not a generalized value and  $R = \mathtt{fail}$ , then E is proper, that is,  $E \neq [\cdot]$ .

PROOF. This is an easy induction on the structure of M.

Deterministic reduction is the relation  $\xrightarrow{\text{det}}$  on closed terms defined in Figure 3.

**Lemma 2** If  $M \xrightarrow{det} M'$  and  $M \xrightarrow{det} M''$  then M' = M''.

PROOF. Since  $M \xrightarrow{\det} M'$  implies that M is not a generalized value, Lemma 1 states that M = E[R] for some unique E, R. If  $R = \mathtt{fail}$ , then E is proper and E[R] can only reduce to  $\mathtt{fail}$ . Otherwise, it follows immediately by inspection of the reduction rules that  $E[R] \xrightarrow{\det} E[N]$  for some N that is uniquely determined by the redex R.

Let us define composition of contexts  $E \circ E'$  inductively as:

$$[\ ] \circ E' \quad \triangleq \quad E'$$
 
$$(E\ M) \circ E' \quad \triangleq \quad (E \circ E')\ M$$
 
$$((\lambda x.M)\ E) \circ E' \quad \triangleq \quad (\lambda x.M)\ (E \circ E')$$

**Lemma 3**  $(E \circ E')[M] = E[E'[M]].$ 

PROOF. By induction on the structure of E.

**Lemma 4** If  $E[R] \xrightarrow{det} E[N]$ , then  $R \xrightarrow{det} N$ .

PROOF. By case analysis on the deterministic reduction rules.

$$\frac{M \xrightarrow{\det} N}{(M, w, s) \to (N, w, s)} \text{ (Red Pure)} \quad \frac{c \in (0, 1]}{(E[\mathsf{score}(c)], w, s) \to (E[\mathsf{true}], c \cdot w, s)} \text{ (Red Score)}$$

$$\frac{w' = \mathrm{pdf}_{\mathsf{D}}(\vec{c}, c) \quad w' > 0}{(E[\mathsf{D}(\vec{c})], w, c :: s) \to (E[c], w \cdot w', s)} \text{ (Red Random)}$$

$$\frac{\mathrm{pdf}_{\mathsf{D}}(\vec{c}, c) = 0}{(E[\mathsf{D}(\vec{c})], w, c :: s) \to (E[\mathsf{fail}], 0, s)} \text{ (Red Random Fail)}$$

Figure 4: Small-step sampling-based operational semantics

**Lemma 5** For any E and M such that  $M \neq E'[fail]$ , if  $M \xrightarrow{det} M'$  then  $E[M] \xrightarrow{det} E[M']$ .

PROOF. Standard, using Lemmas 1 and 2.

Since  $M \xrightarrow{\det} M'$ , M is not a generalized value. By Lemma 1, M = E'[R] for some E', R.

By assumption,  $R \neq \mathtt{fail}$ , so by inspection of the reduction rules  $E'[R] \xrightarrow{\det} E'[N]$  for some N. By Lemma 2, E'[N] = M'. By Lemma 3,  $E[M] = (E \circ E')[R]$  and  $E[M'] = (E \circ E')[N]$ .

Since Lemma 4 gives  $R \xrightarrow{\det} N$ , by case analysis on the derivation of  $R \xrightarrow{\det} N$  we can show that  $(E \circ E')[R] \xrightarrow{\det} (E \circ E')[N]$ , which implies  $E[M] \xrightarrow{\det} E[M']$ .

**Lemma 6** If  $(M, w, s) \rightarrow (M', w', s')$  and  $(M, w, s) \rightarrow (M'', w'', s'')$ , then M' = M'', w' = w'' and s'' = s'.

PROOF. By case analysis. Since there is no rule that reduces generalized values,  $(M, w, s) \rightarrow (M', w', s')$  implies that  $M \notin \mathcal{GV}$ , so by Lemma 1, M = E[R] for some unique E, R.

- If  $(M, w, s) \to (M', w', s')$  was derived with (RED PURE), then M = E[R], where  $R \neq D(\underline{c})$  and  $R \neq \mathtt{score}(c)$ , which implies that  $(M, w, s) \to (M'', w'', s'')$  must also have been derived with (RED PURE). Hence, we have w'' = w' = w, s'' = s' = s,  $M \xrightarrow{\det} M'$  and  $M \xrightarrow{\det} M''$ . By Lemma 2, M'' = M', as required.
- If  $(M, w, s) \to (M', w', s')$  was derived with (RED RANDOM), then  $M = E[\mathsf{D}(\vec{c})], s = c :: s^*$  and  $\mathsf{pdf}_\mathsf{D}(\vec{c}, c) > 0$ . Hence,  $(M, w, s) \to (M'', w'', s'')$  must also have been derived with (RED RANDOM), and so  $M'' = M' = E[c], s'' = s' = s^*$  and  $w'' = w' = w \, \mathsf{pdf}_\mathsf{D}(\vec{c}, c)$ , as required. The (RED RANDOM FAIL) case is analogous.
- If  $(M, w, s) \to (M', w', s')$  was derived with (Red Score), then  $M = E[\mathsf{score}(c)]$  and  $c \in (0, 1]$ , so  $(M, w, s) \to (M'', w'', s'')$  must also have been derived with (Red Score). Hence  $M'' = M' = E[\mathsf{true}]$ ,  $w'' = w' = c \cdot w$  and s'' = s' = s.

Rules of small-step reduction are given in Figure 4. We let *multi-step reduction* be the inductively defined relation  $(M, w, s) \Rightarrow (M', w', s')$  if and only if (M, w, s) = (M', w', s') or  $(M, w, s) \rightarrow (M'', w'', s'') \Rightarrow (M', w', s')$  for some M'', w'', s''. As can be easily verified, the multi-step reduction of a term to a generalized value is deterministic once the underlying trace is kept fixed:

**Lemma 7** If both  $(M, w, s) \Rightarrow (G', w', s')$  and  $(M, w, s) \Rightarrow (G'', w'', s'')$ , then G' = G'', w' = w'' and s' = s''.

PROOF. By induction on the derivation of  $(M, w, s) \Rightarrow (G', w', s')$ , with appeal to Lemma 6.

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- Base case: (M, w, s) = (G', w', s'). Generalized values do not reduce, so G'' = G' = G, w'' = w' = w and s'' = s' = s.
- Induction step:  $(M, w, s) \to (\hat{M}, \hat{w}, \hat{s}) \Rightarrow (G', w', s')$ . Since  $M \neq G''$ , we also have  $(M, w, s) \to (M^*, w^*, s^*) \Rightarrow (G'', w'', s'')$ . By Lemma 6,  $(M^*, w^*, s^*) = (\hat{M}, \hat{w}, \hat{s})$ , and so by induction hypothesis, (G'', w'', s'') = (G', w', s'), as required.

**Lemma 8** For any E and M such that  $M \neq E'[\mathtt{fail}]$ ,  $if(M, w, s) \rightarrow (M', w', s')$  then  $(E[M], w, s) \rightarrow (E[M'], w', s')$ 

PROOF. By inversion of  $\rightarrow$ , using Lemma 5.

- If  $(M, w, s) \to (M', w', s')$  was derived with (RED PURE), then  $M \xrightarrow{\det} M'$ , so by Lemma 5,  $E[M] \xrightarrow{\det} E[M']$ , and by (RED PURE),  $(E[M], w, s) \to (E[M'], w', s')$ .
- If  $(M, w, s) \to (M', w', s')$  was derived with (RED RANDOM), then  $M = E'[\mathsf{D}(\vec{c})], M' = E'[c],$  s = c :: s' and  $w' = w \operatorname{pdf}_{\mathsf{D}}(\vec{c}, c)$ , where  $\operatorname{pdf}_{\mathsf{D}}(\vec{c}, c) > 0$ . By (RED RANDOM) and Lemma 3, we can derive  $(E[M], w, s) \to (E[M'], w', s')$ . Cases (RED RANDOM FAIL) and (RED SCORE) are analogous.

**Lemma 9** If  $(E[R], w, s) \rightarrow (E[N], w', s')$  then  $(R, w, s) \rightarrow (N, w', s')$ 

PROOF. By case analysis.

- If  $(E[R], w, s) \to (E[N], w', s')$  was derived with (Red Pure), then  $E[R] \xrightarrow{\det} E[N]$ , so by Lemma 5,  $R \xrightarrow{\det} N$ , which implies  $(M, w, s) \to (M', w', s')$ . • If  $(E[R], w, s) \to (E[N], w', s')$  was derived with (Red Random), then  $R = \mathsf{D}(\vec{c})$ , N = c,
- If  $(E[R], w, s) \to (E[N], w', s')$  was derived with (Red Random), then  $R = \mathsf{D}(\vec{c}), N = c, s = c :: s'$  and  $w' = w \operatorname{pdf}_{\mathsf{D}}(\vec{c}, c)$ , where  $\operatorname{pdf}_{\mathsf{D}}(\vec{c}, c) > 0$ . Hence, with (Red Random), we can derive  $(\mathsf{D}(\vec{c}), w, s) \to (c, w', s')$ Cases (Red Random Fail) and (Red Score) are analogous.

Reduction can take place in any evaluation context, provided the result is not a failure. Moreover, multi-step reduction is a transitive relation. This is captured by the following lemmas.

**Lemma 10** For any E, if  $(M, w, s) \Rightarrow (M', w', s')$  and  $M' \neq \text{fail}$ , then we have  $(E[M], w, s) \Rightarrow (E[M'], w', s')$ .

PROOF. By induction on the number of steps in the derivation of  $(M, w, s) \Rightarrow (M', w', s')$ , with appeal to Lemma 8.

Since  $M' \neq \mathtt{fail}$ , no expression in the derivation chain (other than the last one) can be of the form  $E'[\mathtt{fail}]$ .

**Lemma 11** For any E, if  $(M, w, s) \Rightarrow (fail, w', s')$  then  $(E[M], w, s) \Rightarrow (fail, w', s')$ .

PROOF. By induction on the number of steps in the derivation, using Lemmas 8 and 10. If  $E = [\ ]$ , the result holds trivially, so let us assume  $E \neq [\ ]$ . If  $(M,w,s) \Rightarrow (\mathtt{fail},w',s')$  was derived in 0 steps, then  $M = \mathtt{fail}, w' = w'$  and s' = s, so by (RED PURE),  $(E[\mathtt{fail}],w,s) \rightarrow (\mathtt{fail},w,s)$ , as required.

If  $(M, w, s) \Rightarrow (fail, w', s')$  was derived in 1 or more steps, then:

- If  $M = E'[\mathtt{fail}]$  and  $E' \neq []$ , then  $((E \circ E')[\mathtt{fail}], w, s) \to (\mathtt{fail}, w', s')$  by (RED PURE).
- Otherwise, there exist  $\hat{M}$ ,  $\hat{w}$ ,  $\hat{s}$  such that  $(M, w, s) \to (\hat{M}, \hat{w}, \hat{s}) \Rightarrow (\mathtt{fail}, w', s')$ , where  $M \notin \mathcal{GV}$ . By induction hypothesis,  $(E[\hat{M}], \hat{w}, \hat{s}) \Rightarrow (\mathtt{fail}, w', s')$  for any E, and by Lemma 8,  $(E[M], w, s) \to (E[\hat{M}], \hat{w}, \hat{s})$ .

**Lemma 12** If  $(M, w, s) \Rightarrow (M', w', s')$  and  $w \ge 0$ , then  $w' \ge 0$ .

PROOF. By induction on the number of steps in the derivation.

- If  $(M, w, s) \Rightarrow (M', w', s')$  was derived in 0 steps, then w' = w, so w' > 0.
- If  $(M, w, s) \Rightarrow (M', w', s')$  was derived in 1 or more steps, then  $(M, w, s) \rightarrow (M^*, w^*, s^*) \Rightarrow (M', w', s')$ .

If  $(M, w, s) \to (M^*, w^*, s^*)$  was derived with (RED PURE), then  $w^* = w \ge 0$ .

If  $(M, w, s) \to (M^*, w^*, s^*)$  was derived with (RED RANDOM), then  $w^* = w \cdot w''$  for some w'' > 0, so  $w^* \ge 0$ .

If  $(M, w, s) \to (M^*, w^*, s^*)$  was derived with (RED SCORE), then  $w^* = w \cdot c$  for some c > 0, so  $w' \ge 0$ .

If  $(M, w, s) \to (M^*, w^*, s^*)$  was derived with (RED RANDOM FAIL), then  $w^* = 0$ .

In either case,  $w^* \geq 0$ , so by induction hypothesis,  $w' \geq 0$ .

**Lemma 13** If  $(M, w, s) \rightarrow (M', w', s')$  was not derived with (RED RANDOM FAIL) and w > 0, then w' > 0.

PROOF. By inspection (similar to the inductive step in the proof of Lemma 12).

**Lemma 14** If  $(M, w, s) \to (M', w', s')$ , then for any  $w^* \ge 0$ ,  $(M, ww^*, s) \to (M', w'w^*, s')$ 

Proof. By case analysis.

**Lemma 15** If  $(M, w, s) \rightarrow (M', w', s')$ , then for any  $s^*$ ,  $(M, w, s@s^*) \rightarrow (M', w', s'@s^*)$ 

Proof. By case analysis.

**Lemma 16** If  $(M, w, s) \to (M', w', s')$ , then there is  $s^*$  such that  $s = s^*@s'$  and  $(M, w, s^*) \to (M', w', [])$ 

Proof. By case analysis.  $\Box$ 

**Lemma 17** If  $(M, w, s) \to^k (M', w', s')$ , then for any  $w^* \ge 0$ ,  $(M, ww^*, s) \to^k (M', w'w^*, s')$ 

PROOF. By induction on k, with appeal to Lemma 14.

**Lemma 18** If  $(M, w, s) \rightarrow^k (M', w', s^*)$ , then for any s',  $(M, w, s@s') \rightarrow^k (M', w', s^*@s')$ 

PROOF. By induction on k, with appeal to Lemma 15.

**Lemma 19** If both  $(M, 1, s) \Rightarrow (M', w', [])$  and  $(M', 1, s') \Rightarrow (M'', w'', [])$ , then  $(M, 1, s@s') \Rightarrow (M'', w' \cdot w'', [])$ .

PROOF. By Lemma 18,  $(M, 1, s@s') \Rightarrow (M', w', s')$  and by lemma 12,  $w' \ge 0$ . Hence, by Lemma 17,  $(M', w', s') \Rightarrow (M'', w'w'', [])$ , which gives  $(M, 1, s@s') \Rightarrow (M'', w'w'', [])$ .

Lemma 20 For any E,  $E[fail] \downarrow_1^{[]} fail$ .

PROOF. By induction on the structure of E.

- Base case: E = [], the result follows by (EVAL VAL).
- Induction step:
  - Case  $E = (\lambda x.L)$  E': By induction hypothesis,  $E'[\text{fail}] \Downarrow_1^{[]}$  fail, and by (EVAL APPL RAISE2),  $(\lambda x.L)$   $E'[\text{fail}] \Downarrow_1^{[]}$  fail, as required.
  - Case E = E' L: By induction hypothesis,  $E'[\mathtt{fail}] \Downarrow_1^{[]} \mathtt{fail}$ , so by (EVAL APPL RAISE1), we get  $E'[\mathtt{fail}] L \Downarrow_1^{[]} \mathtt{fail}$ .

**Lemma 21** For any E, if  $\operatorname{pdf}_D(\vec{c},c)=0$ , then  $E[D(\vec{c})] \downarrow_0^{[c]}$  fail.

PROOF. By induction on the structure of E.

- Base case: E = [], the result follows by (EVAL RANDOM FAIL).
- Induction step:
  - Case  $E = (\lambda x.L)$  E': By induction hypothesis,  $E'[D(\vec{c})] \downarrow_0^{[c]}$  fail, and by (EVAL APPL RAISE2),  $(\lambda x.L)$   $E'[D(\vec{c})] \downarrow_0^{[]}$  fail, as required.
  - Case E = E' L: By induction hypothesis,  $E'[D(\vec{c})] \downarrow_0^{[c]}$  fail, so by (EVAL APPL RAISE1), we get  $E'[D(\vec{c})] \perp \downarrow_0^{[]}$  fail.

The following directly relates the small-step and big-step semantics, saying that the latter is invariant on the former:

**Lemma 22** If  $(M,1,s) \to (M',w,[])$  and  $M' \downarrow_{w'}^{s'} G$ , then  $M \downarrow_{w\cdot w'}^{s@s'} G$ .

PROOF. By induction on the structure of M.

If  $M = E[\mathtt{fail}]$  for some  $E \neq []$ , the result follows immediately by Lemma 20. Now, let us assume that  $M \neq E[\mathtt{fail}]$ .

- Base case: M = R:
  - If  $M = g(\vec{c})$  or M = c V or M = T, then M reduces to a generalized value in 1 step, so the result holds trivially (by one of the evaluation rules).
  - Case  $M = \text{if true then } M_2 \text{ else } M_3$ : We have (if true then  $M_2 \text{ else } M_3, 1, []) \to (M_2, 1, [])$ . By assumption,  $M_2 \Downarrow_{w'}^{s'} G$ . Thus, the desired result holds by (EVAL IF TRUE).
  - Case  $M = \text{if false then } M_2 \text{ else } M_3$ : analogous to the previous case.
  - Case  $M = (\lambda x. N_1) \ V$ : We have  $((\lambda x. N_1) \ V, 1, []) \to (N_1 \{V/x\}, 1, [])$ . Since  $(\lambda x. N_1)$  and V are already values and  $N_1 \{V/x\} \Downarrow_{w'}^{s'} G$  by assumption, (EVAL APPL) yields  $(\lambda x. N_1) \ V \Downarrow_{w'}^{s'} G$ .
  - Case  $M = D(\vec{c})$ :  $(M, 1, s) \to (M', w, [])$  must have been derived with (RED RANDOM) or (RED RANDOM FAIL). In the former case, s = [c], M' = c, and  $w = \mathrm{pdf}_D(\vec{c}, c)$ , where c > 0. The second assumption then takes the form  $c \downarrow \downarrow_1^{[]} c$ , so the required result follows from (EVAL RANDOM). The (RED RANDOM FAIL) case is similar, with the result following from (EVAL RANDOM FAIL).
  - Case  $M = \mathtt{score}(c), c \in (0,1]$ :  $(M,1,s) \to (M',w,[])$  must have been derived with (RED SCORE).so  $M' = \mathtt{true}, w = c$  and s = []. Thus, the result then follows from (EVAL SCORE).
- Induction step:  $M = E[R], E \neq [], R \neq fail$ :
  - Case  $E = (\lambda x.L)$  E':  $M = (\lambda x.L)$  E'[R]. We have  $((\lambda x.L)$   $E'[R], 1, s) \rightarrow ((\lambda x.L)$  E'[N], w, []) for some N, so by lemmas 8 and 9,  $(E'[R], 1, s) \rightarrow (E'[N], w, [])$ . By assumption,  $(\lambda x.L)$   $E'[N] \bigvee_{w'}^{s'} G$ .
    - If  $(\lambda x.L)$   $E'[N] \downarrow_{w'}^{s'} G$  was derived with (EVAL APPL), then  $E'[N] \downarrow_{w_1}^{s_1} V$  and  $(\lambda x.L)$   $V \downarrow_{w_2}^{s_2} G$ , where  $w' = w_1 w_2$  and  $s' = s_1@s_2$ . By induction hypothesis,  $E'[R] \downarrow_{ww_1}^{s@s_1} V$ , so (EVAL APPL) gives  $(\lambda x.L)$   $E'[R] \downarrow_{ww'}^{s@s'} G$ , as required.
    - If  $(\lambda x.L)$   $E'[N] \downarrow_{w'}^{s'} G$  was derived with (EVAL APPL RAISE3), then  $G = \mathtt{fail}$  and  $E'[N] \downarrow_{w'}^{s'}$  fail. By induction hypothesis,  $E'[R] \downarrow_{ww'}^{s@s'}$  fail, so by (EVAL APPL RAISE3),  $(\lambda x.L)$   $E'[R] \downarrow_{ww'}^{s@s'}$  fail
  - Case E = E' L:  $M = E'[M^*]$  L: We have  $(E'[R] L, 1, s) \to (E'[N] L, w, [])$  for some N, so by lemmas 8 and 9,  $(E'[R], 1, s) \to (E'[N], w, [])$ . By assumption,  $E'[N] L \Downarrow_{w'}^{s'} G$ .
    - If  $E'[N] L \Downarrow_{w'}^{s'} G$  was derived with (EVAL APPL), then  $E'[N] \Downarrow_{s_1}^{w_1} (\lambda x. N')$ ,  $L \Downarrow_{s_2}^{w_2} V$  and  $N'[V/x] \Downarrow_{s_3}^{w_3} G$ , where  $w' = w_1 w_2 w_3$  and  $s' = s_1@s_2@s_3$ . By induction hypothesis,  $E'[R] \Downarrow_{ww_1}^{s@s_1} (\lambda x. N')$ , so (EVAL APPL) gives  $E'[R] L \Downarrow_{ww'}^{s@s'} G$ , as required.
    - If E'[N] L  $\psi_{w'}^{s'}$  G was derived with (EVAL APPL RAISE1), then G = fail and E'[N]  $\psi_{w'}^{s'}$  fail. By induction hypothesis, E'[R]  $\psi_{ww'}^{s@s'}$  fail, so by (EVAL APPL RAISE1), E'[R] L  $\psi_{ww'}^{s@s'}$  fail

- If E'[N]  $L \downarrow_{w'}^{s'} G$  was derived with (EVAL APPL RAISE3), then  $E'[N] \downarrow_{w_1}^{s_1} (\lambda x. N')$  and  $L \downarrow_{w_2}^{s_2}$  fail, where  $w' = w_1 w_2$  and  $s' = s_1@s_2$ . By induction hypothesis,  $E'[R] \downarrow_{ww_1}^{s@s_1}$  $(\lambda x.N')$ , so (EVAL APPL RAISE3) gives E'[R]  $L \Downarrow_{ww'}^{s@s'}$  fail, as required.
- If  $E'[N] L \Downarrow_{w'}^{s'} G$  was derived with (EVAL APPL RAISE1), then  $G = \mathtt{fail}$  and  $N_1' \Downarrow_{w'}^{s'} c$ . By induction hypothesis,  $E'[R] \Downarrow_{ww'}^{s@s'} c$ , so by (EVAL APPL RAISE1),  $E'[R] L \Downarrow_{ww'}^{s@s'} c$ fail.

Finally, we have all the ingredients to show that the small-step and the big-step sampling-based semantics both compute the same traces with the same weights.

**Theorem 1**  $M \Downarrow_w^s G$  if and only if  $(M, 1, s) \Rightarrow (G, w, [])$ .

The left to right implication is an induction on the derivation of  $M \downarrow_w^s G$ . The most interesting case is definitely the following:

(EVAL APPL)
$$\frac{M \Downarrow_{w_1}^{s_1} \lambda x.M' \qquad N \Downarrow_{w_2}^{s_2} V \qquad M'[V/x] \Downarrow_{w_3}^{s_3} G}{M N \Downarrow_{w_1,w_2,w_3}^{s_1@s_2@s_3} G}$$

By induction hypothesis,  $(M, 1, s_1) \Rightarrow (\lambda x.M', w_1, []), (N, 1, s_2) \Rightarrow (V, w_2, [])$  and  $(M'[V/x], 1, s_3) \Rightarrow$  $(G, w_3, [])$ . By Lemma 10 (for E = []N),  $(M N, 1, s_1) \Rightarrow ((\lambda x. M') N, w_1, [])$ . By Lemma 10 again (for  $E = (\lambda x.M')$  []),  $((\lambda x.M') N, 1, s_2) \Rightarrow ((\lambda x.M') V, w_2, [])$ . By Lemma 19,  $(M N, 1, s_1@s_2) \Rightarrow$  $((\lambda x.M')\ V, w_1w_2, [])$  By (RED PURE),  $((\lambda x.M')\ V, w_1 \cdot w_2, []) \to (M'[V/x], w_1 \cdot w_2, [])$ , which implies  $(M \ N, 1, s_1@s_2) \Rightarrow ((\lambda x.M') \ V, w_1w_2, [])$  Thus, the desired result follows by Lemma

• Case:  $G \in \mathcal{GV}$   $G \downarrow_1 G$ 

Here, M = V, w = 1 and s = []. so  $(M, w_0, s_0)$  reduces to  $(V, w_0, s_0)$  in 0 steps by the small-step semantics.

(EVAL RANDOM)

 $w = \mathrm{pdf}_{\mathsf{D}}(\vec{c}, c)$ 

• Case: w > 0 $\mathsf{D}(\vec{c}) \Downarrow_w^{[c]} c$ 

By (Red Random) (taking E = []),  $(D(\vec{c}), 1, [c]) \rightarrow (c, w, [])$ . (EVAL RANDOM FAIL)

 $\bullet \ \text{Case:} \ \frac{\operatorname{pdf}_{\mathsf{D}}(\vec{c},c) = 0}{\mathsf{D}(\vec{c}) \ \psi_0^{[c]} \ \mathtt{fail}}$ 

By (Red Random Fail) (taking E = []),  $(D(\vec{c}), 1, [c]) \rightarrow (fail, 0, [])$ . (EVAL PRIM)

• Case:  $\frac{1}{g(\vec{c}) \Downarrow_1^{[]} \sigma_g(\vec{c})}$ 

By (RED PURE) (taking E = []),  $(g(\vec{c}), 1, []) \rightarrow (\sigma_q(\vec{c}), 1, [])$ . (EVAL SCORE)

• Case:  $\frac{c \in (0,1]}{\text{score}(c) \downarrow_c^{\square} \text{true}}$ 

By (Red Score) (taking E = []),  $(D(\vec{c}), 1, []) \rightarrow (c, w, [])$ .

