A Lambda Calculus Foundation for Universal Probabilistic Programming

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Introduction

We want to prove correct a variant of Metropolis-Hastings MCMC on program traces (sequences of random choices made during execution), in the line of the algorithm used by Church.

Why a formal correctness proof of Trace MCMC?

- ...because there is none yet! (for a functional language)
- Can we really trust probabilistic languages and their inference engines?
- Machine learning used in safety-critical applications (medicine, autonomous vehicles etc.)
- Traces are highly nonstandard parameter spaces. Simple textbook proof for MH-MCMC does not apply.
Roadmap

To prove correctness of an inference algorithm for a probabilistic language we need:

- The syntax of the language
- A semantics of the language
- A rigorous definition of the algorithm
- A formal definition of “correct”
This paper consists of two parts:

- Semantics of a probabilistic lambda-calculus with continuous distribution, defined in two ways:
  - Distributional semantics - distribution on return values
  - Sampling-based semantics - distribution on random traces
- A formal proof of correctness of MH-MCMC on this language, with respect to the distributional semantics.
  - Still completing proofs of two measurability lemmas
Untyped lambda-calculus with continuous distributions

Let $x, D, g$ range over countable sets of identifiers, distributions, primitive functions, respectively.

$V ::= c \mid x \mid \lambda x. M$

$M ::= V \mid M N \mid D(V_1, \ldots, V_{|D|}) \mid g(V_1, \ldots, V_{|g|})$

if $V$ then $M$ else $L \mid$ fail

$G ::= V \mid$ fail

We define a metric space on the space $\Lambda$ of terms:

\[
\begin{align*}
    d(c, d) &= |c - d| \\
    d(x, x) &= 0 \\
    d(\lambda x. M, \lambda x. N) &= d(M, N) \\
    d(M N, L P) &= d(M, L) + (N, P) \quad \ldots
\end{align*}
\]

The metric space $(\Lambda, d)$ gives rise to a topology and a Borel $\sigma$-algebra.
Example program

Using standard syntactic sugar for `let`.

```plaintext
let p = uniform() in
let flip = \_.uniform() < p in
if (flip() = 0) and (flip() = 1) then p else fail
```
Distributional Semantics - Small Step

Deterministic reduction: \( M \rightarrow N \)

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

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

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

\[
\ldots
\]

One-step evaluation: \( M \rightarrow \mathcal{D} \)

\[
E[D(\vec{c})] \rightarrow E\{\mu_{D(\vec{c})}\}
\]

\[
E[M] \rightarrow \delta(E[N]) \quad \text{if } M \xrightarrow{\text{det}} N
\]

Step-Indexed approximation semantics: \( M \rightarrow^n \mathcal{D} \).

\[
\frac{n > 0}{G \rightarrow^n \delta(G)}
\]

\[
\frac{M \rightarrow^n 0}{M \rightarrow 0 0}
\]

\[
M \rightarrow \mathcal{D} \quad \{N \rightarrow^n \mathcal{E}_N\}_{N \in \text{supp}(\mathcal{D})}
\]

\[
M \rightarrow^n+1 (A \mapsto \int \mathcal{E}_N(A) \; \mathcal{D}(dN))
\]

Semantics:

\[
\llbracket M \rrbracket \Rightarrow = \sup \{ \mathcal{D} \mid M \rightarrow^n \mathcal{D} \}
\]

Lemma

\( \rightarrow \) is a subprobability kernel

Lemma

\( \rightarrow^n \) is a subprobability kernel for every \( n \geq 0 \).
Distributional Semantics- Big Step

\[
\begin{align*}
M & \downarrow_n \mathcal{D} & N & \downarrow_n \mathcal{E} & \{L \{V/x\} \downarrow_n \mathcal{E}_L,V\} & (\lambda x.L) \in \text{supp}(\mathcal{D}), V \in \text{supp}(\mathcal{E}) \\
M N & \downarrow_{n+1} A & \mathcal{D}^E(A) + \mathcal{D}(\mathbb{R}) \cdot \delta(\text{error}) + \mathcal{D}(\text{V}_\lambda) \cdot \mathcal{E}^E(A) + \\
& & \int \int \mathcal{E}_L,V(A) \mathcal{D}^{\mathcal{V}_\lambda}(\lambda x.dL) \mathcal{E}^\mathcal{V}(dV)
\end{align*}
\]

Semantics: \( [M] \downarrow = \sup \{ \mathcal{D} \mid M \downarrow_n \mathcal{D} \} \)

**Theorem**

For every term \( M \), \( [M] \downarrow = [M] \Rightarrow \).
Sampling Based Semantics - Pseudo-deterministic Evaluation

Small step: \((M, w, s) \rightarrow (M', w', s')\)

\[
\begin{align*}
M \xrightarrow{\text{det}} N \\
(M, w, s) &\rightarrow (N, w, s)
\end{align*}
\]

\[w' = \text{pdf}_D(\bar{c}, c) \quad w' > 0\]

\[(E[D(\bar{c})], w, s) \rightarrow (E[c], w w', s \oplus [c])\]

Big step: \(M \Downarrow^s_w G\)

\[
\begin{align*}
G \in \mathcal{G}& \quad w = \text{pdf}_D(\bar{c}, c) \quad w > 0 \\
G \Downarrow^1_1 G \\
D(\bar{c}) &\Downarrow^{[c]}_w c
\end{align*}
\]

\[g(\bar{c}) \Downarrow^{\sigma}_1 \sigma_g(\bar{c})\]

\[
\begin{align*}
M \Downarrow^{s_1}_{w_1} \lambda x.P & \quad N \Downarrow^{s_2}_{w_2} V & \quad P[V/x] \Downarrow^{s_3}_{w_3} G
\end{align*}
\]

\[M \Downarrow^{s_1 \odot s_2 \odot s_3}_{w_1 w_2 w_3} G\]

\[\ldots\]

**Proposition**

\[M \Downarrow^s_w G \text{ if and only if } (M, 1, []) \rightarrow^* (G, w, s).\]
Sampling Based Semantics: inspired by (Nori, Hur, Rajamani, Samuel 2013)

- Measurable space of program traces: \((\mathcal{S}, S)\), where:
  - \(\mathcal{S} = \biguplus_{n \in \mathbb{N}} \mathbb{R}^n\)
  - \(S = \{\biguplus_{n \in \mathbb{N}} H_n \mid H_n \in \mathcal{R}^n \text{ for all } n\}\)

- Stock measure on program traces: \(\mu(\biguplus_{n \in \mathbb{N}} H_n) = \sum_{n=1}^{\infty} \lambda_n(H_n)