(EVAL APPL)

 $M \Downarrow_{w_1}^{s_1} \lambda x.M'$ 

• Case:  $\frac{N \downarrow_{s_2}^{w_1} V}{M'[V/x] \downarrow_{w_3}^{s_3} G}$   $\frac{M N \downarrow_{w_1 \cdot w_2 \cdot w_3}^{s_1 \cdot @s_2 \cdot @s_3} G}{M N \downarrow_{w_1 \cdot w_2 \cdot w_3}^{s_1 \cdot @s_2 \cdot @s_3} G}$ 

```
(G, w_3, []).
    By Lemma 10 (for E = [] N), (M N, 1, s_1) \Rightarrow ((\lambda x.M') N, w_1, []).
    By Lemma 10 again (for E = (\lambda x.M') []), ((\lambda x.M') N, 1, s_2) \Rightarrow ((\lambda x.M') V, w_2, []).
    By Lemma 19, (M \ N, 1, s_1@s_2) \Rightarrow ((\lambda x.M') \ V, w_1w_2, [])
    By (Red Pure), ((\lambda x.M') V, w_1 \cdot w_2, []) \rightarrow (M'[V/x], w_1 \cdot w_2, []), which implies (M N, 1, s_1@s_2) \Rightarrow
    ((\lambda x.M')\ V, w_1w_2, [])
    Thus, the desired result follows by Lemma 19.
             (EVAL APPL RAISE1)
 \bullet \ {\rm Case:} \ \frac{\stackrel{.}{M} \Downarrow_w^s {\rm fail}}{M \ N \Downarrow_w^s {\rm fail}}
    By induction hypothesis, (M, 1, s) \Rightarrow (fail, w, []).
    By Lemma 11 (with E = [N]), (M N, 1, s) \Rightarrow (fail, w, []).
             (EVAL APPL RAISE2)
 • Case: \frac{M \Downarrow_w^s c}{M N \Downarrow_w^s \text{fail}}
    By induction hypothesis, (M, 1, s) \Rightarrow (c, w, []). By Lemma 10 (with E = []N)), (M, N, 1, s) \Rightarrow
    (c \ N, w, []).
    By (RED PURE), (c N, w, []) \rightarrow (fail, w, []).
    Thus, (M N, 1, s) \Rightarrow (\mathtt{fail}, w, []).
             (EVAL APPL RAISE3)
             M \Downarrow_{w_1}^{s_1} \lambda x.M'
 • Case: N \Downarrow_{w_2}^{s_2} fail
             M N \downarrow_{w_1 \cdot w_2}^{s_1@s_2} fail
    By induction hypothesis, (M, 1, s_1) \Rightarrow (\lambda x. M', w_1, []), and (N, 1, s_2) \Rightarrow (\mathtt{fail}, w_2, []).
    By Lemma 10, (M \ N, 1, s_1) \Rightarrow ((\lambda x. M') \ N, w_1, []).
    By Lemma 11, ((\lambda x.M') N, 1, s_2) \Rightarrow (\text{fail}, w_2, []).
    Thus, by Lemma 19, (M \ N, 1, s_1@s_2) \Rightarrow (fail, w_1 \cdot w_2, []).
             (EVAL IF TRUE)
 • Case: M_2 \Downarrow_w^s G if true then M_2 else M_3 \Downarrow_w^s G
    By (RED PURE) (taking E = []), (if true then M_2 else M_3, 1, s) \to (M_2, 1, s). By induction
    hypothesis, (M_2, 1, s) \Rightarrow (G, w, []).
    Hence (if 1 then M_2 else M_3, 1, s) \Rightarrow (G, w, [])
 • Case (EVAL IF FALSE): analogous to (EVAL IF TRUE)
             (EVAL FAIL)
 • Case: \frac{}{T \Downarrow_1^{\parallel} \text{fail}}
    By (RED PURE), (T, 1, []) \rightarrow (fail, 1, []).
The right to left implication can be proved by an induction on the length of the derivation of
(M,1,s) \Rightarrow (G,w,[]).
 • Base case: If (M, 1, s) = (G, w, []), then M \downarrow_s^w G by (EVAL VAL).
 • Induction step: assume (M,1,s) \to (M',w',s') \to^n (G,w,[]). If (M,1,s) \to (M',w',s') was
    derived with (RED RANDOM FAIL), then M = E[D(\vec{c})], n = 1, s = [c], G = \text{fail} and
    w = w' = \mathrm{pdf}_D(\vec{c}, c) = 0. By Lemma 21, we have M \downarrow^{[c]_0} fail, as required.
    Otherwise, by Lemma 13, w' > 0, so by Lemma 17, (M', 1, s') \to^n (G, w/w', []). By induction hypothesis, M' \downarrow_{w/w'}^{s'} G. By Lemma 16, (M, 1, s^*) \to (M', w', []), where s = s^*@s'.
    Therefore, by Lemma 22, M \Downarrow_w^{s^* @ s'} G, and so M \Downarrow_w^s G.
                                                                                                                                As a corollary of Theorem 1 and Lemma 7 we obtain:
```

By induction hypothesis,  $(M, 1, s_1) \Rightarrow (\lambda x. M', w_1, []), (N, 1, s_2) \Rightarrow (V, w_2, [])$  and  $(M'[V/x], 1, s_3) \Rightarrow$ 

**Lemma 23** If  $M \downarrow_w^s G$  and  $M \downarrow_{w'}^s G'$  then w = w' and G = G'.

At this point, we have defined intuitive operational semantics based on the consumption of an explicit trace of randomness, but we have defined no distributions. In the rest of this section we show that this semantics indeed associates a sub-probability distribution with each term. Before proceeding, however, we need some measure theory.

#### 3.2 Some Measure-Theoretic Preliminaries.

We begin by recapitulating some standard definitions for sub-probability distributions and kernels over metric spaces. For a more complete, tutorial-style introduction to measure theory, see Billingsley [2], Panangaden [29], or another standard textbook or lecture notes.

A  $\sigma$ -algebra (over a set X) is a set  $\Sigma$  of subsets of X that contains  $\emptyset$ , and is closed under complement and countable union (and hence is closed under countable intersection). Let the  $\sigma$ -algebra generated by S, written  $\sigma(S)$ , be the set  $\sigma(S)$   $S \subseteq \mathcal{P}(X)$ , that is the least  $\sigma$ -algebra over  $\cup S$  that is a superset of S. In other words,  $\sigma(S)$  is the least set such that:

- 1. we have  $S \subseteq \sigma(S)$  and  $\emptyset \in \sigma(S)$ ; and
- 2.  $((\cup S) \setminus A) \in \sigma(S)$  if  $A \in \sigma(S)$ ; and
- 3.  $\bigcup_{i\in\mathbb{N}} A_i \in \sigma(S)$  if each  $A_i \in \sigma(S)$ .

An equivalent definition is that  $\sigma(S) \triangleq \bigcap \{\Sigma \mid S \subseteq \Sigma \text{ and } \Sigma \text{ is a } \sigma\text{-algebra} \}.$ 

We write  $\mathbb{R}_+$  for  $[0,\infty]$  and  $\mathbb{R}_{[0,1]}$  for the interval [0,1]. A metric space is a set X with a symmetric distance function  $\delta: X \times X \to \mathbb{R}_+$  that satisfies the triangle inequality  $\delta(x,z) \le \delta(x,y) + \delta(y,z)$  and the axiom  $\delta(x,x) = 0$ . We write  $\mathbf{B}(x,r) \triangleq \{y \mid \delta(x,y) < r\}$  for the open ball around x of radius r. We equip  $\mathbb{R}_+$  and  $\mathbb{R}_{[0,1]}$  with the standard metric  $\delta(x,y) = |x-y|$ , and products of metric spaces with the Manhattan metric (e.g.,  $\delta((x_1,x_2),(y_1,y_2)) = \delta(x_1,y_1) + \delta(x_2,y_2)$ ). The Borel  $\sigma$ -algebra on a metric space  $(X,\delta)$  is  $\mathcal{B}(X,\delta) \triangleq \sigma(\{\mathbf{B}(x,r) \mid x \in X \land r > 0\})$ . We often omit the arguments to  $\mathcal{B}$  when they are clear from the context.

A measurable space is a pair  $(X, \Sigma)$  where X is a set of possible outcomes, and  $\Sigma \subseteq \mathcal{P}(X)$  is a  $\sigma$ -algebra of measurable sets. As an example, consider the extended positive real numbers  $\mathbb{R}_+$  equipped with the Borel  $\sigma$ -algebra  $\mathcal{R}$ , i.e. the set  $\sigma(\{(a,b) \mid a,b \geq 0\})$  which is the smallest  $\sigma$ -algebra containing all open (and closed) intervals. We can create finite products of measurable spaces by iterating the construction  $(X,\Sigma)\times (X',\Sigma')=(X\times X',\sigma(A\times B\mid A\in \Sigma\wedge B\in \Sigma'))$ . If  $(X,\Sigma)$  and  $(X',\Sigma')$  are measurable spaces, then the function  $f:X\to X'$  is measurable if and only if for all  $A\in \Sigma'$ ,  $f^{-1}(A)\in \Sigma$ , where the inverse image  $f^{-1}:\mathcal{P}(X')\to \mathcal{P}(X)$  is given by  $f^{-1}(A)\triangleq \{x\in X\mid f(x)\in A\}$ .

A measure  $\mu$  on  $(X, \Sigma)$  is a function from  $\Sigma$  to  $\mathbb{R}_+$ , that is (1) zero on the empty set, that is,  $\mu(\varnothing) = 0$ , and (2) countably additive, that is,  $\mu(\cup_i A_i) = \Sigma_i \mu(A_i)$  if  $A_1, A_2, \ldots$  are pairwise disjoint. The measure  $\mu$  is called a (sub-probability) distribution if  $\mu(X) \leq 1$  and finite if  $\mu(X) \neq \infty$ . If  $\mu, \nu$  are finite measures and  $\nu \geq 0$ , we write  $\nu \in \mathbb{R}_+$  for the finite measure  $\mu \in \mathbb{R}_+$  for

$$\delta(x)(A) = \begin{cases} 1 & \text{if } x \in A; \\ 0 & \text{otherwise.} \end{cases}$$

A measure space is a triple  $\mathscr{M}=(X,\Sigma,\mu)$  where  $\mu$  is a measure on the measurable space  $(X,\Sigma)$ . Given a measurable function  $f:X\to\mathbb{R}_+$ , the integral of f over  $\mathscr{M}$  can be defined following Lebesgue's theory and denoted as either of

$$\int f \ d\mu = \int f(x) \ \mu(dx) \in \mathbb{R}_+.$$

The Iverson brackets [P] are 1 if predicate P is true, and 0 otherwise. We then write

$$\int_{A} f \ d\mu \triangleq \int f(x) \cdot [x \in A] \ \mu(dx).$$

We equip some measurable spaces  $(X, \Sigma)$  with a stock measure  $\mu$ . We then write  $\int f(s) ds$  (or shorter, f(f) for f(f) d $\mu$  when f is measurable  $f: X \to \mathbb{R}_+$ . In particular, we let the stock measure on  $(\mathbb{R}^n, \mathcal{B})$  be the Lebesgue measure  $\lambda_n$ .

A function f is a density of a measure  $\nu$  (with respect to the measure  $\mu$ ) if  $\nu(A) = \int_A f \, d\mu$  for all measurable A.

Given a measurable set A from  $(X, \Sigma)$ , we write  $\Sigma|_A$  for the restriction of  $\Sigma$  to elements in A, i.e.,  $\Sigma|_A = \{B \cap A \mid B \in \Sigma\}$ . Then  $(A, \Sigma|_A)$  is a measurable space. Any distribution  $\mu$  on  $(X, \Sigma)$ trivially yields a distribution  $\mu|_A$  on  $(A, \Sigma|_A)$  by  $\mu|_A(B) = \mu(B)$ .

#### Measure Space of Program Traces 3.3

In this section, we construct a measure space on the set S of program traces: (1) we define a measurable space ( $\mathbb{S}, \mathcal{S}$ ) and (2) we equip it with a stock measure  $\mu$  to obtain our measure space  $(\mathbb{S}, \mathcal{S}, \mu)$ .

The Measurable Space of Program Traces To define the semantics of a program as a measure on the space of random choices, we first need to define a measurable space of program traces. Since a program trace is a sequence of real numbers of an arbitrary length (possibly 0), the set of all program traces is  $\mathbb{S} = \biguplus_{n \in \mathbb{N}} \mathbb{R}^n$ . Now, let us define the  $\sigma$ -algebra  $\mathcal{S}$  on  $\mathbb{S}$  as follows: let  $\mathcal{B}_n$  be the Borel  $\sigma$ -algebra on  $\mathbb{R}^n$  (we take  $\mathcal{B}_0$  to be  $\{\{[]\}, \{\}\}\}$ ). Consider the class of sets  $\mathcal{S}$  of the form:

$$A = \biguplus_{n \in \mathbb{N}} H_n$$

where  $H_n \in \mathcal{B}_n$  for all n. Then  $\mathcal{S}$  is a  $\sigma$ -algebra, and so  $(\mathbb{S}, \mathcal{S})$  is a measurable space.

Lemma 24 S is a  $\sigma$ -algebra on S.

PROOF. We have  $\mathbb{S} = \biguplus_{n \in \mathbb{N}} \mathbb{R}^n$  and  $\mathbb{R}^n \in \mathcal{R}^n$  for all n, so  $\mathbb{S} \in \mathcal{S}$ . If A is defined as above, then  $\mathbb{S} - A = \biguplus_{n \in \mathbb{N}} (\mathbb{R}^n - H_n)$ , where  $\mathbb{R}^n - H_n \in \mathcal{R}^n$  for all n, so

For closure under countable union, take  $A_i = \biguplus_{n \in \mathbb{N}} H_{in}$  for all  $i \in \mathbb{N}$ , where  $H_{in} \in \mathcal{R}^n$  for all i, n. Then  $\bigcup_{i \in \mathbb{N}} A_i = \bigcup_{i \in \mathbb{N}} \biguplus_{n \in \mathbb{N}} H_{in} = \biguplus_{n \in \mathbb{N}} (\bigcup_{i \in \mathbb{N}} H_{in}) \in \mathcal{S}$ , because  $\bigcup_{i \in \mathbb{N}} H_{in} \in \mathcal{R}^n$ . Thus, S is a  $\sigma$ -algebra on E. 

Stock Measure on Program Traces Since each primitive distribution D has a density, the probability of each random value (and thus of each trace of random values) is zero. Instead, we define the trace and transition probabilities in terms of densities, with respect to the stock measure  $\mu$  on  $(\mathbb{S}, \mathcal{S})$  defined as follows:

$$\mu\left(\biguplus_{n\in\mathbb{N}}H_n\right) = \sum_{n\in\mathbb{N}}\lambda_n(H_n)$$

where  $\lambda_0 = \delta([])$  and  $\lambda_n$  is the Lebesgue measure on  $\mathbb{R}^n$  for n > 0.

**Lemma 25**  $\mu$  is a measure on  $(\mathbb{S}, \mathcal{S})$ .

PROOF. We check the three properties:

- 1. Since for all  $n \in \mathbb{N}$  and  $H_n \in \mathbb{R}^n$ , we have  $\lambda_n(H_n) \in [0,\infty]$ , obviously  $\mu(\biguplus_{n \in \mathbb{N}} H_n) =$  $\sum_{n=1}^{\infty} \lambda_n(H_n) \in [0, \infty]$
- 2. If  $H = \biguplus_{n \in \mathbb{N}} H_n = \emptyset$ , then  $H_n = \emptyset$  for all n, so  $\mu(H) = \sum_{n=1}^{\infty} \lambda_n(\emptyset) = 0$ .

3. Countable additivity: if  $H_1 = \biguplus_{n \in \mathbb{N}} H_{1n}, H_2 = \biguplus_{n \in \mathbb{N}} H_{2n}, \dots$  is a sequence of disjoint sets in  $\mathcal{S}$ , then:

$$\mu(\biguplus_{m=1}^{\infty} H_m) = \mu(\biguplus_{m=1}^{\infty} \biguplus_{n=0}^{\infty} H_{mn})$$

$$= \mu(\biguplus_{n=0}^{\infty} \biguplus_{m=1}^{\infty} H_{mn})$$

$$= \sum_{n=0}^{\infty} \lambda_n(\biguplus_{m=1}^{\infty} H_{mn})$$

$$= \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} \lambda_n(H_{mn})$$

$$= \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} \lambda_n(H_{mn})$$

$$= \sum_{m=1}^{\infty} \mu(H_m)$$

where the equality  $\sum_{n=0}^{\infty} \sum_{m=1}^{\infty} \lambda_n(H_{mn}) = \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} \lambda_n(H_{mn})$  follows from Tonelli's theorem for series (see [36]).

A measure  $\mu$  on  $(X, \Sigma)$  is  $\sigma$ -finite if  $X = \bigcup_i A_i$  for some countable (finite or infinite) sequence of sets  $A_i \in \Sigma$  such that  $\mu(A_i) < \infty$ . If  $\mu$  is a  $\sigma$ -finite measure on  $(X, \Sigma)$ , the measure space  $(X, \Sigma, \mu)$  is also called  $\sigma$ -finite.  $\sigma$ -finite measure spaces behave better with respect to integration than those who are not.

In the following, let  $[a,b]^n = \{(x_1,\ldots,x_n) \mid x_i \in [a,b] \quad \forall i \in 1...n\}.$ 

**Lemma 26** The measure  $\mu$  on  $(\mathbb{S}, \mathcal{S})$  is  $\sigma$ -finite.

PROOF. For every  $n \in \mathbb{N}$ , we have that  $\mathbb{R}^n = \bigcup_{k \in \mathbb{N}} [-k, k]^n$ . Hence,  $\mathbb{S} = \biguplus_{n \in \mathbb{N}} \mathbb{R}^n = \biguplus_{n \in \mathbb{N}} \bigcup_{k \in \mathbb{N}} [-k, k]^n$  is a countable union of sets in  $\mathcal{S}$  of the form  $[-k, k]^n$ . Finally, for all  $k, n \in \mathbb{N}$  we have  $\mu([-k, k]^n) = \lambda_n([-k, k]^n) = (2k)^n < \infty$ .

It follows that  $(\mathbb{S}, \mathcal{S}, \mu)$  is a  $\sigma$ -finite measure space.

**Discrete Random Variables** We have taken the sample space to be the real numbers, but any complete separable metric space will do. For example, in order to add discrete distributions to the language we can change  $\mathbb{S}$  to  $\biguplus_{n\in\mathbb{N}}(\mathbb{R}\uplus\mathbb{N})^n$ . The measurable sets  $H_n$  become  $(\mathcal{R}\uplus\mathcal{P}(\mathbb{N}))^n$ . The stock measure  $\mu$  would become  $\sum_{n=0}^{\infty}(\lambda,\mu_{\#})^n(H_n)$ , where  $\mu_{\#}$  is the counting measure on  $\mathbb{N}$  (that is,  $\mu_{\#}(A) = |A|$  if A is finite, otherwise  $\mu_{\#}(A) = \infty$ ).

Discrete distributions have probability mass functions, that is, densities with respect to the counting measure on  $\mathbb{N}$ , which are trivially zero-extended to densities with respect to  $\mu$ . Given a measurable injection function  $\lceil \cdot \rceil : \mathbb{R} \uplus \mathbb{N} \to \mathcal{V}$  (e.g., mapping natural numbers to the corresponding reals, or to Church numerals), it is easy to update the different semantics to a more general sample space, e.g.,

$$\frac{w = \mathrm{pdf}_{\mathsf{D}}(\vec{c}, z) \qquad w > 0}{\mathsf{D}(\vec{c}) \, \psi_w^{[z]} \, [z]} \, (\text{EVAL RANDOM})$$

## 3.4 Distributions $\langle\!\langle M \rangle\!\rangle$ and $[\![M]\!]_{\mathbb{S}}$ Given by Sampling-Based Semantics

The result of a closed term M on a given trace is

$$\mathbf{O}_M(s) = \begin{cases} G & \text{if } M \downarrow_w^s G \text{ for some } w \in \mathbb{R}_+\\ \text{fail} & \text{otherwise.} \end{cases}$$

The density of termination of a closed term M on a given trace is defined as follows.

$$\mathbf{P}_{M}(s) = \left\{ \begin{array}{ll} w & \text{if } M \Downarrow_{w}^{s} G \text{ for some } G \in \mathcal{GV} \\ 0 & \text{otherwise} \end{array} \right.$$

This density function induces a distribution  $\langle\!\langle M \rangle\!\rangle$  on traces defined as  $\langle\!\langle M \rangle\!\rangle(A) := \int_A \mathbf{P}_M$ .

By inverting the result function  $\mathbf{O}_M$ , we also obtain a distribution  $[\![M]\!]_{\mathbb{S}}$  over generalised values (also called a *result distribution*). It can be computed by integrating the density of termination over all traces that yield the generalised values of interest.

$$\llbracket M \rrbracket_{\mathbb{S}}(A) := \langle \langle M \rangle \rangle (\mathbf{O}_{M}^{-1}(A)) = \int \mathbf{P}_{M}(s) \cdot [\mathbf{O}_{M}(s) \in A] \, ds.$$

As an example, for the geometric distribution example of Section 2.4 we have  $\mathbf{O}_{geometric\ 0.5}(s) = n$  if  $s \in [0.5, 1]^n[0, 0.5)$ , and otherwise  $\mathbf{O}_{geometric\ 0.5}(s) = \mathtt{fail}$ . Similarly, we have  $\mathbf{P}_{geometric\ 0.5}(s) = 1$  if  $s \in [0.5, 1]^n[0, 0.5)$  for some n, and otherwise 0. We then obtain

$$\langle \langle geometric \ 0.5 \rangle \rangle (A) = \sum_{n \in \mathbb{N}} \lambda_{n+1} (A \cap \{[0.5, 1]^n [0, 0.5)\}) \text{ and}$$

$$[[geometric \ 0.5]]_{\mathbb{S}}(\{n\}) = \int [s \in \{[0.5, 1]^n [0, 0.5)\}] ds = \frac{1}{2^{n+1}}.$$

As seen above, we use the exception fail to model the failure of a hard constraint. To restrict attention to normal termination, we modify  $P_M$  as follows.

$$\mathbf{P}_{M}^{\mathcal{V}}(s) = \left\{ \begin{array}{ll} w & \text{if } M \Downarrow_{w}^{s} V \text{ for some } V \in \mathcal{V} \\ 0 & \text{otherwise.} \end{array} \right.$$

As above, this density function generates distributions over traces and values as, respectively

$$\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}(A) := \int_{A} \mathbf{P}_{M}^{\mathcal{V}} = \langle\!\langle M \rangle\!\rangle (A \cap \mathbf{O}_{M}^{-1}(\mathcal{V}))$$
$$(\llbracket M \rrbracket_{\mathbb{S}})|_{\mathcal{V}}(A) := \langle\!\langle M \rangle\!\rangle^{\mathcal{V}}(\mathbf{O}_{M}^{-1}(A)) = \int \mathbf{P}_{M}^{\mathcal{V}}(s) \cdot \left[\mathbf{O}_{M}(s) \in A\right] ds$$

To show that the above definitions make sense measure-theoretically, we first define the measurable space of terms  $(\Lambda, \mathcal{M})$ , where  $\mathcal{M}$  is the set of Borel-measurable sets of terms with respect to the recursively defined metric d in Figure 5.

**Lemma 27** For any closed term M, the functions  $\mathbf{P}_M$ ,  $\mathbf{O}_M$  and  $\mathbf{P}_M^{\mathcal{V}}$  are all measurable;  $\langle\!\langle M \rangle\!\rangle$  and  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}$  are measures on  $(\mathbb{S}, \mathcal{S})$ ;  $[\![M]\!]_{\mathbb{S}}$  is a measure on  $(\mathcal{GV}, \mathcal{M}|_{\mathcal{GV}})$ ; and  $([\![M]\!]_{\mathbb{S}})|_{\mathcal{V}}$  is a measure on  $(\mathcal{V}, \mathcal{M}|_{\mathcal{V}})$ .

Proof. See Appendix A. 
$$\Box$$

# 4 Distribution-Based Operational Semantics

In this section we introduce small- and big-step distribution-based operational semantics, where the small-step semantics is a generalisation of Jones [20] to continuous distributions. We prove correspondence between the semantics using some non-obvious properties of kernels. Moreover, we

```
d(x,x) = 0
d(c,d) = |c-d|
d(MN,LP) = d(M,L) + d(N,P)
d(g(V_1, \dots, V_n), g(W_1, \dots, W_n))
= d(V_1, W_1) + \dots + d(V_n, W_n)
d(\lambda x.M, \lambda x.N) = d(M,N)
d(D(V_1, \dots, V_n), D(W_1, \dots, W_n))
= d(V_1, W_1) + \dots + d(V_n, W_n)
d(\operatorname{score}(V), \operatorname{score}(W)) = d(V, W)
d(\operatorname{if} V \operatorname{then} M \operatorname{else} N, \operatorname{if} W \operatorname{then} L \operatorname{else} P)
= d(V, W) + d(M, L) + d(N, P)
d(\operatorname{fail}, \operatorname{fail}) = 0
d(M, N) = \infty \operatorname{otherwise}
```

Figure 5: Metric d on terms.

will prove that the distribution-based semantics are equivalent to the sampling-based semantics from Section 3. A term will correspond to a distribution over generalised values, below called a result distribution. A term M is said to be *skeleton* iff no real number occurs in M, and each variable occurs at most once in M. The set of skeletons is SK. Any closed term M can be written as  $N\{\vec{c}/\vec{x}\}$ , where N is a skeleton. The set of closed terms corresponding this way to a skeleton  $M \in SK$  is denoted as TM(M). If the underlying term is a skeleton, substitution can be defined also when the substituted terms are *sets* of values rather than mere values, because variables occurs at most once; in that case, we will used the notation  $M\{X/x\}$ , where X is any set of values.

### 4.1 Sub-Probability Kernels

If  $(X, \Sigma)$  and  $(Y, \Sigma')$  are measurable spaces, then a function  $Q: X \times \Sigma' \to \mathbb{R}_{[0,1]}$  is called a (sub-probability) kernel (from  $(X, \Sigma)$  to  $(Y, \Sigma')$ ) if

- 1. for every  $x \in X$ ,  $Q(x, \cdot)$  is a sub-probability distribution on  $(Y, \Sigma')$ ; and
- 2. for every  $A \in \Sigma'$ ,  $Q(\cdot, A)$  is a non-negative measurable function  $X \to \mathbb{R}_{[0,1]}$ .

The measurable function  $q: X \times Y \to \mathbb{R}_+$  is said to be a *density* of kernel Q with respect to a measure  $\mu$  on  $(Y, \Sigma')$  if  $Q(v, A) = \int_A q(v, y) \, \mu(dy)$  for all  $v \in X$  and  $A \in \Sigma'$ . When Q is a kernel, note that  $\int f(y) \, Q(x, dy)$  denotes the integral of f with respect to the measure  $Q(x, \cdot)$ .

Kernels can be composed in the following ways: If  $Q_1$  is a kernel from  $(X_1, \Sigma_1)$  to  $(X_2, \Sigma_2)$  and  $Q_2$  is a kernel from  $(X_2, \Sigma_2)$  to  $(X_3, \Sigma_3)$ , then  $Q_2 \circ Q_1 : (x, A) \mapsto \int Q_2(y, A) Q_1(x, dy)$  is a kernel from  $(X_1, \Sigma_1)$  to  $(X_3, \Sigma_3)$ . Moreover, if  $Q_1$  is a kernel from  $(X_1, \Sigma_1)$  to  $(X_2, \Sigma_2)$  and  $Q_2$  is a kernel from  $(X_1', \Sigma_1')$  to  $(X_2', \Sigma_2')$ , then  $Q_1 \times Q_2 : ((x, y), (A \times B)) \mapsto Q_1(x, A) \cdot Q_2(y, B)$  uniquely extends to a kernel from  $(X_1, \Sigma_1) \times (X_1', \Sigma_1')$  to  $(X_2, \Sigma_2) \times (X_2', \Sigma_2')$ .

### 4.2 Approximation Small-Step Semantics

The first thing we need to do is to generalize deterministic reduction into a relation between closed terms and term distributions. If  $\mu$  is a measure on terms and E is an evaluation context, we let  $E\{\mu\}$  be the push-forward measure  $A \mapsto \mu(\{M \mid E[M] \in A\})$ .

One-step evaluation is a relation  $M \to \mathscr{D}$  between closed terms M and distributions  $\mathscr{D}$  on

terms, defined as follows:

$$\begin{split} E[\mathsf{D}(\vec{c})] &\to E\{\mu_{\mathsf{D}(\vec{c})}\} \\ E[M] &\to \delta(E[N]) \text{ if } M \xrightarrow{\det} N \\ E[\mathsf{score}(c)] &\to c \cdot \delta(E[\mathsf{true}]) \text{ if } 0 < c \leq 1 \end{split}$$

We first of all want to show that one-step reduction is essentially deterministic, and that we have a form of deadlock-freedom.

**Lemma 28** For every closed term M, either M is a generalized value or there is a unique  $\mathscr{D}$  such that  $M \to \mathscr{D}$ .

Proof. An easy consequence of Lemma 1.

We need to prove the just introduced notion of one-step reduction to support composition. This is captured by the following result.

Lemma 29  $\rightarrow$  is a sub-probability kernel.

Let  $R\Lambda_P = \{E[R] \in C\Lambda\}$  be the set of all closed reducible terms.

PROOF. Lemma 28 already tells us that  $\rightarrow$  can be seen as a function  $\hat{\rightarrow}$  defined as follows:

$$\hat{\rightarrow}(M,A) = \left\{ \begin{array}{ll} \mathscr{D}(A) & \text{if } M \rightarrow \mathscr{D}; \\ 0 & \text{otherwise.} \end{array} \right.$$

The fact that  $\hat{\to}(M,\cdot)$  is a distribution is easily verified. On other hand, the fact that  $\hat{\to}(\cdot,A)$  is measurable amounts to proving that  $OS(A,B)=(\hat{\to}(\cdot,A))^{-1}(B)$  is a measurable set of terms whenever B is a measurable set of real numbers. We will do that by showing that for every skeleton N, the set  $OS(A,B)\cap \mathsf{TM}(N)$  is measurable. The thesis then follows by observing that

$$OS(A,B) = \bigcup_{N \in \mathsf{SK}} OS(A,B) \cap \mathsf{TM}(N)$$

and that SK is countable. Now, let us observe that for every skeleton N, the nature of any term L in  $\mathsf{TM}(N)$  as for if being a value, or containing a deterministic redex, or containing a sampling redex, only depends on N and not on the term L. As an example, terms in  $\mathsf{TM}(xy)$  are nothing but deterministic redexes (actually, all of them rewrites deterministically to  $\delta(\mathtt{fail})$ ). This allows us to proceed by distinguishing three cases:

• If all terms in TM(N) are values, then it can be easily verified that

$$OS(A,B) \cap \mathsf{TM}(N) = \left\{ egin{array}{ll} \mathsf{TM}(N) & \text{if } 0 \in B; \\ \varnothing & \text{if } 0 \not \in B. \end{array} \right.$$

Both when  $0 \in B$  and when  $0 \notin B$ , then,  $OS(A, B) \cap TM(N)$  is indeed measurable.

• If all terms in  $\mathsf{TM}(N)$  contain deterministic redexes, then

$$OS(A,B)\cap\mathsf{TM}(N)=\left\{\begin{array}{ll}\to^{-1}(A)\cap\mathsf{TM}(N)&\text{ if }1\in B\\\varnothing&\text{ if }1\not\in B.\end{array}\right.$$

Since deterministic reduction  $\rightarrow$  is known to be measurable, then both when  $1 \in B$  and when  $1 \notin B$ , the set  $OS(A, B) \cap \mathsf{TM}(N)$  is measurable.

- The hardest case is when N is of the form  $G[D(\vec{x})]$ , where G is an evaluation context. In this case, however, we can proceed by decomposing the function we want to prove measurable into three measurable functions:
  - The function  $app : \mathcal{C} \times C\Lambda \to C\Lambda$ , that given an evaluation context E and a term M, returns the term E[M]. This is proved measurable in the Appendix.

$$\frac{n > 0}{G \Rightarrow_n \delta(G)} \text{ (DRED VAL)} \quad \overline{M \Rightarrow_0 \mathbf{0}} \text{ (DRED EMPTY)}$$

$$\frac{M \to \mathscr{D} \qquad \{N \Rightarrow_n \mathscr{E}_N\}_{N \in \text{supp}(\mathscr{D})}}{M \Rightarrow_{n+1} A \mapsto \int \mathscr{E}_N(A) \mathscr{D}(dN)} \text{ (DRED STEP)}$$

Figure 6: Step-Indexed Approximation Small-Step Semantics.

- The function  $deapp: R\Lambda_P \to \mathcal{C} \times C\Lambda$  that "splits" a term in  $R\Lambda_P$  into an evaluation context E and a closed term M. This is proved measurable in the Appendix.
- For every distribution identifier D, the function  $distapp_{D} : \mathbb{R}^{n} \to C\Lambda$  (where n is the arity of D) that, given a tuple of real numbers x, returns the term D(x). This function is a continuous function between two metric spaces, so measurable.
- We know that for every distribution identifier D, there is a kernel  $\mu_{\mathsf{D}}: \mathbb{R}^n \times \Sigma_{\mathbb{R}} \to \mathbb{R}_{[0,1]}$ . Moreover, one can also consider the Dirac kernel on evaluation contexts, namely  $I: \mathcal{C} \times \Sigma_{\mathcal{C}} \to \mathbb{R}_{[0,1]}$  where  $I(E,A) = [A \in E]$ . Then, the product  $\mu_{\mathsf{D}} \times I$  is also a kernel, so measurable.

This concludes the proof.

Given a family  $\{\mathscr{D}_M\}_{M\in A}$  of distributions indexed by terms in a measurable set A of terms, and a measurable set B, we often write, with an abuse of notation,  $\mathscr{D}_M(B)$  for the function that assigns to any term  $M\in A$  the real number  $\mathscr{D}_M(B)$ . The step-indexed approximation small-step semantics is the family of n-indexed relations  $M\Rightarrow_n\mathscr{D}$  between terms and result distributions inductively defined in Figure 6. Since generalised values have no transitions (there is no  $\mathscr{D}$  such that  $G\to\mathscr{D}$ ), the rules above are disjoint and so there is at most one  $\mathscr{D}$  such that  $M\to_n\mathscr{D}$ . Compared to the discrete case [20], the step-index n is needed to ensure that the integral in (DRED STEP) is defined.

**Lemma 30** For every  $n \in \mathbb{N}$ , the function  $\Rightarrow_n$  is a kernel.

PROOF. By induction on n:

- $\Rightarrow_0$  can be seen as the function  $\hat{\rightarrow}_0$  that attributes 0 to any pair (M,A). This is clearly a kernel
- $\Rightarrow_{n+1}$  can be seen as the function  $\Rightarrow_{n+1}$  defined as follows:

$$\hat{\rightarrow}_{n+1}(M,A) = \begin{cases} 1 & \text{if } M \in \mathcal{GV} \text{ and } M \in A; \\ 0 & \text{if } M \in \mathcal{GV} \text{ and } M \notin A; \\ (\int \hat{\rightarrow}_n(N,A) \, \mathscr{D}(dN)) & \text{if } M \to \mathscr{D}. \end{cases}$$

The fact that  $\hat{\rightarrow}_{n+1}(M,\cdot)$  is a measure for every M is clear, and can be proved by case distinction on M. On the other hand, if B is a measurable set of reals, then:

$$(\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) = (\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) \cap \mathcal{GV} \cup (\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) \cap (C\Lambda - \mathcal{GV}).$$

Now, the fact that  $(\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) \cap \mathcal{GV}$  is a measurable set of terms is clear: it is  $A \cap \mathcal{GV}$  if  $1 \in B$  and  $\varnothing$  otherwise. But how about  $(\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) \cap (C\Lambda - \mathcal{GV})$ ? In that case, we just need to notice that

$$(\hat{\rightarrow}_{n+1}(\cdot,A))^{-1}(B) \cap (C\Lambda - \mathcal{GV}) = (\hat{\rightarrow}_n \circ \to)^{-1}(B)$$

where  $\hat{\rightarrow}_n$  and  $\rightarrow$  are kernels (the former by induction hypothesis, the latter by Lemma 29). Since kernels compose, this concludes the proof.

$$\frac{n > 0}{G \Downarrow_n \delta(G)} \text{ (DEVAL VAL)} \qquad \frac{m \Downarrow_0 0}{M \Downarrow_0 0} \text{ (DEVAL EMPTY)} \qquad \frac{n > 0}{T \Downarrow_n \delta(\text{fail})} \text{ (DEVAL FAIL)}$$

$$\frac{n > 0}{D(\vec{c}) \Downarrow_n \mu_{D(\vec{c})}} \text{ (DEVAL SAMP)} \qquad \frac{n > 0}{g(\vec{c}) \Downarrow_n \delta(\sigma_g(\vec{c}))} \text{ (DEVAL FUN)}$$

$$\frac{0 < c \le 1 \qquad n > 0}{\text{score}(c) \Downarrow_n c \cdot \delta(\text{true})} \text{ (DEVAL SCORE)}$$

$$\frac{M \Downarrow_n \mathscr{D}}{\text{if true then } M \text{ else } N \Downarrow_{n+1} \mathscr{D}} \text{ (DEVAL IF TRUE)}$$

$$\frac{N \Downarrow_n \mathscr{D}}{\text{if false then } M \text{ else } N \Downarrow_{n+1} \mathscr{D}} \text{ (DEVAL IF FALSE)}$$

$$\frac{M \Downarrow_n \mathscr{D} \qquad N \Downarrow_n \mathscr{E} \qquad \{L\{V/x\} \Downarrow_n \mathscr{E}_{L,V}\}_{(\lambda x.L) \in \text{supp}(\mathscr{D}), V \in \text{supp}(\mathscr{E})}}{MN \Downarrow_{n+1} A \mapsto \mathscr{D}|_{\{\text{fail}\}}(A) + \mathscr{D}(\mathbb{R}) \cdot [\text{fail} \in A] + \mathscr{D}(V_{\lambda}) \cdot \mathscr{E}|_{\{\text{fail}\}}(A)} \text{ (DEVAL APPL)}$$

$$+ \iint \mathscr{E}_{L,V}(A) \mathscr{D}|_{V_{\lambda}}(\lambda x.dL) \mathscr{E}|_{V}(dV)$$

Figure 7: Step Indexed Approximation Big-Step Semantics.

**Lemma 31** For every closed term M and for every  $n \in \mathbb{N}$  there is a unique distribution  $\mathscr{D}$  such that  $M \Rightarrow_n \mathscr{D}$ .

Proof. This is an easy consequence of Lemma 30.

### 4.3 Approximation Big-Step Semantics

The step-indexed approximation big-step semantics  $M \downarrow_n \mathscr{D}$  is the n-indexed family of relations between terms and result distributions inductively defined by the rules in Figure 7.

Above, the rule for applications is the most complex, with the resulting distribution consisting of three exceptional terms in addition to the normal case. To better understand this rule, one can study what happens if we replace general applications with a let construct plus application of values to values. Then we would end up having the following three rules, instead of the rule for application above:

$$\frac{M \Downarrow_n \mathscr{D} \qquad \{N\{V/x\} \Downarrow_n \mathscr{E}_V\}_{V \in \operatorname{supp}(\mathscr{D})}}{\operatorname{let} x = M \text{ in } N \Downarrow_{n+1} A \mapsto \left(\begin{array}{c} \mathscr{D}|_{\{\text{fail}\}}(A) + \mathscr{D}(\mathbb{R}) \cdot [\text{fail} \in A] \\ + \int \mathscr{E}_V(A) \mathscr{D}|_{\mathcal{V}}(dV) \end{array}\right)}$$
$$\frac{M\{V/x\} \Downarrow_n \mathscr{E}}{(\lambda x.M)V \Downarrow_{n+1} \mathscr{E}} \qquad \frac{n > 0}{c \ V \Downarrow_n \delta(\text{fail})}$$

The existence of the integral in rule (DEVAL APPL) is guaranteed by a lemma analogous to Lemma 30

**Lemma 32** For every  $n \in \mathbb{N}$ , the function  $\downarrow_n$  is a kernel.

This can be proved by induction on n, with the most difficult case being precisely the one of applications. Composition and product properties of kernels are the key ingredients there.

### 4.4 Beyond Approximations

The set of result distributions with the pointwise order forms an  $\omega \mathbf{CPO}$ , and thus any denumerable, directed set of result distributions has a least upper bound. One can define the *small-step* semantics and the big-step semantics as, respectively, the two distributions

$$[\![M]\!]_{\Rightarrow} = \sup \{ \mathscr{D} \mid M \to_n \mathscr{D} \}$$
$$[\![M]\!]_{\downarrow} = \sup \{ \mathscr{D} \mid M \Downarrow_n \mathscr{D} \}$$

It would be quite disappointing if the two object above were different. Indeed, this section is devoted to proving the following theorem:

**Theorem 2** For every term M,  $[M]_{\Rightarrow} = [M]_{\Downarrow}$ .

The following is a fact which will be quite useful in the following:

Lemma 33 (Monotonicity) If 
$$M \Rightarrow_n \mathcal{D}$$
,  $m \geq n$  and  $M \Rightarrow_m \mathcal{E}$ , then  $\mathcal{E} \geq \mathcal{D}$ .

Theorem 2 can be proved by showing that any big-step approximation can itself over-approximated with small-step, and vice versa. Let us start by showing that, essentially, the big-step rule for applications is small-step-admissible:

**Lemma 34** If  $M \Rightarrow_n \mathscr{D}$ ,  $N \Rightarrow_m \mathscr{E}$ , and for all L and V,  $L\{V/x\} \Rightarrow_p \mathscr{E}_{L,V}$ , then  $MN \Rightarrow_{n+m+p} \mathscr{F}$  such that for all A

$$\begin{split} \mathscr{F}(A) & \geq \mathscr{D}|_{\{\mathtt{fail}\}}(A) + \mathscr{D}(\mathbb{R}) \cdot [\mathtt{fail} \in A] + \mathscr{D}(\mathcal{V}_{\lambda}) \cdot \mathscr{E}|_{\{\mathtt{fail}\}}(A) \\ & + \iint \mathscr{E}_{L,V}(A) \, \mathscr{D}|_{\mathcal{V}_{\lambda}}(\lambda x.dL) \, \mathscr{E}|_{\mathcal{V}}(dV). \end{split}$$

PROOF. First of all, one can prove that if  $N \Rightarrow_n \mathscr{D}$  and  $L\{V/x\} \Rightarrow_m \mathscr{E}_V$  for all V then  $(\lambda x.L)N \Rightarrow_{n+m} \mathscr{F}$  where  $\mathscr{F}(A) \geq \mathscr{D}|_{\{\text{fail}\}}(A) + \int \mathscr{E}_V(A) \mathscr{D}|_{\mathcal{V}}(dV)$  for all A. This is an induction on n.

- If n = 0, then  $\mathscr{D}$  is necessarily the zero distribution  $A \mapsto 0$ . Then  $\mathscr{F}(A) \geq 0 = \mathscr{D}|_{\{\text{fail}\}}(A) + \int \mathscr{E}_V(A) \mathscr{D}|_V(dV))$ .
- Suppose the thesis holds for n, and let's try to prove the thesis for n + 1. We proceed by further distinguishing some subcases:
  - If N is a value W, then  $\mathcal{D} = \delta(W)$ ,  $\mathcal{D}|_{\{\text{fail}\}}$  is the zero distribution and thus

$$(\lambda x.L)N \Rightarrow_{m+1} (A \mapsto \mathscr{D}|_{\{\text{fail}\}}(A) + \int \mathscr{E}_V(A) \mathscr{D}|_{\mathcal{V}}(dV)).$$

The thesis follows by monotonicity.

• If N is an exception fail, then  $\mathscr{D} = \delta(\mathtt{fail})$ , and since  $(\lambda x.L)\mathtt{fail} \to \mathtt{fail}$ , we can conclude that, since  $\mathscr{D}|_{\mathcal{V}}$  is the zero distribution,

$$(\lambda x.L)N \Rightarrow_2 \delta(\mathtt{fail}) = (A \mapsto \mathscr{D}|_{\{\mathtt{fail}\}}(A) + \int \mathscr{E}_V(A)\,\mathscr{D}|_{\mathcal{V}}(dV)).$$

The thesis again follows by monotonicity.

• If N is not a generalized value, then, necessarily  $\mathscr{D}(A) = \int \mathscr{G}_P(A) \mathscr{H}(dP)$ , where  $N \to \mathscr{H}$  and  $P \Rightarrow_n \mathscr{G}_P$  for every P. By induction hypothesis, there are distributions  $\mathscr{I}_P$  such that  $(\lambda x.L)P \Rightarrow_{n+m} \mathscr{I}_P$ , and, for all A,

$$\mathscr{I}_P(A) \geq \mathscr{G}_P|_{\{\mathtt{fail}\}} + \int \mathscr{E}_V(A) \mathscr{G}_P|_{\mathcal{V}}(dV)$$

Let now E be the evaluation context  $(\lambda x.L)[\cdot]$ . Then, it holds that  $(\lambda x.L)N \to E\{\mathcal{H}\}$  and thus:

$$(\lambda x.L)N \Rightarrow_{n+m+1} (A \mapsto \int \mathscr{I}_P(A) (E\{\mathscr{H}\}((\lambda x.L)dP))).$$

We can now observe that:

$$\begin{split} \int \mathscr{I}_{P}(A) \left( E\{\mathscr{H}\}((\lambda x.L)dP) \right) &= \int \mathscr{I}_{P}(A) \,\mathscr{H}(dP) \\ &\geq \int \mathscr{G}_{P}|_{\{\mathtt{fail}\}}(A) \,\mathscr{H}(dP) + \iint \mathscr{E}_{V}(A) \,\mathscr{G}_{P}|_{\mathcal{V}}(dV) \,\mathscr{H}(dP) \\ &= \mathscr{D}|_{\{\mathtt{fail}\}}(A) + \iint \mathscr{E}_{V}(A) \,\mathscr{G}_{P}|_{\mathcal{V}}(dV) \,\mathscr{H}(dP) \\ &= \mathscr{D}|_{\{\mathtt{fail}\}}(A) + \int \mathscr{E}_{V}(A) \,\mathscr{D}|_{\mathcal{V}}(dV). \end{split}$$

Then one can prove the statement of the lemma, again by induction on n, following the same strategy as above.

**Lemma 35** If  $M \downarrow_n \mathscr{D}$  there is  $\mathscr{E}$  s.t.  $M \Rightarrow_{3^n} \mathscr{E}$  and  $\mathscr{E} > \mathscr{D}$ .

PROOF. By induction on n, we can prove that if  $M \downarrow_n \mathscr{D}$ , then  $M \Rightarrow_{\mathscr{E}}$  where  $\mathscr{E} \geq \mathscr{D}$ . The only interesting case is when M is an application, and there we simply use Lemma 34.

At this point, we already know that  $[\![M]\!]_{\Rightarrow} \geq [\![M]\!]_{\downarrow}$ . The symmetric inequality can be proved by showing that the big-step rule for applications can be *inverted* in the small-step:

**Lemma 36** If  $MN \Rightarrow_{n+1} \mathscr{D}$ , then  $M \Rightarrow_n \mathscr{E}$ ,  $N \Rightarrow_n \mathscr{F}$  and for all P and V,  $P\{V/x\} \Rightarrow_n \mathscr{G}_{P,V}$ such that for all A,

$$\begin{split} \mathscr{D}(A) &\leq \mathscr{E}|_{\{\mathtt{fail}\}}(A) + \mathscr{E}(\mathbb{R}) \cdot [\mathtt{fail} \in A] + \mathscr{E}(\mathcal{V}_{\lambda}) \cdot \mathscr{F}|_{\{\mathtt{fail}\}}(A) \\ &+ \iint \mathscr{G}_{P,V}(A) \, \mathscr{E}|_{\mathcal{V}_{\lambda}}(\lambda x.dP) \, \mathscr{F}|_{\mathcal{V}}(dV). \end{split}$$

PROOF. By induction on n.

- If n = 0, then  $\mathcal{D}$  is the zero distribution, and so are  $\mathcal{E}, \mathcal{F}$  and all  $\mathcal{G}_{P,V}$ .
- Suppose the thesis holds for every natural number smaller than n and prove it for n. Let us distinguish a few cases, and examine the most relevant ones:
  - If M is an abstraction  $\lambda x.L$  and N is a value W, then  $M \to \delta(L\{W/x\})$  and  $L\{W/x\} \Rightarrow_n \mathscr{D}$ . We can then observe that

$$\begin{split} \mathscr{E} &= \delta(\lambda x.L) \\ \mathscr{F} &= \delta(W) \\ \mathscr{G}_{P,V} &= \mathscr{D} \text{ whenever } P = L \text{ and } V = W \end{split}$$

Just observe that

$$\mathscr{D}(A) = \iint \mathscr{G}_{P,V}(A)\,\mathscr{E}(\lambda x.dP)\,\mathscr{F}(dV)$$

and that  $\mathscr{E}|_{\{\mathtt{fail}\}} = \mathscr{E}|_{\mathbb{R}} = \mathscr{F}|_{\{\mathtt{fail}\}} = \mathbf{0}$ .

• If none of M and N are values, then  $M \to \mathscr{L}$  and thus  $MN \to E\{\mathscr{L}\}$  where  $E = [\cdot]N$ . Moreover,  $LN \Rightarrow_n \mathscr{H}_L$ , where

$$\mathscr{D}(A) = \int \mathscr{H}_L(A) \, E\{\mathscr{L}\}((dL)N) = \int \mathscr{H}_L(A) \, \mathscr{L}(dL)$$

We apply the induction hypothesis (and monotonicity) to each of the  $LN \Rightarrow_n \mathscr{H}_L$ , and we obtain that  $L \Rightarrow_{n-1} \mathscr{I}_L$ ,  $N \Rightarrow_n \mathscr{F}$  and  $P\{V/x\} \Rightarrow_n \mathscr{G}_{P,V}$ , where

$$\begin{split} \mathscr{H}_L(A) &\leq \mathscr{I}_L|_{\{\mathtt{fail}\}}(A) + \mathscr{I}_L(\mathbb{R}) \cdot [\mathtt{fail} \in A] + \mathscr{I}_L(\mathcal{V}_\lambda) \cdot \mathscr{F}|_{\{\mathtt{fail}\}}(A) \\ &+ \iint \mathscr{G}_{P,V}(A) \, \mathscr{I}_L|_{\mathcal{V}_\lambda}(\lambda x.dP) \, \mathscr{F}|_{\mathcal{V}}(dV) \end{split}$$

Now let  $\mathcal E$  be the distribution

$$A \mapsto \int \mathscr{I}_L(A) \mathscr{L}(dL).$$

Clearly,  $M \Rightarrow_n \mathscr{E}$ . Moreover,

$$\begin{split} \mathscr{D}(A) &= \int \mathscr{H}_L(A)\,\mathscr{L}(dL) \\ &\leq \int \mathscr{I}_L|_{\{\mathtt{fail}\}}(A)\,\mathscr{L}(dL) + \int \mathscr{I}_L(\mathbb{R}) \cdot [\mathtt{fail} \in A]\,\mathscr{L}(dL) \\ &+ \int \mathscr{I}_L(\mathcal{V}_\lambda) \cdot \mathscr{F}|_{\{\mathtt{fail}\}}(A)\,\mathscr{L}(dL) \\ &+ \iiint \mathscr{G}_{P,V}(A)\,\mathscr{I}_L|_{\mathcal{V}_\lambda}(\lambda x.dP)\,\mathscr{F}|_{\mathcal{V}}(dV)\,\mathscr{L}(dL) \\ &= \mathscr{E}|_{\{\mathtt{fail}\}}(A) + \mathscr{E}(\mathbb{R}) \cdot [\mathtt{fail} \in A] + \mathscr{E}(\mathcal{V}_\lambda) \cdot \mathscr{F}|_{\{\mathtt{fail}\}}(A) \\ &+ \iint \mathscr{G}_{P,V}(A)\,\mathscr{E}|_{\mathcal{V}_\lambda}(\lambda x.dP)\,\mathscr{F}|_{\mathcal{V}}(dV) \end{split}$$

**Lemma 37** If  $M \Rightarrow_n \mathscr{D}$ , then there is  $\mathscr{E}$  such that  $M \downarrow_n \mathscr{E}$  and  $\mathscr{E} \geq \mathscr{D}$ .

PROOF. Again, this is an induction on n that makes essential use, this time, of Lemma 36.  $\square$ 

Restatement of Theorem 2. For all M,  $[M]_{\Rightarrow} = [M]_{\Downarrow}$ .

PROOF. This is a consequence of Lemma 35 and Lemma 37.

In subsequent sections we let [M] stand for  $[M]_{\Rightarrow}$  or  $[M]_{\Downarrow}$ .

### 4.5 Geometric Distribution, Revisited

Let's consider again the geometric distribution of Section 2.4. There is a monotonically increasing map  $f: \mathbb{N} \to \mathbb{N}$  such that for every n, it holds that

$$(geometric\ 0.5) \Rightarrow_{f(n)} \sum_{i=0}^{n} \frac{1}{2^{i+1}} \delta(i)$$

As a consequence,  $[geometric\ 0.5] = \sum_{i=0}^{\infty} \frac{1}{2^{i+1}} \delta(i)$ .

### 4.6 Distribution-based and Sampling-based Semantics are Equivalent

This section is a proof of the following theorem.

**Theorem 3** For every term M,  $[\![M]\!]_{\mathbb{S}} = [\![M]\!]$ .

The way to prove Theorem 3 is by looking at traces of bounded length. For every  $n \in \mathbb{N}$ , let  $\mathbb{S}_n$  be the set of sample traces of length at most n, which itself has the structure of a measure space with measurable sets  $\mathcal{S}|_{\mathbb{S}_n}$ . We define the result distribution  $[\![M]\!]_{\mathbb{S}}^n$  as follows:

$$[\![M]\!]_{\mathbb{S}}^n(A) = \int_{\mathbb{S}_-} \mathbf{P}_M(s) \cdot [\mathbf{O}_M(s) \in A] \, ds$$

The integral over all traces can be seen as the limit of all integrals over bounded-length traces:

**Lemma 38** If  $f: \mathbb{S} \to \mathbb{R}_+$  is measurable then  $\int f = \sup_n \int_{\mathbb{S}_n} f$ .

PROOF. Let  $g_n(s) = f(s) \cdot [s \in \mathbb{S}_n]$ , so  $\int_{\mathbb{S}_n} f = \int g_n$  by definition. Since the  $g_n$  are converging to f pointwise from below, we have  $\int f = \sup_n \int g_n$  by the monotone convergence theorem.

A corollary is that  $[\![M]\!]_{\mathbb{S}} = \sup_{n \in \mathbb{N}} [\![M]\!]_{\mathbb{S}}^n$ .

**Lemma 39** If  $M \to \mathcal{D}$ , then  $[\![M]\!] = A \mapsto \int [\![N]\!] (A) \mathcal{D}(dN)$ 

PROOF. For every n and for every term N, let  $\mathcal{E}_N^n$  be the unique value distribution such that  $N \Rightarrow_n \mathscr{E}_N^n$ . By definition, we have that

$$\mathscr{E}_M^{n+1}(A) = \int \mathscr{E}_N^n(A) \, \mathscr{D}(dN).$$

By the monotone convergence theorem, then,

$$\begin{split} [\![M]\!](A) &= \sup_n \mathscr{E}_M^{n+1}(A) = \sup_n \int \mathscr{E}_N^n(A) \; \mathscr{D}(dN) \\ &= \int (\sup_n \mathscr{E}_N^n(A)) \; \mathscr{D}(dN) = \int [\![N]\!](A) \; \mathscr{D}(dN). \end{split}$$

The following is a useful technical lemma.

**Lemma 40**  $[E[D(\vec{c})]]_{\mathbb{S}}^{n+1}(A) = \int [N]_{\mathbb{S}}^{n}(A) E\{\mu_{D}(\vec{c})\}(dN).$ 

**Lemma 41** If  $M \to \mathcal{D}$ , then  $[\![M]\!]_{\mathbb{S}} = A \mapsto \int [\![N]\!]_{\mathbb{S}}(A) \, \mathcal{D}(dN)$ 

A program M is said to deterministically diverge iff  $(M,1,s) \Rightarrow (N,w,[])$  implies that w=1, s = [], and N is not a generalized value. Terms that deterministically diverge have very predictable semantics, both distribution- and sampling-based.

**Lemma 42** If M deterministically diverges then  $[M] = [M]_{\mathbb{S}} = 0$ .

PROOF. One can easily prove, by induction on n, that if M deterministically diverges, then  $M \Rightarrow_n \mathbf{0}$ :

- If n=0, then  $M \Rightarrow_n \mathbf{0}$  by definition.
- About the inductive case, since M cannot be a generalized value, it must be that  $M \to \delta(N)$ (where N deterministically diverges) and that  $M \Rightarrow_{n+1} \mathcal{D}$ , where  $N \Rightarrow_n \mathcal{D}$ . By induction hypothesis,  $\mathcal{D} = \mathbf{0}$ .

The fact that  $[\![M]\!]_S = \mathbf{0}$  is even simpler to prove, since if M deterministically diverges, then there cannot be any s, w, V such that  $M \downarrow_w^s V$ , and thus  $\mathbf{P}_M(s)$  is necessarily 0.

A program M is said to deterministically converge to a program N iff  $(M, 1, []) \Rightarrow (N, 1, [])$ . Any term that deterministically converges to another term has the same semantics as the latter.

**Lemma 43** Let M deterministically converge to N. Then:

- $\mathscr{D} \leq \mathscr{E}$  whenever  $M \Rightarrow_n \mathscr{D}$ ; and  $N \Rightarrow_n \mathscr{E}$ ;
- $\bullet \ \llbracket M \rrbracket_{\mathbb{S}}^n = \llbracket N \rrbracket_{\mathbb{S}}^n; \\ \bullet \ \llbracket M \rrbracket = \llbracket N \rrbracket \ and \ \llbracket M \rrbracket_{\mathbb{S}} = \llbracket N \rrbracket_{\mathbb{S}}$

PROOF. The first point is an induction on the structure of the proof that M deterministically converge to N. Let us consider the second and third points. Since equality is transitive, we can assume, without losing any generality, that  $(M,1,[]) \to (N,1,[])$ , namely that  $M \xrightarrow{\det} N$ . With the latter hypothesis, it is easy to realize that  $M \downarrow_s^w V$  iff  $N \downarrow_s^w V$  and that  $M \Rightarrow_{n+1} \mathscr{D}$  iff  $N \Rightarrow_n \mathscr{D}$ . The thesis easily follows.

**Lemma 44** For every generalized value G, it holds that  $\llbracket G \rrbracket = \llbracket G \rrbracket_{\mathbb{S}} = \delta(G)$ .

If a term does not diverge deterministically, then it converges either to a generalized value or to a term that performs a sampling.

**Lemma 45** For every program M, exactly one of the following conditions holds:

- M deterministically diverges;
- There is generalized value G such that M deterministically converges to G
- There are  $E, D, c_1, \ldots, c_{|D|}$  such that M deterministically converges to  $E[D(c_1, \ldots, c_{|D|})]$ .

We are finally ready to give the two main lemmas that lead to a proof of Theorem 3. The first one tells us that any distribution-based approximation is smaller than the sampling based semantics:

Lemma 46 If  $M \Rightarrow_n \mathcal{D}$ , then  $\mathcal{D} \leq [\![M]\!]_{\mathbb{S}}$ .

PROOF. By induction on n:

- If n=0, then  $\mathcal{D}$  is necessarily  $\mathbf{0}$ , and we are done.
- About the inductive case, let's distinguish three cases depending on the three cases of Lemma 45, applied to M:
  - If M deterministically diverges, then by Lemma 42,  $\mathscr{D} \leq [M] = [M]_{\mathbb{S}}$ .
  - If M deterministically converges to a generalized value G, then by Lemma 43 and Lemma 44, it holds that

$$\mathscr{D} \leq \llbracket M \rrbracket = \llbracket G \rrbracket = \delta(G) = \llbracket G \rrbracket_{\mathbb{S}} = \llbracket M \rrbracket_{\mathbb{S}}.$$

• If M deterministically converges to  $E[\mathsf{D}(\vec{c})]$ , let  $\mathscr{E}$  be such that  $E[\mathsf{D}(\vec{c})] \Rightarrow_{n+1} \mathscr{E}$ . By Lemma 43 and Lemma 40 we have, by induction hypothesis, that

$$\mathcal{D}(A) \le \mathcal{E}(A) = \int \mathcal{F}_N(A) \ E\{\mu_{\mathsf{D}}(\vec{c})\}(dN)$$
$$\le \int [N]_{\mathbb{S}}(A) \ E\{\mu_{\mathsf{D}}(\vec{c})\}(dN)$$
$$= [M]_{\mathbb{S}}$$

where 
$$N \Rightarrow_n \mathscr{F}_N$$
.

The second main lemma tells us that if we limit our attention to traces of length at most n, then we stay below distribution-based semantics:

**Lemma 47** For every  $n \in \mathbb{N}$ ,  $[M]_{\mathbb{S}}^n \leq [M]$ .

PROOF. By induction on n:

- In the base case, then let us distinguish three cases depending on the three cases of Lemma 45, applied to M:
  - If M deterministically diverges, then by Lemma 42,  $[M]_{\mathbb{S}}^0 \leq [M]_{\mathbb{S}} = [M]$ .
  - If M deterministically converges to a generalized value G, then by Lemma 43 and Lemma 44, it holds that

$$[M]_{\mathbb{S}}^{0} = [G]_{\mathbb{S}}^{0} \le [G]_{\mathbb{S}} = \delta(G) = [G] = [M].$$

- If M deterministically converges to  $E[\mathsf{D}(\vec{c})]$ , then  $[M]_{\mathbb{S}}^0 = [E[\mathsf{D}(\vec{c})]]_{\mathbb{S}}^0 = \mathbf{0} \leq [M]$ .
- About the inductive case, let us again distinguish three cases depending on the three cases of Lemma 45, applied to M:

  - If M deterministically diverges, then by Lemma 42,  $[\![M]\!]_{\mathbb{S}}^{n+1} \leq [\![M]\!]_{\mathbb{S}} = [\![M]\!]$ . If M deterministically converges to a generalized value G, then by Lemma 43 and Lemma 44, it holds that

$$[\![M]\!]_{\mathbb{S}}^{n+1} = [\![G]\!]_{\mathbb{S}}^{n+1} \le [\![G]\!]_{\mathbb{S}} = \delta(G) = [\![G]\!] = [\![M]\!].$$

• If M deterministically converges to  $E[\mathsf{D}(\vec{c})]$ , by Lemma 43 and Lemma 40 we have, by induction hypothesis, that

$$\begin{split} [\![M]\!]_{\mathbb{S}}^{n+1}(A) &= [\![E[\mathsf{D}(\vec{c})]]\!]_{\mathbb{S}}^{n+1}(A) \\ &= \int [\![N]\!]_{\mathbb{S}}^{n}(A) \ E\{\mu_{\mathsf{D}}(\vec{c})\}(dN) \\ &\leq \int [\![N]\!](A) \ E\{\mu_{\mathsf{D}}(\vec{c})\}(dN) \\ &= [\![M]\!]. \end{split}$$

Restatement of Theorem 3.  $[\![M]\!]_{\mathbb{S}} = [\![M]\!]$ .

Proof.

**Corollary 1** The measures  $\langle\!\langle M \rangle\!\rangle$  and  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}$  are sub-probability distributions.

## 4.7 An Application of the Distribution-Based Semantics

It is routine to show that for all values V, it holds that  $[score(V)]|_{\mathcal{V}} = [MV]|_{\mathcal{V}}$ , where M is the term

$$\lambda x. \texttt{if } (0 < x) \land (x \leq 1)$$
 then (if  $flip(x)$  then true else fail) else fail

This shows that even though  $\mathtt{score}(V)$  and MV do not have the same sampling-based semantics, they can be used interchangeably whenever only their extensional, distribution-based behaviour on values is important. We use the equation to our advantage by encoding soft constraints with  $\mathtt{score}$  instead of  $\mathtt{flip}$  (as discussed in Section 2.5), as the fewer the nuisance parameters the better for inference.

Whenever the stronger equation  $\llbracket \mathtt{score}(V) \rrbracket = \llbracket MV \rrbracket$  is needed, we could replace M by the following one:

$$\lambda x. \texttt{if } (0 < x) \land (x \leq 1)$$
 then (if  $flip(x)$  then true else  $\Omega$ ) else fail

### 4.8 Rejection Sampling

The same (normalized) distribution on successful runs would be obtained by re-evaluating the entire program from the beginning whenever the Boolean predicate fails, as in:

This corresponds to a basic inference algorithm known as rejection sampling.

#### 4.9 Motivation for 1-Bounded Scores

Recall that we only consider score(c) for  $c \in (0,1]$ . Admitting score(2) (say), we exhibit an anomaly by constructing a recursive program that intuitively terminates with probability 1, but where the expected value of its score is infinite. Let

$$inflate := fix \ f \ \lambda x.if \ flip(0.5) \ then \ score(2); (f \ x) \ else \ x.$$

Since [score(2)] = [fail] we have  $[inflate\ V] = 0.5 \cdot \delta(V) + 0.5 \cdot \delta(fail)$  for any V. However, evaluating inflate V in a version of our trace semantics where the argument to score may be 2 yields

$$\langle\langle inflate\ V\rangle\rangle(\mathbb{S}_n) = \sum_{k=1}^n 1/2 = n/2$$

and so there  $[inflate\ V]_{\mathbb{S}}(A) = \infty$  if  $V \in A$ , otherwise 0.

More strikingly, in the modified semantics we would also have  $\llbracket inflate \ \mathsf{Gaussian}(0,1) \rrbracket_{\mathbb{S}}([q,r]) = \infty$  for all real numbers q < r. These examples show that even statically bounded scores in combination with recursion may yield return value measures that are not even  $\sigma$ -finite, causing many standard results in measure theory not to apply. For this reason, we restrict attention to positive scores bounded by one. An alternative approach would be to admit unbounded scores, and restrict attention to those programs for which  $\llbracket M \rrbracket_{\mathbb{S}}(\mathcal{V}) < \infty$ .

### 5 Inference

In this section, we present a variant of the Metropolis-Hastings (MH) algorithm [26, 17] for sampling the return values of a particular closed term  $M \in C\Lambda$ . This algorithm yields consecutive samples from a Markov chain over  $\mathbb{S}$ , such that the density of the samples s converges to  $\mathbf{P}_{M}^{\mathcal{V}}(s)$  up to normalization. We can then apply the function  $\mathbf{O}_{M}$  to obtain the return value of M for a given trace.

We prove correctness of this algorithm by showing that as the number of samples goes to infinity, the distribution of the samples approaches the distributional semantics of the program.

### 5.1 A Metropolis-Hastings Sampling Algorithm

We begin by outlining a generic Metropolis-Hastings algorithm for probabilistic programs, parametric in a proposal density function q(s,t). The algorithm consists of three steps:

- 1. Pick an initial state s with  $\mathbf{P}_{M}^{\mathcal{V}}(s) \neq 0$  (e.g., by running M).
- 2. Draw the next state t at random with probability density q(s,t).
- 3. Compute  $\alpha$  as below.

$$\alpha = \min\left(1, \frac{\mathbf{P}_{M}^{\mathcal{V}}(t)}{\mathbf{P}_{M}^{\mathcal{V}}(s)} \cdot \frac{q(t, s)}{q(s, t)}\right) \tag{1}$$

- With probability  $\alpha$ , output t and repeat from 2 with s := t.
- Otherwise, output s and repeat from 2 with s unchanged.

The formula used for the number  $\alpha$  above is often called the Hastings acceptance probability. Different probabilistic programming language implementations use different choices for the density q above, based on pragmatics. The trivial choice would be to let  $q(s,t) = \mathbf{P}_M^{\mathcal{V}}(t)$  for all s, which always yields  $\alpha = 1$  and so is equivalent to rejection sampling. We here define another simple density function q (based on Hur et al. [19]), giving emphasis to the conditions that it needs to satisfy in order to prove the convergence of the Markov chain given by the Metropolis-Hastings algorithm (Theorem 4).

$$q(s,t) = (\prod_{i=1}^k \operatorname{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i)) \cdot \mathbf{P}_N^{\mathcal{V}}(t_{k+1..|t|})$$
if  $|t| \neq 0$ , where  $k = \min\{|s|, |t|\}$ 
and  $N = \operatorname{peval}(M, t_{1..k})$ 

$$q(s, []) = 1 - \int_A q(s,t) \, dt, \text{ where } A = \{t \mid |t| \neq 0\}$$

$$Q(s,A) = \int_A q(s,t) \, dt$$

Figure 8: Proposal Density q(s,t) and Kernel Q(s,A) for Program M

#### **Proposal Density** 5.2

In the following, let M be a fixed program. Given a trace  $s = [c_1, \ldots, c_n]$ , we write  $s_{i...j}$  for the trace  $[c_i, \ldots, c_j]$  when  $1 \le i \le j \le n$ . Intuitively, the following procedure describes how to obtain the proposal kernel density (q above):

- 1. Given a trace s of length n, let  $t = [t_1, \ldots, t_n]$  where each  $t_i$  is drawn independently from a normal distribution with mean  $s_i$  and variance  $\sigma^2$ , and let  $p_i$  be the probability density of  $t_i$ .
- 2. Let  $k \leq n$  be the largest number such that  $(M, 1, t_{1...k}) \Rightarrow (M', w, [])$ . There are three cases:
  - If k = n, run  $M' \downarrow_{t'}^{w'} V$ , and let  $q(s, t@t') = p_1 \dots p_n w'$ . If k < n and  $M' \downarrow_{\parallel}^{1} V$ , let  $q(s, t_{1...k}) = p_1 \dots p_k$ .

  - Otherwise, let  $q(s, t_{1...k}) = 0$  and propose the trace ||...|

To define this density formally, we first give a function that partially evaluates M given a trace. Let peval be a function taking a closed term M and trace s and returning the closed term M'obtained after applying just as many reduction steps to M as required to use up the entire trace s (or fail if this cannot be done).

$$\mathtt{peval}(M,s) = \begin{cases} M & \text{if } s = []\\ M' & \text{if } (M,1,s) \Rightarrow (M_k,w_k,s_k) \to (M',w',[])\\ & \text{for some } M_k,w_k,s_k,w' \text{ such that } s_k \neq []\\ \texttt{fail} & \text{otherwise} \end{cases}$$

Lemma 48 For every  $M \in C\Lambda$ ,  $c \in \mathbb{R}$ ,  $s \in \mathbb{S}$ , peval(peval(M, [c]), s) = peval(M, c :: s).

PROOF. By splitting the equality into two inequalities, substituting the alternative definition of peval (described in the appendix) and using Scott induction.

Lemma 49 For every  $M \in C\Lambda$ ,  $c \in \mathbb{R}$ ,  $s \in \mathbb{S}$ , peval(peval(M, s), t) = peval(M, s@t).

PROOF. By induction on |s|, with appeal to Lemma 48.

#### A Metropolis-Hastings Proposal Kernel 5.3

We define the transition kernel Q(s,A) of the Markov chain constructed by the algorithm by integrating a density q(s,t) (as a function of t) over A with respect to the stock measure  $\mu$  on program traces. For technical reasons, we need to ensure that Q is a probability kernel, i.e., that  $Q(s,\mathbb{S})=1$  for all s. We normalize  $q(s,\cdot)$  by giving non-zero probability q(s,[]) to transitions ending in [] (which is not a completed trace of M by assumption). All this is in Figure 8.

The integral  $\int_A q(s,t)dt$  is well-defined if and only if  $q(s,\cdot)$  is non-negative and measurable for every s. In order to show that this property is satisfied, we first need to prove that the peval function, used in the definition of q, is measurable:

**Lemma 50** peval is a measurable function  $C\Lambda \times \mathbb{S} \to C\Lambda$ .

Using this result, we can show that q, as a function defined on pairs of traces, is measurable.

**Lemma 51** For any closed program M, the transition density  $q(\cdot,\cdot):(\mathbb{S}\times\mathbb{S})\to\mathbb{R}_+$  is measurable.

By a well-known result in measure theory [2, Theorem 18.1], it follows that  $q(s, \cdot)$  is measurable for every  $s \in \mathbb{S}$ . To define the transition kernel for the algorithm in terms of the proposal kernel Q, we need to show that Q is a probability kernel.

**Lemma 52** The function Q is a probability kernel on (S, S).

The proofs of lemmas 50, 51 and 52 can be found in the long version of this paper [4].

#### 5.4 Transition Kernel of the Markov Chain

We now use the proposal kernel Q to construct the transition kernel of the Markov chain induced by the algorithm. To avoid trivial cases, we assume that M has positive success probability and does not behave deterministically, i.e., that  $[M](\mathcal{V}) > 0$  and  $\langle\!\langle M \rangle\!\rangle(\{[]\}) = 0$ .

Hastings' Acceptance Probability  $\alpha$  is defined as in Equation (1) on page 32, where we let  $\alpha(s,t)=0$  if  $\mathbf{P}_{M}^{\mathcal{V}}(t)=0$  and otherwise  $\alpha(s,t)=1$  if  $\mathbf{P}_{M}^{\mathcal{V}}(s)\cdot q(s,t)=0$ . Given the proposal transition kernel Q and the acceptance ratio  $\alpha$ , the Metropolis-Hastings algorithm yields a Markov chain over traces with the following transition probability kernel.

$$P(s,A) = \int_{A} \alpha(s,t) Q(s,dt) + [s \in A] \cdot \int (1 - \alpha(s,t)) Q(s,dt). \tag{2}$$

Define  $P^n(s,A)$  to be the probability of the n:th element of the chain with transition kernel P starting at s being in A:

$$P^{0}(s,A) = [s \in A]$$

$$P^{n+1}(s,A) = \int P(t,A)P^{n}(s,dt)$$

**Lemma 53** If  $s_0 \in \mathbf{O}_M^{-1}(\mathcal{V})$  then  $P^n(s_0, \mathbf{O}_M^{-1}(\mathcal{V})) = 1$ .

PROOF. By induction on n. The base case holds, since  $s_0 \in \mathbf{O}_M^{-1}(\mathcal{V})$  by assumption. For the induction case, we have  $P^{n+1}(s_0, \mathbf{O}_M^{-1}(\mathcal{V})) = \int P(s, \mathbf{O}_M^{-1}(\mathcal{V})) P^n(s_0, ds)$ . If  $s \in \mathbf{O}_M^{-1}(\mathcal{V})$  we have

$$\begin{split} P(s, \mathbf{O}_{M}^{-1}(\mathcal{V})) &= \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} \alpha(s,t) \, Q(s,dt) + \int (1 - \alpha(s,t)) \, Q(s,dt) \\ &= \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} q(s,t) \, dt + (1 - \alpha(s,[])) q(s,[]) \\ &= \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} q(s,t) \, dt + (1 - \alpha(s,[])) (1 - \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} q(s,t) \, dt) \\ &= 1 - \alpha(s,[]) (1 - \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} q(s,t) \, dt) \end{split}$$

where  $\alpha(s, ||) = 0$  since  $\mathbf{P}_{M}^{\mathcal{V}}(||) = 0$  by assumption. Then

$$\int P(s, \mathbf{O}_{M}^{-1}(\mathcal{V})) P^{n}(s_{0}, ds) = \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} P(s, \mathbf{O}_{M}^{-1}(\mathcal{V})) P^{n}(s_{0}, ds)$$

$$= \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} 1 P^{n}(s_{0}, ds)$$

$$= 1$$

where the first and the third equality follow from the induction hypothesis.

**Lemma 54** There is  $0 \le c < 1$  such that  $P^n([], \mathbf{O}_M^{-1}(\mathcal{V})) = 1 - c^n$  and  $P^n([], \{[]\}) = c^n$ .

PROOF. Let  $c = 1 - \langle\!\langle M \rangle\!\rangle^{\mathcal{V}}(\mathbb{S} \setminus \{[]\})$ . By assumption  $[] \notin \mathbf{O}_M^{-1}(\mathcal{V})$  and c < 1, and since  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}$  is a sub-probability distribution we have  $0 \le c$ . We proceed by induction on n. The base case is trivial. For the induction case, we have  $P(s, \mathbb{S} \setminus \{[]\}) = 1$  for all  $s \in \mathbf{O}_M^{-1}(\mathcal{V})$ . Finally

$$P([], \mathbf{O}_{M}^{-1}(\mathcal{V})) = \int_{\mathbf{O}_{M}^{-1}(\mathcal{V})} \mathbf{P}_{M}^{\mathcal{V}} = \langle \langle M \rangle \rangle^{\mathcal{V}} (\mathbf{O}_{M}^{-1}(\mathcal{V})) = \langle \langle M \rangle \rangle^{\mathcal{V}} (\mathbb{S} \setminus \{[]\}).$$

Based on Lemma 53 and 54, we below consider the Markov chain with kernel P restricted to  $\mathbf{O}_M^{-1}(\mathcal{V}) \cup \{[]\}$ .

### 5.5 Correctness of Inference

By saying that the inference algorithm is correct, we mean that as the number of steps goes to infinity, the distribution of generated samples approaches the distribution specified by the sampling-based semantics of the program.

Formally, we define  $T^n(s,A) = P^n(s,\mathbf{O}_M^{-1}(A))$  as the value sample distribution at step n of the Metropolis-Hastings Markov chain. For two measures defined on the same measurable space  $(X,\Sigma)$ , we also define the variation norm  $||\mu_1 - \mu_2||$  as:

$$||\mu_1 - \mu_2|| = \sup_{A \in \Sigma} |\mu_1(A) - \mu_2(A)|$$

We want to prove the following theorem:

Theorem 4 (Correctness) For every trace s with  $\mathbf{P}_{M}^{\mathcal{V}}(s) \neq 0$ ,

$$\lim_{n \to \infty} ||T^n(s, \cdot) - [M]||_{\mathcal{V}}|| = 0.$$

To do so, we first need to investigate the convergence of  $P^n$  to our target distribution  $\pi$ , defined as follows:

$$\pi(A) = \langle \langle M \rangle \rangle^{\mathcal{V}}(A) / \langle \langle M \rangle \rangle^{\mathcal{V}}(\mathbb{S}).$$

We use a sequence of known results for Metropolis-Hastings Markov chains [38] to prove that  $P^n$  converges to  $\pi$ . We say that a Markov chain transition kernel P is  $\mathscr{D}$ -irreducible if  $\mathscr{D}$  is a non-zero sub-probability distribution on  $(\mathbb{S}, \mathcal{S})$ , and for all  $x \in \mathbb{S}$ ,  $A \in \mathcal{S}$  there exists an integer n > 0 such that  $\mathscr{D}(A) > 0$  implies  $P^n(x, A) > 0$ . We say that P is  $\mathscr{D}$ -aperiodic if there do not exist  $d \geq 2$  and disjoint  $B_1, \ldots, B_d$  such that  $\mathscr{D}(B_1) > 0$ , and  $x \in B_d$  implies  $P(x, B_1) = 1$ , and  $x \in B_i$  implies that  $P(x, B_{i+1}) = 1$  for  $i \in \{1, \ldots, d-1\}$ .

**Lemma 55 (Tierney [38], Theorem 1 and Corollary 2)** Let K be the transition kernel of a Markov chain given by the Metropolis-Hastings algorithm with target distribution  $\mathscr{D}$ . If K is  $\mathscr{D}$ -irreducible and aperiodic, then for all s,  $\lim_{n\to\infty} ||K^n(s,\cdot)-\mathscr{D}||=0$ .

Lemma 56 (Strong Irreducibility) If  $\mathbf{P}_{M}^{\mathcal{V}}(s) > 0$  and  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}(A) > 0$  then P(s, A) > 0.

PROOF. There is n such that  $\mathbf{P}_{M}^{\mathcal{V}}(A \cap \mathbb{S}_{n}) > 0$ . Write  $A|_{n} = A \cap \mathbb{S}_{n}$ . For all  $t \in A|_{n}$ , q(s,t) > 0 by case analysis on whether  $n \leq |s|$ . If  $n \leq |s|$ , then for all  $t \in A|_{n}$ ,

$$q(s,t) = \prod_{i=1}^{n} \operatorname{pdf}_{\mathsf{Gaussian}}(s_{i}, \sigma^{2}, t_{i}) > 0$$
 and 
$$q(t,s) = (\prod_{i=1}^{n} \operatorname{pdf}_{\mathsf{Gaussian}}(t_{i}, \sigma^{2}, s_{i})) \cdot \mathbf{P}_{\mathsf{peval}(M,s_{1-n})}^{\mathcal{V}}(s_{(n+1)}, \dots, s_{n}) > 0.$$

Similarly, if n > |s|, then for all  $t \in A|_n$ ,

$$\begin{split} q(s,t) &= (\Pi_{i=1}^{|s|}\operatorname{pdf}_{\mathsf{Gaussian}}(s_i,\sigma^2,t_i)) \cdot \mathbf{P}^{\mathcal{V}}_{\mathtt{peval}(M,t_{1..|s|})}(t_{(|s|+1)},\ldots,t_{|s|}) > 0 \qquad \text{and} \\ q(t,s) &= \Pi_{i=1}^{|s|}\operatorname{pdf}_{\mathsf{Gaussian}}(t_i,\sigma^2,s_i) > 0. \end{split}$$

Since  $\mu(A|_n) > 0$  and  $\mathbf{P}_M^{\mathcal{V}}(t) > 0$  for all  $t \in A|_n$ ,

$$\begin{split} P(s,A) &\geq P(s,A|_n) \\ &\geq \int_{A|_n} \alpha(s,t) \, Q(s,dt) \\ &= \int_{A|_n} \alpha(s,t) q(s,t) \, dt \\ &= \int_{A|_n} \min\{q(s,t), \frac{\mathbf{P}_M^{\mathcal{V}}(t) q(t,s)}{\mathbf{P}_M^{\mathcal{V}}(s)}\} \, dt \\ &> 0. \end{split}$$

Corollary 2 (Irreducibility) P as given by Equation (2) is  $\pi$ -irreducible.

Lemma 57 (Aperiodicity) P as given by Equation (2) is  $\pi$ -aperiodic.

PROOF. Assume that  $B_1, B_2$  are disjoint sets such that  $\pi(B_1) > 0$  and  $P(s, B_2) = 1$  for all  $s \in B_1$ . If  $s \in B_1$ , Lemma 56 gives that  $P(s, B_1) > 0$ , so  $P(s, B_2) < P(s, \mathbb{S}) = 1$ , which is a contradiction. A fortiori, P is  $\pi$ -aperiodic.

**Lemma 58** If  $\mu_1$  and  $\mu_2$  are measures on  $(X_1, \Sigma_1)$  and  $f: X_1 \to X_2$  is measurable  $\Sigma_1/\Sigma_2$ , then

$$||\mu_1 f^{-1} - \mu_2 f^{-1}|| \le ||\mu_1 - \mu_2||$$

PROOF. We have  $\sup_{B\in\Sigma_2}|\mu_1f^{-1}(B)-\mu_2f^{-1}(B)|=\sup_{A\in\Sigma_1'}||\mu_1(A)-\mu_2(A)||$ , where  $\Sigma_1'=\{f^{-1}(B)|B\in\Sigma_2\}$ . By measurability of f we get  $\Sigma_1'\subseteq\Sigma_1$ , so by monotonicity of sup we get  $\sup_{A\in\Sigma_1'}|\mu_1(A)-\mu_2(A)|\leq\sup_{A\in\Sigma_1}|\mu_1(A)-\mu_2(A)|$ .  $\square$ 

RESTATEMENT OF THEOREM 4. For every trace s with  $\mathbf{P}_{M}^{\mathcal{V}}(s) \neq 0$ ,

$$\lim_{n \to \infty} ||T^n(s, \cdot) - [M]||_{\mathcal{V}}|| = 0.$$

PROOF. By Corollary 2, P is  $\pi$ -irreducible, and by Lemma 57, P is  $\pi$ -aperiodic. Lemma 55 then yields that

$$\lim_{n \to \infty} ||P^n(x, \cdot) - \pi|| = 0.$$

By definition,  $T^n(s,A) = P^n(s,\mathbf{O}_M^{-1}(A))$  and  $[\![M]\!]|_{\mathcal{V}}(A) = [\![M]\!](A \cap \mathcal{V})/[\![M]\!](\mathcal{V})$ . By Theorem 3,  $[\![M]\!](A \cap \mathcal{V}) = [\![M]\!]_{\mathbb{S}}(A \cap \mathcal{V}) = \langle\![M]\!](\mathbf{O}_M^{-1}(A \cap \mathcal{V})) = \langle\![M]\!](\mathbf{O}_M^{-1}(A) \cap \mathbf{O}_M^{-1}(\mathcal{V})) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V}) = \langle\![M]\!](\mathcal{V})$ , which gives  $[\![M]\!]|_{\mathcal{V}}(A) = \pi((O_M^{-1}(A)))$ . Thus, by Lemma 58 and the squeeze theorem for limits we get

$$\lim_{n\to\infty}||T^n(s,\cdot)-[\![M]\!]|_{\mathcal{V}}||\leq \lim_{n\to\infty}||P^n(s,\cdot)-\pi||=0.$$

### 5.6 Examples

To illustrate how inference works, we revisit the geometric distribution and linear regression examples from Section 2. Before discussing the transition kernels for these models, note that the products of Gaussian densities always cancel out in the acceptance probability  $\alpha$ , because  $\operatorname{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i) = \operatorname{pdf}_{\mathsf{Gaussian}}(t_i, \sigma^2, s_i)$  by the definition of the Gaussian PDF.

Geometric Distribution Let us begin with the implementation of the geometric distribution, described in 2.4, which we will call  $M_1$ . Since the only random primitive used in  $M_1$  is rnd, whose density is 1 on all its support, and there are no calls to score, the weight of any trace that yields a value must be 1. Because the *geometric* function applied to 0.5 returns a value immediately when the call to rnd returns a number smaller than 0.5, and recursively calls itself otherwise, otherwise returns a value immediately

The function geometric applied to 0.5 calls itself recursively if the call to rnd returned a value greater or equal to a half, and returns a value immediately otherwise. Hence, every valid trace consists of a sequence of numbers in [0.5, 1], followed by a number in [0, 0.5), and so the set of valid traces is  $S_1 = \{s \mid s_i \in [0, 0.5) \text{ for } i < |s| \land s_{|s|} \in [0.5, 1] \land |s| > 0\}$ . The proposal density is

$$q(s,t) = [t \in S_1] \prod_{i=1}^k \mathrm{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i)$$

where  $k = \min\{|s|, |t|\}$ . The term  $[t \in S_1]$  reflects the fact that for every non-valid trace,

 $\mathbf{P}_{\mathtt{peval}(M,t_{1...k})}^{\mathcal{V}}(t_{k+1..|t|}) = 0.$ As noted above, the Gaussians cancel out in the acceptance ratio, and the density of every valid trace is 1, so  $\alpha(s,t) = [t \in S_1]$ . This means that every valid trace is accepted. The transition kernel of the Markov chain induced by the MH algorithm is

$$\begin{split} P(s,A) &= \int_{A \cap S_1} \Pi_{i=1}^{\min\{|s|,|t|\}} \operatorname{pdf}_{\mathsf{Gaussian}}(s_i,\sigma^2,t_i) \mu(dt) \\ &+ [s \in A] \int_{\mathbb{S} \backslash S_1} \Pi_{i=1}^{\min\{|s|,|t|\}} \operatorname{pdf}_{\mathsf{Gaussian}}(s_i,\sigma^2,t_i) \mu(dt) \end{split}$$

Linear Regression with flip Now, consider the linear regression model from section 2.6, which can be translated from Church to the core calculus by applying the rules in Figure 2 (details are omitted, but the translation is straightforward as there is no recursion).

In every trace in this translated model, which we call  $M_2$ , we have two draws from  $\mathsf{Gaussian}(0,2)$ , whose values are assigned to variables m and b. They are followed by four calls to rnd made while evaluating the four calls to softeq. The conditioning statement at the end sets the return value to false if at least one call to softed evaluates to false. Since softed x y returns true if and only if the corresponding call to rnd returned a value less than squash x y, it follows from the definitions of squash and f that the element of the trace consumed by softeq (f x) y must be in the interval  $[1, \frac{1}{e^{(m \cdot x + b - y)^2}})]$ . Note that since the pdf of rnd is flat, the weight of any trace depends only on the first two random values, drawn from the Gausians, as long as the remaining four random values are in the right intervals.

The full density for this model is

$$\begin{split} \mathbf{P}^{\mathcal{V}}_{M_2}(s) &= \left(\Pi_{i=1}^2 \operatorname{pdf}_{\mathsf{Gaussian}}(0,2,s_i)\right) \cdot \\ & \left(\Pi_{i=1}^4 \left[s_{i+2} \in \left[1, \frac{1}{e^{(s_i \cdot x_i + s_2 - y_i)^2}}\right)\right]\right) \end{split}$$

if  $s \in \mathbb{R}^6$  and  $\mathbf{P}_{M_2}^{\mathcal{V}}(s) = 0$  if  $s \notin \mathbb{R}^6$ .

Note that the partial derivative of  $\mathbf{P}_{M_2}^{\mathcal{V}}(s)$  with respect to each of  $s_3, s_4, s_5, s_6$  is zero wherever defined, precluding the use of efficient gradient-based methods for searching over these components of the trace.

Now, let us derive the density q(s,t), assuming that  $\mathbf{P}_{M_2}^{\mathcal{V}}(s) > 0$  (which implies  $s \in \mathbb{R}^6$ , as shown above) and  $t \in \mathbb{R}^6$ . Since we have |s| = |t| = 6, the formula for q reduces to:

$$q(s,t) = (\Pi_{i=1}^6 \operatorname{pdf}_{\mathsf{Gaussian}}(s_i,\sigma^2,t_i) \mathbf{P}_{M_2'}^{\mathcal{V}}([])$$

where  $M_2' = peval(M_2, t)$ . Because there cannot be more than six random draws in any run of the program,  $M_2'$  is determinstic. This means that  $\mathbf{P}_{M_2'}^{\mathcal{V}}([]) = 0$  if  $M_2' \downarrow_1^{[]}$  fail and  $\mathbf{P}_{M_2'}^{\mathcal{V}}([]) = 1$ if  $M_2' \downarrow_1^{[]}$  fail for some V.

It is easy to check that if  $t \notin \mathbb{R}^6$ , then q(s,t) = 0—since there is no trace of length other than 6 leading to a value, the value of  $\mathbf{P}_{M_2'}^{\mathcal{V}}(t_{k+1..|t|})$  in the definition of q must be 0 in this case.

Thus, the proposal density is

$$\begin{array}{lcl} q(s,t) &=& \left(\Pi_{i=1}^6 \operatorname{pdf}_{\mathsf{Gaussian}}(s_i,\sigma^2,t_i)\right) \cdot \\ && \left(\Pi_{i=1}^4 [t_{i+2} \in [0,\frac{1}{e^{(t_i \cdot x_1 + t_2 - y_i)^2}})]\right) \end{array}$$

for  $t \in \mathbb{R}^6$  and q(s,t) = 0 for  $t \notin \mathbb{R}^6$ .

Hence, the acceptance ratio reduces to

$$\begin{array}{lcl} \alpha(s,t) & = & \min\{1, \frac{\prod_{i=1}^2 \mathrm{pdf}_{\mathsf{Gaussian}}(0,2,t_i)}{\prod_{i=1}^2 \mathrm{pdf}_{\mathsf{Gaussian}}(0,2,s_i)} \, \cdot \\ & & \quad \Pi_{i=1}^4[t_{i+2} \in [0, \frac{1}{e^{(t_1 \cdot x_i + t_2 - y_i)^2}})]\} \end{array}$$

if  $t \in \mathbb{R}^6$  and  $\alpha(s,t) = 0$  otherwise.

Note that  $\alpha(s,t)$  is only positive if each of  $t_3, t_4, t_5, t_6$  are within a certain (small) interval. This is problematic for an implementation, since it will need to find suitable values for all these components of the trace for every new trace to be proposed, leading to inefficiencies due to a slowly mixing Markov chain.

Linear Regression with score In this alternative version  $M_3$  of the previous model, we also have two draws from  $\mathsf{Gaussian}(0,2)$  at the beginning, but the calls to flip are replaced with calls to  $\mathsf{score}$ , which multiply the trace density by a positive number without consuming any elements of the trace. Because the support of the Gaussian PDF is  $\mathbb R$  and there are precisely two random draws (both from Gaussians) in every trace leading to a value, the set of valid traces is  $\mathbb R^2$ . We have  $\mathbf P^{\mathcal V}_{M_3}(s) = \Pi^2_{i=1} \operatorname{pdf}_{\mathsf{Gaussian}}(0,2,s_i) \ \Pi^4_{i=1} e^{-(s_1 \cdot x_i + s_2 - y_i)^2}$  if  $s \in \mathbb R^2$  and  $\mathbf P^{\mathcal V}_{M_3}(s) = 0$  otherwise. Assuming  $\mathbf P^{\mathcal V}_{M_3}(s) > 0$  and  $t \in \mathbb R^2$ , we get the proposal density

$$q(s,t) = \prod_{i=1}^{2} pdf_{\mathsf{Gaussian}}(s_{i}, \sigma^{2}, t_{i}) \prod_{i=1}^{4} \frac{1}{e^{(t_{1} \cdot x_{i} + t_{2} - y_{i})^{2}}}$$

where x = [0, 1, 2, 3] and y = [0, 1, 4, 6]. If  $t \notin \mathbb{R}^2$ , then q(s, t) = 0, because otherwise there would be a trace of length different than 2 leading to a value.

Thus, the acceptance ratio is

$$\alpha(s,t) = \frac{\prod_{i=1}^{2} \operatorname{pdf}_{\mathsf{Gaussian}}(0,2,t_{i})}{\prod_{i=1}^{2} \operatorname{pdf}_{\mathsf{Gaussian}}(0,2,s_{i})}$$

if  $t \in \mathbb{R}^2$  and  $\alpha(s,t) = 0$  otherwise.

In contrast to the previous example, here the acceptance ratio is positive for all proposals, non-zero gradients exist almost everywhere, and there are four fewer nuisance parameters to deal with (one per data point!). This makes inference for this version of the model much more tractable in practice.

### 6 Related Work

To the best of our knowledge, the only previous theoretical justification for trace MCMC is the recent work by Hur et al. [19], who show correctness of trace MCMC for the imperative probabilistic language R2 [27]. Their result does not apply to higher-order languages such as CHURCH or our  $\lambda$ -calculus, nor to programs that do not almost surely terminate [9]. Their algorithm is different from ours in that it exploits the explicit storage locations found in imperative programs, keeping one sample trace per location. The authors do state that the space of traces in their language is

equipped with a "stock" measure, and that the distributions of program traces and transitions are given by densities with respect to that measure. They do not, however, show that these densities are measurable. Their proof of correctness only shows that the acceptance ratio  $\alpha$  computed by their algorithm matches Hasting's formula: the authors do not prove convergence of the resulting Markov chain. Indeed, properties such as irreducibility and aperiodicity depend on the choices of parameters in the algorithm.

Other probabilistic language implementations also use trace MCMC inference, including Church [15], Venture [25], Webpel [13], and Anglican [39]. These works focusing on efficiency and convergence properties, and do not state formal correctness claims for their implementations.

Wingate et al. [42] give a general program transformation for a probabilistic language to support trace MCMC, with a focus on labelling sample points in order to maximise sample reuse. Extending our trace semantics with such labelling is important future work, given that Kiselyov [22] points out some difficulties with the transformation and proposes alternatives.

Many recent probabilistic languages admit arbitrary non-negative scores. This is done either by having an explicit score-like function, as in WEBPPL (called factor), or by observing that a particular value V was drawn from a given distribution  $D(\vec{c})$  (without adding it to the trace), as in WEB CHURCH (written (D  $\vec{c}$  V)) or Anglican (observe (D  $\vec{c}$ ) V). In recent work for a non-recursive  $\lambda$ -calculus with score, Staton et al. [35] note that unbounded scores introduce the possibility of "infinite model evidence errors". As seen in Section 4.9, even statically bounded scores exhibit this problem in the presence of recursion.

Kozen [23] gives a semantics of imperative probabilistic programs as partial measurable functions from infinite random traces to final states, which serves as the model for our trace semantics. Kozen also proves this semantics equivalent to a domain-theoretic one. Park et al. [30] give an operational version of Kozen's trace-based semantics for a  $\lambda$ -calculus with recursion, but "do not investigate measure-theoretic properties". Cousot and Monerau [5] generalise Kozen's trace-based semantics to consider probabilistic programs as measurable functions from a probability space into a semantics domain, and study abstract interpretation in this setting. Toronto et al. [41] use a pre-image version of Kozen's semantics to obtain an efficient implementation using rejection sampling. Scibior et al. [34] define a monadic embedding of probabilistic programming in Haskell along the lines of Kozen's semantics; their paper describes various inference algorithms but has no formal correctness results.

Ramsey and Pfeffer [32] provide a monadic denotational semantics for a first-order functional language with discrete probabilistic choice, and a Haskell implementation of the expectation monad using variable elimination. Bhat et al. [1] define a denotational semantics based on density functions for a restricted first-order language with continuous distributions. They also present a type system ensuring that a given program has a density.

Jones [20, Chapter 8] defines operational and domain-theoretic semantics for a  $\lambda$ -calculus with discrete probabilistic choice and a fixpoint construct. Our distribution-based operational semantics generalises Jones's to deal with continuous distributions. Like Kozen's and Jones's semantics, our operational semantics makes use of the partially additive structure on the category of subprobability kernels [28] in order to treat programs that make an unbounded number of random draws. Staton et al. [35] give a domain-theoretic semantics for a  $\lambda$ -calculus with continuous distributions and unbounded score, but without recursion. While giving a fully abstract domain theory for probabilistic  $\lambda$ -calculi with recursion is known to be hard [21], there have been recent advances using probabilistic coherence spaces [6, 8] and game semantics [7], which in some cases are fully abstract. We see no strong obstacles in applying any of these to a typed version of our calculus, but it is beyond the scope of this work. Another topic for future work are methodologies for equivalence checking in the style of logical relations or bisimilarity, which have been recently shown to work well in discrete probabilistic calculi [3].

## 7 Conclusions and Remarks

As a foundation for probabilistic inference in languages such as Church, we defined a probabilistic  $\lambda$ -calculus with draws from continuous probability distributions and both hard and soft constraints, defined its semantics as distributions on terms, and proved correctness of a trace MCMC inference algorithm via a sampling semantics for the calculus.

Although our emphasis has been on developing theoretical underpinnings, we also implemented our algorithm in F# to help develop our intuitions and indeed to help debug definitions. The algorithm is correct and effective, but not optimized. In future, we aim to extend our proofs to cover more efficient algorithms, inspired by Wingate et al. [42] and Kiselyov [22], for example.

# A Proofs of Measurability

This appendix contains the proofs of measurability of  $\mathbf{P}_M$ ,  $\mathbf{O}_M$ ,  $\mathbf{P}_M^{\mathcal{V}}$ , peval and q, as well as a proof that Q is a probability kernel.

The proofs usually proceed by decomposing the functions into simpler operations. However, unlike Toronto [40], we do not define these functions entirely in terms of general measurable operators, because the scope for reuse is limited here. We would have, for instance, to define multiple functions projecting different subexpressions of different expressions, and prove them measurable. Hence, the overhead resulting from these extra definitions would be greater than the benefits.

First we recap some useful results from measure theory:

- A function  $f: X_1 \to X_2$  between metric spaces  $(X_1, d_1)$  and  $(X_2, d_2)$  is continuous if for every  $x \in X_1$  and  $\epsilon > 0$ , there exists  $\delta$  such that for every  $y \in X_1$ , if  $d_1(x, y) < \delta$ , then  $d_2(f(x), f(y)) < \epsilon$ .
- A subset A of a metric space (X, d) is dense if

$$\forall x \in X, \epsilon > 0 \ \exists y \in A \quad d(x, y) < \epsilon$$

- A metric space is *separable* if it has a countable dense subset.
- Given a sequence of points  $x_n$  in a metric space (X, d), we say that x is the *limit* of  $x_n$  if for all  $\epsilon > 0$ , there exists an N such that  $d(x_n, x) < \epsilon$ .
- A subset A of a metric space is *closed* if it contains all the limit points, that is if  $x_n \in A$  for all n and  $x_n \to x$ , then  $x \in A$ .

**Lemma 59 (Billingsley [2, ex. 13.1])** Let  $(\Omega, \Sigma)$  and  $(\Omega', \Sigma')$  be two measurable spaces,  $T: \Omega \to \Omega'$  a function and  $A_1, A_2, \ldots$  a countable collection of sets in  $\Sigma$  whose union is  $\Omega$ . Let  $\Sigma_n = \{A \mid A \subseteq A_N, A \in \Sigma\}$  be a  $\sigma$ -algebra in  $A_n$  and  $T_n: A_n \to \Omega'$  a restriction of T to  $A_n$ . Then T is measurable  $\Sigma/\Sigma'$  if and only if  $T_n$  is measurable  $\Sigma_n/\Sigma'$  for every n.

A convenient way of showing that a function is Borel-measurable is to show that it is continuous as a function between metric spaces.

Let us represent the product  $\sigma$ -algebra  $\mathcal{M} \times \mathcal{R} \times \mathcal{S}$  as a Borel  $\sigma$ -algebra induced by a metric. First, we define the standard metric on  $\mathbb{R}$ , and the disjoint union of Manhattan metrics for  $\mathbb{S}$ :

$$d_{\mathbb{R}}(w, w') \triangleq |w - w'|$$

$$d_{\mathbb{S}}(s, s') \triangleq \begin{cases} \sum_{i=1}^{|s|} |s_i - s'| & \text{if } |s| = |s'| \\ \infty & \text{otherwise} \end{cases}$$

We can easily verify that  $(\mathbb{S}, d)$  generates  $\mathcal{S}$ . We define the metric on  $\Lambda \times \mathbb{R} \times \mathbb{S}$  to be the Manhattan metric:

$$d((M, w, s), (M', w', s')) \triangleq d_{\Lambda}(M, M') + d_{\mathbb{R}}(w, w') + d_{\mathbb{S}}(s, s')$$

The following is a standard result in measure theory:

Lemma 60 (Gallay [10, Proposition 4.2 b)]) If  $X_1, X_2$  are separable metric spaces then

$$\mathcal{B}(X_1 \times X_2) = \mathcal{B}(X_1) \times \mathcal{B}(X_2)$$

It is obvious that  $(\mathbb{R}, d)$  and  $(\mathbb{S}, d)$  are separable. Now, let  $\Lambda_Q$  be the subset of  $\Lambda_P$  in which all constants are rational. Then, it is easy to show that  $\Lambda_Q$  is countable.

**Lemma 61**  $\Lambda_Q$  is a dense subset of  $(\Lambda_P, d)$ 

PROOF. We need to prove that

$$\forall M \in \Lambda_P, \epsilon > 0 \ \exists M_Q \in \Lambda_Q \quad d(M, M_q) < \epsilon$$

This can be easily shown by induction (the base case follows from the fact that  $\mathbb{Q}$  is a dense subset of  $\mathbb{R}$ .

**Lemma 62** The metric space  $(\Lambda_P, d)$  is separable.

Proof. Corollary of Lemma 61.

Corollary 3 The  $\sigma$ -algebra on  $\Lambda \times \mathbb{R} \times \mathbb{S}$  generated by the metric d is  $\mathcal{M} \times \mathcal{R} \times \mathcal{S}$ .

Throughout this section, we call a function "measurable" if it is Borel measurable and "continuous" if it is continuous as a function between metric spaces.

We can use lemma 59 to split the space  $\mathcal{M}$  of expressions into subspaces of expressions of different type, and restrict functions (such as the reduction relation) to a given type of expression, to process different cases separately.

We write  $\mathbf{Subst}(M, x, v)$  for  $M\{V/x\}$ , to emphasize the fact that substitution is a function.

#### Detailed definition of substitution

```
\begin{aligned} \mathbf{Subst}(c,x,V) &\triangleq c \\ \mathbf{Subst}(x,x,V) &\triangleq V \\ \mathbf{Subst}(x,y,V) &\triangleq y \quad \text{if } x \neq y \\ \mathbf{Subst}(\lambda x.M,x,V) &\triangleq \lambda x.M \\ \mathbf{Subst}(\lambda x.M,y,V) &\triangleq \lambda x.(\mathbf{Subst}(M,y,V)) \quad \text{if } x \neq y \\ \mathbf{Subst}(M,x,V) &\triangleq \mathbf{Subst}(M,x,V) \quad \mathbf{Subst}(N,x,V) \\ \mathbf{Subst}(D(V_1,\ldots,V_{|D|}),x,V) &\triangleq D(\mathbf{Subst}(V_1,x,V),\ldots,\mathbf{Subst}(V_{|D|},x,V)) \\ \mathbf{Subst}(g(V_1,\ldots,V_{|g|}),x,V) &\triangleq g(\mathbf{Subst}(V_1,x,V),\ldots,\mathbf{Subst}(V_{|g|},x,V)) \\ \mathbf{Subst}(\text{if } W \text{ then } M \text{ else } L,x,V) &\triangleq \\ &\quad \text{if } \mathbf{Subst}(W,x,V) \text{ then } \mathbf{Subst}(M,x,V) \text{ else } \mathbf{Subst}(L,x,V) \\ \mathbf{Subst}(\text{score}(V'),x,V) &\triangleq \text{score}(\mathbf{Subst}(V',x,V)) \\ \mathbf{Subst}(\text{fail},x,V) &\triangleq \text{fail} \end{aligned}
```

For convenience, let us also define a metric on contexts:

$$\begin{array}{ccc} d([\cdot],[\cdot]) & \triangleq & 0 \\ d(EM,FN) & \triangleq & d(E,F)+d(M,N) \\ d((\lambda x.M)E,(\lambda x.N)F) & \triangleq & d(M,N)+d(E,F) \\ d(E,F) & \triangleq & \infty & \text{otherwise} \end{array}$$

**Lemma 63**  $d(E[M], F[N]) \le d(E, F) + d(M, N)$ .

PROOF. By induction on the structure of E.

If  $d(E,F)=\infty$ , then the result is obvious, since  $d(M',N')\leq\infty$  for all M',N'.

Now let us assume  $d(E,F) \neq \infty$  and prove the result by simultaneous induction on the structure on E and F:

- Case  $E = F = [\cdot]$ : in this case, E[M] = M, F[N] = N, and d(E, F) = 0, so obviously d(E[M], F[N]) = d(E, F) + d(M, N)
- Case  $E = E' L_1$ ,  $F = F' L_2$ : We have  $d(E[M], F[N]) = d(E'[M] L_1, F'[N] L_2) = d(E'[M], F'[N]) + d(L_1, L_2)$ . By induction hypothesis,  $d(E'[M], F'[N]) \le d(E', F') + d(M, N)$ , so  $d(E[M], F[N]) \le d(E', F') + d(M, N) + d(L_1, L_2) = d(E, F) + d(M, N)$ .
- Case  $E = (\lambda x. L_1) \ E', \ F = (\lambda x. L_2) \ F'$ : We have  $d(E[M], F[N]) = d((\lambda x. L_1)(E'[M]), (\lambda x. L_2)(F'[N])) = d(\lambda x. L_1, \lambda x. L_2) + d(E'[M], F'[N])$ . By induction hypothesis,  $d(E'[M], F'[N]) \le d(E', F') + d(M, N)$ , so  $d(E[M], F[N]) \le d(E', F') + d(\lambda x. L_1, \lambda x. L_2) + d(M, N) = d(E, F) + d(M, N)$ .

**Lemma 64** If  $d(E,F) = \infty$ , then for all  $R_1$ ,  $R_2$ ,  $d(E[R_1], F[R_2])$ .

PROOF. By induction on the structure of E:

- If E = [], then  $d(E, F) = \infty$  implies  $F \neq []$ :
  - If  $F = (\lambda x.M)$  F', then  $d(E[R_1], F[R_2]) = d(R_1, (\lambda x.M))$   $F'[R_2]) = \infty$ , because  $R_1$  is either not an application or of the form  $V_1$   $V_2$ , and  $F'[R_2]$  is not a value.
  - If F = F' N, then  $d(E[R_1], F[R_2]) = d(R_1, F'[R_2] N) = \infty$ , because  $R_1$  is either not an application or of the form  $V_1 V_2$ , and  $F'[R_2]$  is not a value.
- If  $E = (\lambda x.M) E'$ , then:
  - If F = F' N, then  $d(E[R_1], F[R_2]) = d(\lambda x.M, F'[R_2]) + d(E'[R_1], N) = \infty$ , because  $d(\lambda x.M, F'[R_2]) = \infty$ , as  $F'[R_2]$  cannot be a lambda-abstraction.
  - If  $F = (\lambda x.N)$  F', then  $d(E,F) = \infty$  implies that either  $d(M,N) = \infty$  or  $d(E',F') = \infty$ . We have  $d(E[R_1],F[R_2]) = d(M,N) + d(E'[R_1],F'[R_2])$ . If  $d(M,N) = \infty$ , then obviously  $d(E[R_1],F[R_2]) = \infty$ . Otherwise, by induction hypothesis,  $d(E',F') = \infty$  gives  $d(E'[R_1],F'[R_2]) = \infty$ , and so  $d(E[R_1],F[R_2]) = \infty$ .
- If E = E' M and F = F' N, then  $d(E, F) = \infty$  implies that either  $d(M, N) = \infty$  or  $d(E', F') = \infty$ . We have  $d(E[R_1], F[R_2]) = d(M, N) + d(E'[R_1], F'[R_2])$ , so  $d(E'[R_1], F'[R_2]) = \infty$  follows like in the previous case.

The property also holds in all remaining cases by symmetry of d.

**Lemma 65**  $d(E[R_1], F[R_2]) = d(E, F) + d(R_1, R_2).$ 

PROOF. If  $d(E, F) = \infty$ , then  $d(E[R_1], F[R_2]) = \infty$  by Lemma 64, otherwise the proof is the same as the proof of lemma 63, with inequality replaced by equality when applying the induction hypothesis.

**Lemma 66**  $d(\mathbf{Subst}(M, x, V), \mathbf{Subst}(N, x, W)) \leq d(M, N) + k \cdot d(V, W)$  where k is the max of the multiplicaties of x in M and N

PROOF. By simultaneous induction on the structure of M and N.

Let  $\mathcal C$  denote the set of contexts and  $\mathcal G$  the set of primitive functions. Let:

- $\Lambda_{appl} \triangleq \{ E[(\lambda x.M)V] \mid E \in \mathcal{C}, (\lambda x.M) \in C\Lambda, V \in \mathcal{V} \}$
- $\Lambda_{applc} \triangleq \{ E[c \ V] \mid E \in \mathcal{C}, c \in \mathbb{R}, V \in \mathcal{V} \}$
- $\bullet \ \Lambda_{iftrue} \triangleq \{ E[ \text{if true then } M \ \text{else } N] \mid E \in \mathcal{C}, M, N \in C\Lambda \}$
- $\Lambda_{iffalse} \triangleq \{E[\text{if false then } M \text{ else } N] \mid E \in \mathcal{C}, M, N \in C\Lambda\}$
- $\Lambda_{fail} \triangleq \{ E[\mathtt{fail}] \mid E \in \mathcal{C} \setminus \{[\ ]\} \}$
- $\Lambda_{prim}(g) \triangleq \{ E[g(\vec{c})] \mid E \in \mathcal{C}, \vec{c} \in \mathbb{R}^{|g|} \}$
- $\Lambda_{prim} \triangleq \bigcup_{g \in \mathcal{G}} \Lambda_{prim}(g)$
- $A\Lambda_{if} \triangleq \{E[\text{if } G \text{ then } M \text{ else } N] \mid E \in \mathcal{C}, M, N \in C\Lambda, G \in \mathcal{GV}\}$
- $\Lambda_{dist}(D) \triangleq \{ E[D(\vec{c})] \mid E \in \mathcal{C}, \vec{c} \in \mathbb{R}^{|D|} \}$
- $\Lambda_{dist} \triangleq \bigcup_{D \in \mathcal{D}} P_{rnd}(D)$
- $A\Lambda_{prim} \triangleq \bigcup_{g \in \mathcal{G}} E[g(G_1, \dots, G_{|g|})] \mid E \in \mathcal{C}, G_1, \dots, G_{|g|} \in \mathcal{GV}$
- $A\Lambda_{dist} \triangleq \bigcup_{D \in \mathcal{D}} E[D(G_1, \dots, G_{|D|})] \mid E \in \mathcal{C}, G_1, \dots, G_{|D|} \in \mathcal{GV}$
- $A\Lambda_{scr} \triangleq \{E[\mathtt{score}(c)] \mid E \in \mathcal{C}, c \in \mathbb{R}\}$
- $\Lambda_{scr} \triangleq \{ E[\mathtt{score}(c)] \mid E \in \mathcal{C}, c \in (0,1] \}$

Lemma 67 All the sets above are measurable.

PROOF. All these sets except for  $\Lambda_{scr}$  are closed, so they are obviously measurable. The set  $\Lambda_{scr}$  is not closed (for example, we can define a sequence of points in  $\Lambda_{scr}$  whose limit is  $score(0) \notin \Lambda_{scr}$ ), but it is still measurable:

Define a function  $i_{scr}: A\Lambda_{scr} \to \mathbb{R}$  by  $i_{scr}(E[\mathtt{score}(c)]) = c$ . This function is continuous and so measurable. Since the interval (0,1] is a Borel subset of  $\mathbb{R}$ ,  $i_{scr}^{-1}((0,1]) = \Lambda_{scr}$  is measurable.  $\square$ 

Now, we need to define the set of erroneous redexes of all types.

- $R\Lambda_{if} \triangleq A\Lambda_{if} \setminus (\Lambda_{iftrue} \cup \Lambda_{iffalse})$
- $R\Lambda_{prim} \triangleq A\Lambda_{prim} \setminus \Lambda_{prim}$
- $R\Lambda_{dist} \triangleq A\Lambda_{dist} \setminus \Lambda_{dist}$
- $R\Lambda_{scr} \triangleq A\Lambda_{scr} \setminus \Lambda_{scr}$
- $\Lambda_{error} \triangleq R\Lambda_{if} \cup R\Lambda_{prim} \cup R\Lambda_{dist} \cup R\Lambda_{scr}$

**Lemma 68** The set  $\Lambda_{error}$  is measurable.

Proof. It is constructed from measurable sets by operations preserving measurability.  $\Box$ 

Define

 $\Lambda_{det} = \Lambda_{appl} \cup \Lambda_{cappl} \cup \Lambda_{iftrue} \cup \Lambda_{iffalse} \cup \Lambda_{fail} \cup \Lambda_{prim} \cup \Lambda_{error}$ 

**Lemma 69**  $\Lambda_{det}$  is measurable.

Proof.  $\Lambda_{det}$  is a union of measurable sets.

Lemma 70 GV is measurable.

PROOF. It is easy to see that  $\mathcal{GV}$  is precisely the union of sets of all closed expressions of the form c,  $\lambda x.M$ , x and fail, so it is closed, and hence measurable.

Lemma 71 V is measurable.

PROOF.  $\mathcal{V}$  is the union of sets of all closed expressions of the form c,  $\lambda x.M$  and x, so it is closed, and hence measurable.

#### A.1 Deterministic reduction as a measurable function

Let us define a function performing one step of the reduction relation. This function has to be defined piecewise. Let us start with sub-functions reducing deterministic redexes of the given type.

$$\begin{array}{ccc} g_{appl} & : & \Lambda_{appl} \to C \Lambda \\ g_{appl}(E[(\lambda x.M) \ V]) & = & E[\mathbf{Subst}(M,x,v)] \end{array}$$

Lemma 72  $g_{appl}$  is measurable.

PROOF. By Lemma 65, we have  $d(E[(\lambda x.M)V], F[(\lambda x.N)W]) = d(E, F) + d(M, N) + d(V, W)$  and by Lemma 66,  $d(E[\mathbf{Subst}(M, x, V)], F[\mathbf{Subst}(N, x, W)]) \leq d(E, F) + d(M, N) + k \cdot d(V, W)$ , where k is the maximum of the multiplicities of x in M and N.

For any  $\epsilon > 0$ , take  $\delta = \frac{\epsilon}{k+1}$ . Then, if  $d(E[(\lambda x.M)V], F[(\lambda x.N)W]) < \delta$ , then

$$\begin{array}{ll} d(E[\mathbf{Subst}(M,x,V)], F[\mathbf{Subst}(N,x,W)]) & \leq & d(E,F) + d(M,N) + k \cdot d(V,W) \\ & \leq & (k+1) \cdot (d(E,F) + d(M,N) + d(V,W)) \\ & = & (k+1) \cdot d(E[(\lambda x.M)V], F[(\lambda x.N)W]) \\ & < & \epsilon \end{array}$$

Thus,  $g_{appl}$  is continuous, and so measurable.

$$\begin{array}{ccc} g_{applc} & : & \Lambda_{applc} \to C \Lambda \\ g_{applc}(E[c~M]) & = & E[{\tt fail}] \end{array}$$

Lemma 73  $g_{applc}$  is measurable.

PROOF. It is easy to check that  $g_{applc}$  is continous.

$$\begin{array}{ccc} g_{prim} & : & \Lambda_{prim} \to C \Lambda \\ g_{prim}(E[g(\vec{c})]) & = & E[\sigma_g(\vec{c})] \end{array}$$

Lemma 74  $g_{prim}$  is measurable.

PROOF. By assumption, every primitive function g is measurable.  $g_{prim}$  is a composition of a function splitting a context and a redex, g and a function combining a context with a redex, all of which are measurable.

$$g_{iftrue}$$
 :  $\Lambda_{iftrue} o C \Lambda$   $g_{iftrue}(E[ ext{if true then } M_1 ext{ else } M_2]) = E[M_1]$   $g_{iffalse}$  :  $\Lambda_{iffalse} o C \Lambda$ 

 $g_{\it iffalse}(E[{\it if false then}\ M_1\ {\it else}\ M_2])\ =\ E[M_2]$ 

**Lemma 75**  $g_{iftrue}$  and  $g_{iffalse}$  are measurable.

PROOF. We have  $d(E[\text{if true then } M_1 \text{ else } N_1], F[\text{if true then } M_2 \text{ else } N_2]) = d(E, F) + d(M_1, M_2) + d(N_1, N_2) \ge d(E[M_1], F[M_2])$ , so  $g_{iftrue}$  is continuous, and so measurable, and similarly for  $g_{iffalse}$ .

$$g_{fail}$$
 :  $\Lambda_{fail} o C \Lambda$   $g_{fail}(E[{ t fail}])$  =  ${ t fail}$ 

Lemma 76  $g_{fail}$  is measurable.

PROOF. Obvious, since it is a constant function.

$$egin{array}{ll} g_{error} &:& \Lambda_{error} 
ightarrow C \Lambda \ g_{error}(E[T]) &=& E[ extsf{fail}] \end{array}$$

Lemma 77  $g_{error}$  is measurable.

PROOF. We have  $d(E[T_1], F[T_2]) \ge d(E, F) = d(E[\mathtt{fail}], F[\mathtt{fail}])$ , so  $g_{error}$  is continuous and hence measurable.

$$\begin{array}{lcl} g'_{det} & : & \Lambda_{det} \to C\Lambda \\ g'_{det} & = & g_{appl} \cup g_{applc} \cup g_{prim} \cup g_{iftrue} \cup g_{iffalse} \cup g_{fail} \cup g_{error} \end{array}$$

Lemma 78  $g'_{det}$  is measurable.

PROOF. Follows directly from Lemma 59.

**Lemma 79**  $M \xrightarrow{det} N$  if and only if  $g'_{det}(M) = N$ .

Proof. By inspection.

#### A.2 Small- step reduction as a measurable function

Let

$$\begin{split} \mathcal{T}_{val} &= \mathcal{GV} \times \mathbb{R} \times \mathbb{S} \\ \mathcal{T}_{det} &= \Lambda_{det} \times \mathbb{R} \times \mathbb{S} \\ \mathcal{T}_{scr} &= \Lambda_{scr} \times \mathbb{R} \times \mathbb{S} \\ \mathcal{T}_{rnd} &= \{ (E[D(\vec{c})], w, c :: s) \mid E \in \mathcal{C}, D \in \mathcal{D}, \vec{c} \in \mathbb{R}^{|D|}, w \in \mathbb{R}, s \in \mathbb{S}, c \in \mathbb{R}, \\ &\quad \text{pdf}_{D}(\vec{c}, c) > 0 \} \end{split}$$

**Lemma 80**  $\mathcal{T}_{val}$ ,  $\mathcal{T}_{det}$ ,  $\mathcal{T}_{scr}$  and  $\mathcal{T}_{rnd}$  are measurable.

PROOF. The measurability of  $\mathcal{T}_{val}$ ,  $\mathcal{T}_{det}$  and  $\mathcal{T}_{scr}$  is obvious (they are products of measurable sets), so let us focus on  $\mathcal{T}_{rnd}$ .

For each distribution D, define a function  $i_D: \Lambda_{rnd}(D) \times \mathbb{R} \times (\mathbb{S} \setminus \{[]\}) \to \mathbb{R}^{|D|} \times \mathbb{R}$  by  $i_D(E[D(\vec{c})], w, c :: s) = (c, \vec{c})$ . This function is continuous, and so measurable. Then, since for each D, pdf  $_D$  is measurable by assumption, the function  $j_d = \operatorname{pdf}_D \circ i_D$  is measurable. Then,  $\mathcal{T}_{rnd} = \bigcup_{D \in \mathcal{D}} j_D^{-1}((0, \infty))$ , and since the set of distributions is countable,  $\mathcal{T}_{rnd}$  is measurable.  $\square$ 

Let  $\mathcal{T} = C\Lambda \times \mathbb{R} \times \mathbb{S}$  and let  $\mathcal{T}_{blocked} = \mathcal{T} \setminus (\mathcal{T}_{val} \cup \mathcal{T}_{det} \cup \mathcal{T}_{scr} \cup \mathcal{T}_{rnd})$  be the set of non-reducible ("stuck") triples, whose first components are not values. Obviously,  $\mathcal{T}_{blocked}$  is measurable. Define:

$$g_{val}$$
 :  $\mathcal{T}_{val} \to \mathcal{T}$   $g_{val}(G, w, s) = (fail, 0, [])$ 

Obviously,  $g_{val}$  is measurable.

$$g_{det}$$
 :  $\mathcal{T}_{det} \to \mathcal{T}$   
 $g_{det}(M, w, s) = (g'_{det}(M), w, s)$ 

Lemma 81  $g_{det}$  is measurable.

Proof. All components of  $g_{det}$  are measurable.

$$\begin{array}{ccc} g_{rnd} & : & \mathcal{T}_{rnd} \to \mathcal{T} \\ g_{rnd} & \triangleq & (g_1,g_2,g_3) \\ g_1(E[\mathsf{D}(\vec{c})],w,c::s) & \triangleq & E[c] \\ g_2(E[\mathsf{D}(\vec{c})],w,c::s) & \triangleq & w \cdot \operatorname{pdf}_{\mathsf{D}}(\vec{c},c), \\ g_3(E[\mathsf{D}(\vec{c})],w,c::s) & \triangleq & s \end{array}$$

Lemma 82  $g_{rnd}$  is measurable.

PROOF. For  $g_1$ , we have  $d(E[c], E'[c']) \leq d(E, E') + d(c, c') \leq d(E, E') + d(\vec{c}, \vec{c'}) + d(w, w') + d(s, s') = d((E[D(\vec{c})], w, c :: s), (E'[D(\vec{c'})], w', c' :: s'))$  and  $d((E[D(\vec{c})], w, c :: s), (E'[E(\vec{c'})], w', c' :: s')) = \infty$  if  $D \neq E$ , so  $g_1$  is continuous and hence Borel-measurable.

For  $g_2$ , we have  $g_2(E[\mathsf{D}(\vec{c})], w, c :: s) = g_w(E[\mathsf{D}(\vec{c})], w, c :: s) \times (\mathsf{pdf}_{\mathsf{D}} \circ g_c)(E[\mathsf{D}(\vec{c})], w, c :: s)$ , where  $g_w(E[\mathsf{D}(\vec{c})], w, c :: s) = w$  and  $g_c(E[\mathsf{D}(\vec{c})], w, c :: s) = (\vec{c}, c)$ . The continuity (and so measurability) of  $g_w$  and  $g_c$  can be easily checked (as for  $g_1$  above). Thus,  $\mathsf{pdf}_{\mathsf{D}} \circ g_c$  is a composition of measurable functions (since distributions are assumed to be measurable), and so  $g_2$  is a pointwise product of measurable real-valued functions, so it is measurable.

The continuity (and so measurability) of  $g_3$  can be shown in a similar way to  $g_1$ .

Hence, all the component functions of  $g_{rnd}$  are measurable, so  $g_{rnd}$  is itself measurable.

$$\begin{array}{rcl} g_{scr} & : & \mathcal{T}_{scr} \to \mathcal{T} \\ g_{scr}(E[\mathtt{score}(c)], w, s) & \triangleq & (E[\mathtt{true}], c \cdot w, s) \end{array}$$

Lemma 83  $g_{scr}$  is measurable.

PROOF. The first component function of  $g_{scr}$  can easily be shown continuous, and so measurable, and ditto for the third component. The second component is a pointwise product of two measurable functions, like in the  $g_{rnd}$  case. Hence,  $g_{scr}$  is measurable.

For completeness, we also define:

$$g_{blocked}$$
 :  $\mathcal{T}_{blocked} o \mathcal{T}$ 
 $g_{blocked}(M, w, s) riangleq ext{(fail, 0, [])}$ 

This function is trivially measurable.

Define

$$g: \mathcal{T} \to \mathcal{T}$$
 $g \triangleq g_{val} \cup g_{det} \cup g_{scr} \cup g_{blocked}$ 

Lemma 84 g is measurable.

PROOF. Follows from Lemma 59.

**Lemma 85** For every  $(M, w, s) \in \mathcal{T}$ ,

1. If 
$$(M, w, s) \to (M', w', s')$$
, then  $g(M, w, s) = (M', w', s')$ .

2. If 
$$g(M, w, s) = (M', w', s') \neq (fail, 0, [])$$
, then  $(M, w, s) \rightarrow (M', w', s')$ .

PROOF. By inspection.

#### A.3 Measurability of P and O

It is easy to check that the sets  $\mathcal{GV}$  and  $\mathbb{R}_+$  (nonnegative reals) form  $\omega \mathbf{CPO}$ s with the orderings  $\mathtt{fail} \leq M$  for all M and  $0 \leq x$ , respectively. This means that functions into  $\mathcal{GV}$  and  $\mathbb{R}_+$  also form  $\omega \mathbf{CPO}$ s with pointwise ordering.

Define:

$$\Theta_{\Lambda}(f)(M, w, s) \triangleq \begin{cases} M & \text{if } M \in \mathcal{GV}, s = [] \\ f(g(M, w, s)) & \text{otherwise} \end{cases}$$

$$\Theta_{w}(f)(M, w, s) \triangleq \begin{cases} w & \text{if } M \in \mathcal{GV}, s = [] \\ f(g(M, w, s)) & \text{otherwise} \end{cases}$$

It can be shown that these functions are continuous, so we can define:

$$egin{aligned} egin{aligned} oldsymbol{\perp}_{\Lambda} &= (M, w, s) \mapsto \mathtt{fail} \\ egin{aligned} oldsymbol{\perp}_{w} &= (M, w, s) \mapsto 0 \end{aligned}$$

$$\mathbf{O}'(M,s) \triangleq \sup_{n} \Theta_{\Lambda}^{n}(\bot_{\Lambda})(M,1,s)$$
$$\mathbf{P}'(M,s) \triangleq \sup_{n} \Theta_{w}^{n}(\bot_{w})(M,1,s)$$

**Lemma 86** If  $(M, w_0, s) \Rightarrow (G, w, [])$ , then  $\sup_n \Theta_w^n(\bot_w)(M, w_0, s) = w$  and  $\sup_n \Theta_\Lambda^n(\bot_\Lambda)(M, w_0, s) = G$ .

PROOF. By induction on the derivation of  $(M, w_0, s) \Rightarrow (G, w, [])$ :

- If  $(M, w_0, s) \to^0 (G, w, [])$ , and so  $M \in \mathcal{GV}$  and s = [], then the equalities follow directly from the definitions of  $\Theta_w$  and  $\Theta_{\Lambda}$ .
- If  $(M, w_0, s) \to (M', w', s') \Rightarrow (G, w, [])$ , assume that  $\sup_n \Theta_w^n(\bot_w)(M', w', s') = w$  and  $\sup_n \Theta_\Lambda^n(\bot_\Lambda)(M', w', s') = G$ , We have  $M \notin \mathcal{GV}$ . By Lemma 85,  $g(M, w_0, s) = (M', w', s')$ . Hence  $\sup_n \Theta_w^n(\bot_w)(M, w_0, s) = \sup_n \Theta_w^n(\bot_w)(g(M, w_0, s)) = \sup_n \Theta_w^n(\bot_w)(M', w', s') = w$  by induction hypothesis. Similarly,  $\sup_n \Theta_\Lambda^n(\bot_\Lambda)(M, w_0, s) = G$ .

Corollary 4 If  $(M, 1, s) \Rightarrow (G, w, [])$ , then  $\mathbf{P}'(M, s) = w$  and  $\mathbf{O}'(M, s) = G$ .

**Lemma 87** If  $\sup_n \Theta_w^n(\bot_w)(M, w_0, s) = w \neq 0$ , then  $(M, w_0, s) \Rightarrow (G, w, [])$  for some  $G \in \mathcal{GV}$ .

PROOF. Because the supremum is taken with respect to a flat  $\omega \mathbf{CPO}$ ,  $\sup_n \Theta_w^n(\bot_w)(M, w_0, s) = w > 0$  implies  $\Theta_w^k(\bot_w)(M, w_0, s) = w$  for some k > 0. We can then prove the result by indiction on k:

- Base case, k = 1: We must have  $\Theta_w(\bot_w)(M, w_0, s) = w_0$ ,  $M = G \in \mathcal{GV}$  and s = [] as otherwise we would obtain  $\bot_w(M, w_0, s) = 0$ . Hence  $(M, w_0, s)$  reduces to  $(G, w_0, [])$  in 0 steps.
- Induction step:  $\Theta_w^{k+1}(\bot_w)(M, w_0, s) = w$ . If  $M \in \mathcal{GV}$  and s = [], then  $w = w_0$  and  $(M, w_0, s)$  reduces to itself in 0 steps, like in the base case. Otherwise, we have  $\Theta_w^k(\bot_w)((M', w', s')) = w$ , where  $g(M, w_0, s) = (M', w', s')$ . We know that  $(M', w', s') \neq (\mathtt{fail}, 0, [])$ , because otherwise we would have w = 0. Thus, by Lemma 85,  $(M, w_0, s) \rightarrow (M', w', s')$ . By induction hypothesis,  $(M', w', s') \Rightarrow (G, w, [])$ , which implies  $(M, w_0, s) \Rightarrow (G, w, [])$ .

**Lemma 88** If  $\sup_n \Theta^n_{\Lambda}(\bot_w)(M, w_0, s) = V \in \mathcal{V}$ , then  $(M, w_0, s) \Rightarrow (V, w, [])$  for some  $w \in \mathbb{R}$ .

PROOF. Similar to the proof of Lemma 87.

Corollary 5 If there are no G, w such that  $(M,1,s) \Rightarrow (G,w,[])$ , then  $\mathbf{P}'(M,s) = 0$  and  $\mathbf{O}'(M,s) =$ fail.

Corollary 6 For any M,  $\mathbf{P}_M = \mathbf{P}'(M, \cdot)$  and  $\mathbf{O}_M = \mathbf{O}'(M, \cdot)$ .

**Lemma 89** If  $(X, \Sigma_1)$  and  $(Y, \Sigma_2)$  are measurable spaces, Y forms a flat  $\omega \mathbf{CPO}$  with a bottom element  $\bot$  such that  $\{\bot\} \in \Sigma_2$  and  $f_1, f_2, \ldots$  is a  $\omega$ -chain of  $\Sigma_1/\Sigma_2$  measurable functions (on the  $\omega \mathbf{CPO}$  with pointwise ordering), then  $\sup_i f_i$  is  $\Sigma_1/\Sigma_2$  measurable.

PROOF. Since  $f^{-1}(A \cup \{\bot\}) = f^{-1}(A) \cup f^{-1}(\{\bot\})$ , we only need to show that  $(\sup_i f_i)^{-1}(\{\bot\}) \in \Sigma_1$  and  $(\sup_i f_i)^{-1}(A) \in \Sigma_1$  for all  $A \in \Sigma_2$  such that  $\bot \notin A$ .

We have  $(\sup_i f_i)^{-1}(\{\bot\}) = \bigcap_i f_i^{-1}(\{\bot\})$ , which is measurable by definition. If  $\bot \notin A$ , then  $\sup_i f_i(x) \in A$  if and only if  $f_i(x) \in A$  for some i, so by extensionality of sets,  $\sup_i f_i^{-1}(A) = \bigcup_i f_i^{-1}(A) \subseteq \Sigma_1$ .

Lemma 90 P' is measurable  $(C\Lambda \times S)/\mathcal{R}|_{\mathbb{R}_+}$ .

PROOF. First, let us show by induction on n that  $\Theta_w^n(\perp_w)$  is measurable for every n:

• Base case, n=0:  $\Theta_w^0(\perp_w)=\perp_w$  is a constant function, and so trivially measurable.

• Induction step: suppose  $\Theta_w^n(\bot_w)$  is measurable. Then we have  $\Theta_w^{n+1}(\bot_w) = \Theta_w(\Theta_w^n(\bot_w))$ , so it is enough to show that  $\Theta_w(f)$  is measurable if f is measurable:

The domain of the first case is  $\mathcal{GV} \times \mathbb{R} \times \{[]\}$ , which is clearly measurable. The domain of the second case is measurable as the complement of the above set in  $\mathcal{T}$ .

The sub-function corresponding to the first case returns the second component of its argument, so it is continuous and hence measurable. The second case is a composition of two measurable functions, hence measurable.

Thus,  $\Theta_w(f)$  is measurable for any measurable f, and so  $\Theta_w^{n+1}(\bot_w)$  is measurable.

By Lemma 89,  $\sup_n \Theta_w^n(\bot_w)$  is measurable. Since  $\mathbf{P}'$  is a composition of  $\sup_n \Theta_w^n(\bot_w)$  and a continuous function mapping (M,s) to (M,1,s), it is a composition of measurable functions, and so it is measurable.

Lemma 91 O' is measurable  $(C\Lambda \times S)/\mathcal{M}|_{GV}$ .

PROOF. Similar to the proof of Lemma 90.

**Lemma 92** For any closed term M, the function  $\mathbf{P}_M$  is measurable  $\mathcal{S}/\mathcal{R}|_{\mathbb{R}_+}$ .

PROOF. Since  $\mathbf{P}'$  is measurable,  $\mathbf{P}_M = \mathbf{P}'(M,\cdot)$  is measurable for every  $M \in C\Lambda$ .

**Lemma 93** For each M, the function  $\mathbf{O}_M$  is measurable  $\mathcal{S}/\mathcal{M}|_{\mathcal{GV}}$ .

PROOF. Since  $\mathbf{O}'$  is measurable,  $\mathbf{O}_M = \mathbf{O}'(M, \cdot)$  is measurable for every  $M \in C\Lambda$ .

Lemma 94 For all M, s,  $\mathbf{P}_{M}^{\mathcal{V}}(s) = \mathbf{P}_{M}(s)[\mathbf{O}_{M}(s) \in \mathcal{V}]$ 

PROOF. By Lemma 23, if  $M \Downarrow_s^w G$ , then w, G are unique. If  $M \Downarrow_s^w V$ , then  $\mathbf{P}_M(s) = w$ ,  $\mathbf{P}_M^{\mathcal{V}}(s)$  and  $\mathbf{O}_M(s) \in \mathcal{V}$ , so the equality holds. If  $M \Downarrow_s^w \mathtt{fail}$ , then  $\mathbf{P}_M(s) = w$ ,  $\mathbf{P}_M^{\mathcal{V}}(s) = 0$  and  $\mathbf{O}_M(s) \notin \mathcal{V}$ ), so both sides of the equation are 0. If there is no G such that  $M \Downarrow_s^w G$ , then both sides are also 0.

**Lemma 95**  $\mathbf{P}_{M}^{\mathcal{V}}$  is measurable for every M.

PROOF. By Lemma 94,  $\mathbf{P}_{M}^{\mathcal{V}}(s) = \mathbf{P}_{M}(s)[\mathbf{O}_{M}(s) \in \mathcal{V}]$ , so  $\mathbf{P}_{M}^{\mathcal{V}}$  is a pointwise product of a measurable function and a composition of  $\mathbf{O}_{M}$  and an indicator function for a measurable set, hence it is measurable.

RESTATEMENT OF LEMMA 92. For any closed term M, the functions  $\mathbf{P}_M$ ,  $\mathbf{O}_M$  and  $\mathbf{P}_M^{\mathcal{V}}$  are all measurable;  $\langle\!\langle M \rangle\!\rangle$  and  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}$  are measures on  $(\mathbb{S}, \mathcal{S})$ ;  $[\![M]\!]_{\mathbb{S}}$  is a measure on  $(\mathcal{GV}, \mathcal{M}|_{\mathcal{GV}})$ ; and  $([\![M]\!]_{\mathbb{S}})|_{\mathcal{V}}$  is a measure on  $(\mathcal{V}, \mathcal{M}|_{\mathcal{V}})$ .

PROOF. For all  $M \in C\Lambda$ ,  $\mathbf{P}_M$ ,  $\mathbf{O}_M$  and  $\mathbf{P}_M^{\mathcal{V}}$  are measurable by lemmas 92, 93 and 95, respectively. Since  $\mathbf{P}_M$ , and  $\mathbf{P}_M^{\mathcal{V}}$  are obviously nonnegative, the functions  $\langle\!\langle M \rangle\!\rangle$  and  $\langle\!\langle M \rangle\!\rangle^{\mathcal{V}}$  are measures of densities  $\mathbf{P}_M$  and  $\mathbf{P}_M^{\mathcal{V}}$  with respect to the stock measure  $\mu$  [10, Section 2.3.3]. The function  $[\![M]\!]_{\mathbb{S}}$  is a transformation of the measure  $\langle\!\langle M \rangle\!\rangle$  on  $(\mathbb{S}, \mathcal{S})$  by the  $\mathcal{S}/\mathcal{M}|_{\mathcal{GV}}$  -measurable function  $\mathbf{O}_M$ , so it is a measure on  $(\mathcal{GV}, \mathcal{M}|_{\mathcal{GV}})$  [2, Section 13, Transformations of Measures]. Since  $([\![M]\!]_{\mathbb{S}})|_{\mathcal{V}}(A) = [\![M]\!]_{\mathbb{S}}(A \cap \mathcal{V})$  for every measurable set  $A \in \mathcal{M}|_{\mathcal{GV}}$ , the function  $([\![M]\!]_{\mathbb{S}})|_{\mathcal{V}}$  is a restriction of  $[\![M]\!]_{\mathbb{S}}$  to  $\mathcal{V}$ , so it is a measure on  $(\mathcal{V}, \mathcal{M}|_{\mathcal{V}})$ .

#### A.4 Measurability of peval

Like in the previous section, we start by giving an alternative definition of peval, using the function g instead of referring to the reduction relation directly.

The set of closed terms  $C\Lambda$  is a  $\omega \mathbf{CPO}$  with respect to the partial order defined by  $\mathtt{fail} \leq G$  for all G. Hence the set  $\mathbf{F}$  of all functions  $(C\Lambda \times \mathbb{R} \times \mathbb{S}) \to C\Lambda$  is a  $\omega \mathbf{CPO}$  with respect to the pointwise order. Define  $\Phi : \mathbf{F} \to \mathbf{F}$  as:

$$\Phi(f)(M, w, s) = \begin{cases} M & \text{if } s = []\\ f(g(M, w, s)) & \text{otherwise} \end{cases}$$

It is easy to check that  $\Phi$  is monotone and preserves suprema of  $\omega$ -chains, so it is continuous. Hence, we can define:

$$\operatorname{\mathtt{peval}}'(M,s) = \sup_k \Phi^k(\bot_\Lambda)(M,1,s)$$

where  $\perp_{\Lambda}(M, w, s) = \text{fail}$ , as before.

We first need to show that the original peval function is well-defined.

**Lemma 96** If  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', [])$  and  $s_k \neq []$  and  $(M, w_0, s) \Rightarrow (M_l, w_l, s_l) \rightarrow (M'', w'', [])$  and  $s_l \neq []$ , then M' = M'' and w' = w''.

PROOF. By induction on the derivation of  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k)$ :

- If  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k)$  was derived in 0 steps, we have  $M_k = M$ ,  $w_k = w$  and  $s_k = s$ , and so  $(M, w_0, s) \rightarrow (M', w', [])$ , where  $s \neq []$ .
  - If  $(M, w_0, s) \Rightarrow (M_l, w_l, s_l)$  was derived in 0 steps, then  $(M_l, w_l, s_l) = (M, w_0, s)$ , and so M'' = M' and w'' = w' by Lemma 6.
  - If  $(M, w_0, s) \Rightarrow (M_l, w_l, s_l)$  was derived in 1 or more steps, we have  $(M, w_0, s) \rightarrow (\hat{M}, \hat{w}, \hat{s}) \Rightarrow (M_l, w_l, s_l) \rightarrow (M'', w'', [])$  and  $s_l \neq []$ , for some  $\hat{M}$ ,  $\hat{w}$ ,  $\hat{s}$ . By Lemma 6,  $\hat{s} = []$ . We have  $(\hat{M}, \hat{w}, []) \Rightarrow (M_l, w_l, s_l)$ , where  $s_l \neq []$ . This leads to a contradiction, as it is easy to show that reducing a term with an empty trace cannot yield a triple with a non-empty trace (there is no rule which adds an element to a trace)
- If  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k)$  was derived in 1 on more steps, we have  $(M, w_0, s) \rightarrow (M^*, w^*, s^*) \rightarrow^k (M_k, w_k, s_k) \rightarrow (M', w', [])$  for some  $k \geq 0$ ,  $M^*$ ,  $w^*$ ,  $s^*$ . Now, if  $(M, w_0, s) \Rightarrow (M_l, w_l, s_l)$  was derived in 1 or more steps, we have  $(M, w_0, s) \rightarrow (\hat{M}, \hat{W}, \hat{s}) \Rightarrow (M_l, w_l, s_l) \rightarrow (M'', w'', [])$  and  $s_l \neq []$  for some  $\hat{M}$ ,  $\hat{w}$ ,  $\hat{s}$ , where  $(\hat{M}, \hat{W}, \hat{s}) = (M^*, w^*, s^*)$  by Lemma 6. Hence, the result follows by the induction hypothesis.

If  $(M, w_0, s) \Rightarrow (M_l, w_l, s_l)$  was derived in 0 steps, then  $(M_l, w_l, s_l) = (M, w_0, s)$ , and so  $(M, w_0, s) \rightarrow (M'', w'', [])$ . By Lemma 6, this implies  $s^* = []$ , so  $(M^*, w^*, []) \Rightarrow (M_k, w_k, s_k)$  for  $s_k \neq []$ , which is impossible, as explained in the previous case.

**Lemma 97** If  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', [])$  and  $s_k \neq []$ , then  $\sup_n \Phi^n(\bot_{\Lambda})(M, w_0, s) = M'$ .

PROOF. By induction on the length of derivation of  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', [])$ . Suppose  $(M, w_0, s) \rightarrow^k (M_k, w_k, s_k) \rightarrow (M', w', [])$ .

- Base case, k=0: We have  $(M,w_0,s)\to (M',w',[])$  and  $s\neq []$ . Hence, by Lemma 85,  $g(M,w_0,s)=(M',w',[])$ , and so, by monotonicity of  $\Phi$ ,  $\sup_k\Phi^k(\bot_\Lambda)(M,w_0,s)=\sup_k\Phi(\Phi^k(\bot_\Lambda))(M,w_0,s)=\sup_k\Phi(\Phi^k(\bot_\Lambda))(M',w',[])=M'$ , as required.
- Induction step: Let  $(M, w_0, s) \to^{k+1} (M_k, w_k, s_k) \to (M', w', [])$ . Then there exist  $M^*$ ,  $w^*$ ,  $s^*$  such that  $(M, w_0, s) \to (M^*, w^*, s^*) \to^k (M_k, w_k, s_k) \to (M', w', [])$ . Now, we have  $\sup_k \Phi^k(\bot_\Lambda)(M, w_0, s) = \sup_k \Phi(\Phi^k(\bot_\Lambda))(M, w_0, s) = \sup_k \Phi^k(\bot_\Lambda)(M^*, w^*, s^*)$ , and  $\sup_k \Phi^k(\bot_\Lambda)(M^*, w^*, s^*) = M'$  by induction hypothesis, which ends the proof.

Corollary 7 If  $(M, 1, s) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', \parallel)$  and  $s_k \neq \parallel$ , then peval'(M, s) = M'.

**Lemma 98** If  $\sup_n \Phi^n(\bot_\Lambda)(M, w_0, s) = M' \neq \texttt{fail}$ , then either s = [] or  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', [])$  for some  $M_k, w_k, s_k, w'$ , where  $s_k \neq []$ .

PROOF. Like in lemma 87, for every M,  $w_0$ , s, we must have  $\Phi^k(\perp_{\Lambda})(M, w_0, s) = M'$  for some k > 0, and we can prove the result by induction on k.

- Base case. k=1: we must have s=[] as otherwise we would have M'= fail.
- Induction step: suppose  $\Phi^{k+1}(\bot_{\Lambda})(M, w_0, s) = M'$ . By definition of  $\Phi$ , if  $s \neq []$ , we have  $\Phi^k(\bot_{\Lambda})(M^*, w^*, s^*) = M'$ , where  $g(M, w_0, s) \to (M^*, w^*, s^*)$ . Since  $M' \neq \mathtt{fail}$  by assumption, Lemma 85 yields  $(M, w_0, s) \to (M^*, w^*, s^*)$ . By induction hypothesis, either  $s^* = []$  or  $(M^*, w^*, s^*) \Rightarrow (M^{**}, w^{**}, s^{**}) \to (M', w'', [])$  for some  $M^{**}, w^{**}, s^{**}, w''$ , where  $s^{**} \neq []$ . In the former case, we have  $(M, w_0, s) \Rightarrow (M_k, w_k, s_k) \to (M', w', [])$  with  $(M, w_0, s) = (M_k, w_k, s_k), (M^*, w^*, s^*) = (M', w', [])$  and  $s_k \neq []$ , as required. In the latter case, we have  $(M, w_0, s) \Rightarrow (M^{**}, w^{**}, s^{**}) \to (M', w'', [])$ , with  $s^{**} \neq []$ .

Lemma 99 peval = peval'

PROOF. We need to show that peval(M, s) = peval'(M, s) for all  $M \in C\Lambda$ ,  $s \in S$ . If s = [], then the equality follows trivially from the two definitions. Now, assume  $s \neq []$ .

If  $peval'(M, s) = M' \neq fail$ , then it follows from Lemma 98 that peval(M, s) = M',

Now, let  $\mathtt{peval}'(M,s) = \mathtt{fail}$  and suppose that  $\mathtt{peval}(M,s) = M' \neq \mathtt{fail}$ . Since  $s \neq []$ , by definition of  $\mathtt{peval}$  there must be  $M_k, w_k, s_k, w'$  such that  $(M,1,s) \Rightarrow (M_k, w_k, s_k) \to (M', w', [])$  and  $s_k \neq []$ . But by Corollary 7, this implies that  $\mathtt{peval}'(M,s) = M' \neq \mathtt{fail}$ , which yields a contradiction. Hence  $\mathtt{peval}(M,s) = \mathtt{fail}$ .

**Lemma 100** For every k, peval<sub>k</sub> =  $\Phi^k(\perp^{\lambda})$  is measurable.

PROOF. By induction on k:

- Base case: k=0: peval<sub>0</sub> =  $\perp^{\lambda}$  is a constant function on  $C\Lambda \times \mathbb{S}$ , so trivially measurable.
- Induction step: we have  $peval_{k+1} = \Phi(peval_k)$ , so it is enough to show that  $\Phi(f)$  is measurable if f is measurable.  $\Phi(f)$  is defined in pieces, so we want to use Lemma 59.

The domain of the first case is  $C\Lambda \times \{[]\}$ , so obviously measurable. The domain of the second case is  $p^{-1}(g^{-1}(C\Lambda \times \mathbb{R} \times \mathbb{S}) \cap (C\Lambda \times \{1\} \times (\mathbb{S} \setminus \{[]\})))$ , and p(M,s) = (M,1,s) is continuous, and so measurable. Hence, the domain is measurable. Finally, the domain of the last case is the complement of the union of the two above measurable sets, which means it is also measurable.

Thus, we only need to show that the functions corresponding to these three cases are measurable. This is obvious in the first and third case, because the corresponding functions are constant. The function for the second case is  $\phi(M,s) = f(g(p(M,s)))$ , where p is as defined above and g' is the restriction of g to  $g^{-1}(C\Lambda \times \mathbb{R} \times \mathbb{S})$ , which is measurable since restrictions preserve measurablety. Since composition of measurable functions is measurable,  $\phi$  is measurable.

Thus,  $peval_{k+1}$  is measurable, as required.

**Lemma 101** peval' is a measurable function  $C\Lambda \times \mathbb{S} \to C\Lambda$ .

PROOF. Corollary of Lemmas 100 and 89.

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Restatement of Lemma 50. peval is a measurable function  $C\Lambda \times \mathbb{S} \to C\Lambda$ .

Proof. Corollary of Lemma 101 and Lemma 99.

 $\textbf{Lemma 102} \ \textit{For every } M \in C\Lambda, c \in \mathbb{R}, s \in \mathbb{S}, \ \texttt{peval}(\texttt{peval}(M, [c]), s) \leq \texttt{peval}(M, c :: s)$ 

PROOF. Define a property  $P \subseteq F$ :

$$P(f) \Leftrightarrow \sup_{L} \Phi^{k}(\perp^{\lambda})(\Phi(f)(M,[c]),s) \leq \sup_{L} \Phi^{k}(\perp^{\lambda})(M,c::s) \quad \forall M,c,s$$

Since  $\sup_k \Phi^k(\perp^{\lambda})$  is a fix point of  $\Phi$ ,  $\Phi(\sup_k \Phi^k(\perp^{\lambda})) = \sup_k \Phi^k(\perp^{\lambda})$ , so

$$P(\sup_k \Phi^k(\bot^\lambda)) \iff \sup_k \Phi^k(\bot^\lambda)(\sup_l \Phi^l(\bot^\lambda)(M,[c]),s) \le \sup_k \Phi^k(\bot^\lambda)(M,c::s) \quad \forall M,c,s$$

So we only need to prove  $P(\sup_k \Phi^k(\perp^{\lambda}))$ .

To show that the property P is  $\omega$ -inductive, let  $f_1 \leq f_2 \leq \ldots$  be a  $\omega$ -chain and  $\sup_i f_i$  its limit. Then  $\Phi(f_1) \leq \Phi(f_2) \leq \ldots$  and  $\sup_i \Phi(f_i) = \Phi(\sup_i f_i)$ . For all M, s, we have

$$\Phi(\sup_{i} f_i)(M,s) = (\sup_{i} \Phi(f_i))(M,s) = \sup_{i} (\Phi(f_i)(M,s))$$

Note that either  $\Phi(f_i)(M,s) = \text{fail}$  for all i or there is some n such that  $\Phi(f_n)(M,s) \in \mathcal{V}$  and  $\Phi(f_m)(M,s) = \Phi(f_n)(M,s)$  for all m > n. In either case, there is a n(M,s) such that  $\sup_i(\Phi(f_i)(M,s)) = \Phi(f_{n(M,s)})(M,s)$ . Hence

$$P(\sup_{i} f_{i}) \Leftrightarrow \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(\sup_{i} f_{i})(M, [c]), s) \leq \sup_{k} \Phi^{k}(\perp^{\lambda})(M, c :: s) \quad \forall M, c, s$$

$$\Leftrightarrow \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(f_{n(M, [c])})(M, [c]), s) \leq \sup_{k} \Phi^{k}(\perp^{\lambda})(M, c :: s) \quad \forall M, c, s$$

$$\Leftrightarrow P(f_{n(M, [c])})$$

as required.

Now we can prove the desired property by Scott induction:

• Base case:

$$P(\bot^{\lambda}) \quad \Leftrightarrow \quad \sup_{k} \Phi^{k}(\bot^{\lambda})(\Phi(\bot^{\lambda})(M,[c]),s) \leq \sup_{k} \Phi^{k}(\bot^{\lambda})(M,c::s) \quad \forall M,c,s$$

For any M, c, s, we have

$$\sup_k \Phi^k(\bot^\lambda)(\Phi(\bot^\lambda)(M,[c]),s) = \sup_k \Phi^k(\bot^\lambda)(\mathtt{fail},s) = \mathtt{fail} \leq \sup_k \Phi^k(\bot^\lambda)(M,c :: s)$$

as required.

• Induction step: We need to show that for all f such that P(f),  $P(\Phi(f))$  holds, that is

$$\sup_k \Phi^k(\bot^\lambda)(\Phi(\Phi(f))(M,[c]),s) \leq \sup_k \Phi^k(\bot^\lambda)(M,c :: s) \quad \forall M,c,s$$

- Case  $(M, 1, [c]) \to (M', w, [c])$ :

$$LHS = \sup_{k} \Phi^{k}(\bot^{\lambda})(\Phi(\Phi(f))(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\bot^{\lambda})(\Phi(f)(M', [c]), s)$$
(by assumption)  $\leq \sup_{k} \Phi^{k}(\bot^{\lambda})(M', c :: s)$ 

$$= \Phi(\sup_{k} \Phi^{k}(\bot^{\lambda}))(M, c :: s)$$

$$= (\sup_{k} \Phi^{k}(\bot^{\lambda})(M, c :: s)$$

$$= RHS$$

- Case 
$$(M, 1, [c]) \rightarrow (M', w, [])$$
:
$$LHS = \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(\Phi(f))(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(f)(M', []), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(M', s)$$

$$= \Phi(\sup_{k} \Phi^{k}(\perp^{\lambda}))(M, c :: s)$$

$$= (\sup_{k} \Phi^{k}(\perp^{\lambda})(M, c :: s)$$
$$= RHS$$

- Case  $(M, 1, [c]) \not\rightarrow$ :

$$\begin{split} LHS &= \sup_k \Phi^k(\bot^\lambda)(\Phi(\Phi(f))(M,[c]),s) \\ &= \sup_k \Phi^k(\bot^\lambda)(\mathtt{fail},s) \\ &= \Phi(\sup_k \Phi^k(\bot^\lambda))(M,c :: s) \\ &= (\sup_k \Phi^k(\bot^\lambda)(M,c :: s) \\ &= RHS \end{split}$$

Therefore,  $P(\sup_k \Phi^k(\perp^{\lambda}))$ , holds, and so  $\operatorname{peval}(\operatorname{peval}(M,[c]),s) \leq \operatorname{peval}(M,c:s)$  for all closed M,c,s.

Lemma 103 For every  $M \in C\Lambda$ ,  $c \in \mathbb{R}$ ,  $s \in \mathbb{S}$ , peval(peval(M, [c]), s)  $\geq$  peval(M, c :: s)

PROOF. Like in the previous lemma, we use Scott induction. Define the property:

$$Q(f) \Leftrightarrow f(M, c :: s) \leq \sup_{k} \Phi^{k}(\bot^{\lambda})(\sup_{l} \Phi^{l}(\bot^{\lambda})(M, [c]), s) \quad \forall M, c, s$$

$$\wedge f \leq \sup_{k} \Phi^{k}(\bot^{\lambda})$$

We need to show that  $Q(\sup_k \Phi^k(\perp^{\lambda}))$  holds.

First, we need to verify that Q is  $\omega$ -inductive. This is obvious for the second conjunct, so let us concentrate on the first. Once again, we use the property that for all  $\omega$ -chains  $f_1 \leq f_2 \leq \ldots$  and M, s, the chain  $f_1(M,s) \leq f_2(M,s) \leq \ldots$  will eventually be stationary. For all M,c,s, we have  $(\sup_i f_i)(M,c::s) = f_{n(M,c,s)}(M,c::s)$  for some n(M,c,s). Then for every M,c,s, the inequality

$$(\sup_{i} f_{i})(M, c :: s) \leq \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M, [c]), s)$$

follows from  $Q(f_{n(M,c,s)})$ .

• Base case:

$$\begin{split} Q(\bot^{\lambda}) & \Leftrightarrow & \bot^{\lambda}(M,c::s) \leq \sup_{k} \Phi^{k}(\bot^{\lambda}) (\sup_{l} \Phi^{l}(\bot^{\lambda})(M,[c]),s) & \forall M,c,s \\ & \wedge \bot^{\lambda} \leq \sup_{k} \Phi^{k}(\bot^{\lambda}) \end{split}$$

Both inequalities are obvious, because the LHS is always fail.

• Induction step: Give Q(f), for every M, c, s we need to show:

$$\begin{array}{lcl} \Phi(f)(M,c :: s) & \leq & \displaystyle \sup_k \Phi^k(\bot^\lambda)(\sup_l \Phi^l(\bot^\lambda)(M,[c]), s) & \forall M, c, s \\ \\ \Phi(f) & \leq & \displaystyle \sup_k \Phi^k(\bot^\lambda) \end{array}$$

Again, the second inequality is obvious, so let us concentrate on the first.

- Case 
$$(M, 1, [c]) \to (M', w, [c])$$
:

$$LHS = f(M', c :: s)$$
(by first assumption)  $\leq \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M', [c]), s)$ 

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(\sup_{l} \Phi^{l}(\perp^{\lambda}))(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M, [c]), s)$$

$$= RHS$$

- Case  $(M, 1, [c]) \to (M', w, [])$ :

$$LHS = f(M', s)$$
(by second assumption)  $\leq \sup_{k} \Phi^{k}(\perp^{\lambda})(M', s)$ 

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(\sup_{l} \Phi^{l}(\perp^{\lambda}))(M', []), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M', []), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\Phi(\sup_{l} \Phi^{l}(\perp^{\lambda}))(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M, [c]), s)$$

$$= \sup_{k} \Phi^{k}(\perp^{\lambda})(\sup_{l} \Phi^{l}(\perp^{\lambda})(M, [c]), s)$$

- Case  $(M, 1, [c]) \not\rightarrow$ :

$$\begin{array}{ccc} LHS & = & \mathtt{fail} \\ & \leq & RHS \end{array}$$

As required.  $\Box$ 

RESTATEMENT OF LEMMA 48. peval(peval(M, [c]), s) = peval(M, c :: s)

PROOF. Follows from Lemmas 102 and 103.  $\hfill\Box$ 

RESTATEMENT OF LEMMA 49. For all closed M, s, t, peval(peval(M, s), t) = peval(M, <math>s@t) PROOF. By induction on |s|.

- Base case: s = []. We have peval(M, []) = M (by definition of peval), so the result is trivial.
- Induction step: s=c::s'. We want peval(peval(M,c::s),t) = peval(M,c::s@t). We have:

$$\begin{array}{rcl} LHS &=& \mathtt{peval}(\mathtt{peval}(M,c::s),t) \\ (\mathtt{by}\ \mathtt{Lemma}\ 48) &=& \mathtt{peval}(\mathtt{peval}(\mathtt{peval}(M,[c]),s),t) \\ (\mathtt{by}\ \mathtt{induction}\ \mathtt{hypothesis}) &=& (\mathtt{peval}(\mathtt{peval}(M,[c]),s@t) \\ (\mathtt{by}\ \mathtt{Lemma}\ 48) &=& \mathtt{peval}(M,[c]::s@t) \end{array}$$

#### A.5 Measurability of q and Q

**Lemma 104** For all  $s \in \mathbb{S}$  and  $M \in C\Lambda$ ,  $\int_{\mathbb{S} \setminus []} q_M(s,t) \mu(dt) \leq 1$ 

To prove this lemma, we need some auxiliary results:

**Lemma 105** If  $M \downarrow_w^{\parallel} G$  and  $M \downarrow_{w'}^s G'$ , then  $s = \parallel$ .

PROOF. By induction on the derivation of  $M \downarrow_{n}^{\square} G$ .

**Lemma 106** If  $\mathbf{P}_{M}^{V}([]) > 0$ , then  $\mathbf{P}_{M}^{V}(t) = 0$  for all  $t \neq []$ .

PROOF. Follows directly from Lemma 105.

Lemma 107 (Tonelli's theorem for sums and integrals, 1.4.46 in [36]) If  $(\Omega, \Sigma, \mu)$  is a measure space and  $f_1, f_2, \ldots$  a sequence of non-negative measurable functions, then

$$\int_{\Omega} \sum_{i=1}^{\infty} f_i(x) \ \mu(dx) = \sum_{i=1}^{\infty} \int_{\Omega} f_i(x) \ \mu(dx)$$

PROOF. Follows from the monotone convergence theorem.

Lemma 108 (Linearity of Lebesgue integral, 1.4.37 ii) from [36]) If  $(\Omega, \Sigma)$  is a measurable space, f a non-negative measurable function, and  $\mu_i, \mu_2, \ldots$  a sequence of measures on  $\Sigma$ , then

$$\int_{\Omega} f(x) \sum_{i=1}^{\infty} \mu_i(dx) = \sum_{i=1}^{\infty} \int_{\Omega} f(x) \mu_i(dx)$$

**Lemma 109 (Ex. 1.4.36 xi) from [36])** If  $(\Omega, \Sigma, \mu)$  is a measure space and f a nonnegative measurable function on  $\Omega$  and  $B \in \Sigma$  and  $f^B$  a restriction of f to B, then

$$\int_{\Omega} f(x)[x \in B] \ \mu(dx) = \int_{B} f(x) \ \mu^{B}(dx)$$

Below we write q(s,t) as  $q_M(s,t)$ , to make the dependency on M explicit. Let  $q_M^*$  be defined as follows:

$$q_M^*(s,t) = \begin{cases} \mathbf{P}_M^{\mathcal{V}}([]) & \text{if } t = []\\ q_M(s,t) & \text{otherwise} \end{cases}$$

**Lemma 110** For all  $M \in C\Lambda$  and  $s, y \in \mathbb{S}$ 

$$q_M^*(s,t) = \begin{cases} \mathbf{P}_M^{\mathcal{V}}(t) & \textit{if } s = [] \textit{ or } t = [] \\ \mathrm{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1)q_{\mathtt{peval}(M,[s_1])}^*([s_2,\ldots s_{|s|}],[t_2,\ldots t_{|t|}]) & \textit{otherwise} \end{cases}$$

PROOF. By induction on |s|:

- Case s = []: If t = [], the result follows directly from the definition of  $q_M^*$ . Otherwise,  $q_M^*([],t) = q_M([],t) = P_M^{\mathcal{V}}(t)$ , as required.
- Case |s| = n + 1 > 0: Again, if t = [], the result follows immediately. Otherwise, we have

$$q_M^*(s,t) = q_M(s,t) = \prod_{i=1}^k (\operatorname{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i)) \mathbf{P}_{\mathsf{peval}(M,[t_1,...,t_k])}^{\mathcal{V}}(t)$$

where  $k = \min(|s|, |t|) > 0$ . Hence

$$\begin{array}{lcl} q_{M}^{*}(s,t) & = & \mathrm{pdf}_{\mathsf{Gaussian}}(s_{1},\sigma^{2},t_{1})\Pi_{i=2}^{k}(\mathrm{pdf}_{\mathsf{Gaussian}}(s_{i},\sigma^{2},t_{i}))\mathbf{P}_{\mathrm{peval}(M,[t_{1},...,t_{k}])}^{\mathcal{V}}([t_{k+1},...,t_{|t|}]) \\ (\mathrm{by\ Lemma\ }48) & = & \mathrm{pdf}_{\mathsf{Gaussian}}(s_{1},\sigma^{2},t_{1})\Pi_{i=2}^{k}(\mathrm{pdf}_{\mathsf{Gaussian}}(s_{i},\sigma^{2},t_{i}))\mathbf{P}_{\mathrm{peval}(\mathrm{peval}(M,[t_{1}]),[t_{2},...,t_{k}])}^{\mathcal{V}}([t_{k+1},...,t_{|t|}]) \\ & = & (\mathrm{pdf}_{\mathsf{Gaussian}}(s_{1},\sigma^{2},t_{1}))q_{\mathrm{peval}(M,[s_{1}])}^{*}([s_{2},...,s_{|s|})],[t_{2},...,t_{|t|}]) \end{array}$$

**Lemma 111** If  $\mathbf{P}_{M}^{\mathcal{V}}([]) > 0$ , then peval(M, t) = fail for every  $t \neq []$ .

PROOF. It  $\mathbf{P}_{M}^{\mathcal{V}}([]) = w > 0$ , then we must have  $M \downarrow_{w}^{[]} V$  for some  $V \in \mathcal{V}$ , which implies  $(M,1,[]) \Rightarrow (G,w,[])$ . Using Lemma 15, we can easily show by induction that  $(M,1,t) \Rightarrow (G,w,t)$  for any  $t \neq []$ . Because the reduction relation is deterministic, this implies that there are no M', w' such that  $(M,1,t) \Rightarrow (M',w',[])$  (if there were, we would have  $(M',w',[]) \Rightarrow (G,w,t)$ , but no reduction rule can add an element to a trace). This means that  $\mathbf{peval}$ , by applying reduction repeatedly, will never reach (M',[]) for any M', so  $\mathbf{peval}(M,t) = \mathbf{fail}$ .

**Lemma 112** If  $\mathbf{P}_{M}^{\mathcal{V}}([]) > 0$ , then  $q_{M}^{*}(s,t) = 0$  for all  $s \in \mathbb{S}, t \neq []$ .

PROOF. Follows easily from Lemma 111.

Restatement of Lemma 104 . For all  $s\in\mathbb{S}$  and  $M\in C\Lambda$ ,  $\int_{\mathbb{S}\backslash\mathbb{T}}q_M(s,t)\mu(dt)\leq 1$ 

PROOF. By induction on |s|.

• Base case: s = []

as required.

$$\int_{\mathbb{S}\backslash\{[]\}} q_{M}([],t) \ \mu(dt)$$

$$= \int_{\mathbb{S}\backslash\{[]\}} \mathbf{P}_{M}^{\mathcal{V}}(t) \ \mu(dt)$$

$$\leq \int_{\mathbb{S}} \mathbf{P}_{M}(t) \ \mu(dt)$$

$$= \langle\!\langle M \rangle\!\rangle(\mathbb{S})$$

$$= \langle\!\langle M \rangle\!\rangle(\mathbf{O}_{M}^{-1}(\mathcal{GV}))$$

$$= [\![M]\!]_{\mathbb{S}}(\mathcal{GV})$$
by Theorem 3 =  $[\![M]\!](\mathcal{GV})$ 

$$\leq 1$$

because  $\llbracket M \rrbracket$  is a sub-probability distribution.

• Induction step:  $s \neq []$ 

We have:

$$\int_{\mathbb{S}\backslash\{[]\}} q_M(s,t) \; \mu(dt)$$

$$= \int_{\mathbb{S}\backslash\{[]\}} q_M^*(s,t) \; \mu(dt)$$
(by Thm 16.9 from Billingsley) 
$$= \sum_{i=1}^{\infty} \int_{\mathbb{R}^i} q_M^*(s,t) \; \mu(dt)$$

$$= \sum_{i=1}^{\infty} \int_{\mathbb{R}^i} q_M^*(s,t) \; \lambda^i(dt)$$

$$= \sum_{i=1}^{\infty} \int_{\mathbb{R}^i} \operatorname{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1) q_{\mathsf{peval}(M,[t_1])}^*([s_2,\ldots,s_{|s|}],[t_2,\ldots,t_{|t|}]) \; \lambda^i(dt)$$
(by Fubini's theorem) 
$$= \sum_{i=1}^{\infty} \int_{\mathbb{R}} \operatorname{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1) \int_{\mathbb{R}^{i-1}} q_{\mathsf{peval}(M,[t_1])}^*(s',t') \; \lambda^{i-1}(dt') \; \lambda(dt_1)$$
(by Lemma 107) 
$$= \int_{\mathbb{R}} \operatorname{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1) \sum_{i=0}^{\infty} \int_{\mathbb{R}^i} q_{\mathsf{peval}(M,[t_1])}^*(s',t') \; \lambda^i(dt') \; \lambda(dt_1)$$

$$= \int_{\mathbb{R}} \operatorname{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1) \left( \int_{\{[]\}} \mathbf{P}_{\mathsf{peval}(M,[t_1])}^{\mathcal{V}}(t') \; \mu(dt') + \int_{\mathbb{R}^{N} \cap \mathbb{R}^d} q_{\mathsf{peval}(M,[t_1])}^*(s',t') \; \mu(dt') \right) \; \lambda(dt_1)$$

Now, we need to show that for all N,

$$\int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt') + \int_{\mathbb{S}\setminus\{[]\}} q_N^*(s',t') \ \mu(dt') \le 1$$
 (3)

First, note that  $\int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt') \leq \int_{\mathbb{S}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt') \leq 1$ , by the same property as the one used in the base case. We also have  $\int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt) = \mathbf{P}_N^{\mathcal{V}}([])$ , so by Lemma 112, if  $\mathbf{P}_N^{\mathcal{V}}([]) > 0$ , then

$$\int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt') + \int_{\mathbb{S}\setminus\{[]\}} q_N^*(s',t') \ \mu(dt') = \int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \ \mu(dt') \le 1$$

On the other hand, if  $\mathbf{P}_N^{\mathcal{V}}([]) = 0$ , then

$$\int_{\{[]\}} \mathbf{P}_N^{\mathcal{V}}(t') \, \mu(dt') + \int_{\mathbb{S}\backslash\{[]\}} q_N^*(s',t') \, \mu(dt') = \int_{\mathbb{S}\backslash\{[]\}} q_N^*(s',t') \, \mu(dt') = \int_{\mathbb{S}\backslash\{[]\}} q_N(s',t') \, \mu(dt') \leq 1$$

by induction hypothesis.

Hence:

$$\begin{split} & \int_{\mathbb{S}\backslash\{[]\}} q_M(s,t) \ \mu(dt) \\ & \leq & \int_{\mathbb{R}} \mathrm{pdf}_{\mathsf{Gaussian}}(s_1,\sigma^2,t_1) \ \lambda(dt_1) \\ & = & 1 \end{split}$$

as required.  $\Box$ 

RESTATEMENT OF LEMMA 51. For any closed program M, the transition density  $q(\cdot, \cdot) : (\mathbb{S} \times \mathbb{S}) \to \mathbb{R}_+$  is measurable.

PROOF. It is enough to show that q(s,t) is measurable for every |s| = n and |t| = m, then the result follows from Lemma 59.

Note that a function taking a sequence s and returning any subsequence of it is trivially continuous and measurable, so for any function of s and t to be measurable, it is enough to show that it is measurable as a function of some projections of s and t.

• If m > 0 and n < m, then we have  $q(s,t) = \prod_{i=1}^n \operatorname{pdf}_{\mathsf{Gaussian}}(s_1, \sigma^2, t_i) \mathbf{P}^{\mathcal{V}}_{\mathsf{peval}(M, t_{1..n})}(t_{n+1..m}) = \prod_{i=1}^n \operatorname{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i) \mathbf{P}'(\mathsf{peval}(M, t_{1..n}), t_{n+1..m}) [\mathbf{O}'(\mathsf{peval}(M, t_{1..n}), t_{n+1..m}) \in \mathcal{V}].$  Each  $\operatorname{pdf}_{\mathsf{Gaussian}}(s_i, \sigma^2, t_i)$  is measurable, as a composition of a function projecting  $(s_i, t_i)$  from (s, t) and the Gaussian pdf, so their pointwise product must be measurable. Now,  $\mathbf{P}'$  is measurable, and the function mapping (s, t) to  $(\operatorname{peval}(M, t_{1..n}), t_{n+1..m})$  is a pair

Now,  $\mathbf{P}'$  is measurable, and the function mapping (s,t) to  $(\mathtt{peval}(M,t_{1..n}),t_{n+1..m})$  is a pair of two measurable functions, one of which is a composition of the measurable  $\mathtt{peval}(M,\cdot)$  and a projection of  $t_{1..n}$ , and the other just a projection of  $t_{n+1..m}$ ). Hence, the function mapping (s,t) to  $\mathbf{P}'(\mathtt{peval}(M,t_{1..n}),t_{n+1..m})$  is a composition of measurable functions.

Finally,  $[\mathbf{O}'(\mathtt{peval}(M, t_{1..n}), t_{n+1..m}) \in \mathcal{V}]$  is a composition of the measurable function mapping (s,t) to  $(\mathtt{peval}(M, t_{1..n}), t_{n+1..m})$  and the indicator function for the measurable set  $\mathcal{V}$ , thus it is measurable.

Hence, q(s,t) is a pointwise product of measurable functions, so it is measurable.

- If m > 0 and n ≥ m, then q(s,t) = Π<sup>m</sup><sub>i=1</sub> pdf<sub>Gaussian</sub>(s<sub>1</sub>, σ², t<sub>i</sub>) P<sup>V</sup><sub>peval(M,t)</sub>([])
  = Π<sup>m</sup><sub>i=1</sub> pdf<sub>Gaussian</sub>(s<sub>i</sub>, σ², t<sub>i</sub>) P'(peval(M,t), []) [O'(peval(M,t), []) ∈ V].
  Now, the function mapping (s,t) to Π<sup>m</sup><sub>i=1</sub> pdf<sub>Gaussian</sub>(s<sub>i</sub>, σ², t<sub>i</sub>) is measurable like in the previous case. The function mapping (s,t) to (peval(M,t), []) is a pairing of two measurable functions, one being a composition of the projection of t and peval(M,·), the other being a constant function returning []. Hence, P'(peval(M,t), []) is a composition of two measurable functions. Meanwhile, [O'(peval(M,t), []) ∈ V] is a composition of a measurable function and an indicator function.
- If m=0, then  $q(s,[])=1-\int_{\mathbb{S}\backslash\{[]\}}q(s,t)\,\mu(dt)$ . Since we have already shown that q(s,t) is measurable on  $\mathbb{S}\times(\mathbb{S}\backslash[])$ ,  $\int_{\mathbb{S}\backslash\{[]\}}q(s,t)\,\mu(dt)$  is measurable by Fubini's theorem, so q(s,[]) is a difference of measurable functions, and hence it is measurable.

RESTATEMENT OF LEMMA 52. The function Q is a probability kernel on (S, S).

PROOF. We need to verify the two properties of probability kernels:

- 1. For every  $s \in \mathbb{S}$ ,  $Q(s,\cdot)$  is a probability distribution on  $\mathbb{S}$ . Since for every  $s \in \mathbb{S}$ ,  $q(s,\cdot)$  is non-negative measurable  $\mathcal{S}$  (by [2, Theorem 18.1]),  $Q(s,B) = \int_B q(s,y)\mu(dy)$  (as a function of B) is a well-defined measure for all  $s \in \mathbb{S}$ . Finally,  $Q(s,\mathbb{S}) = Q(s,[]) + Q(s,\mathbb{S} \setminus \{[]\}) = 1$ .
- 2. For every  $B \in \mathcal{S}$ ,  $Q(\cdot, B)$  is a non-negative measurable function on  $\mathbb{S}$ : Since  $(\mathbb{S}, \mathcal{S}, \mu)$  is a  $\sigma$ -finite measure space,  $q(\cdot, \cdot)$  is non-negative and measurable  $\mathcal{S} \times \mathcal{S}$  and  $Q(s, B) = \int_B q(s, y) \mu(ds)$ , this follows from [2, Theorem 18.3].

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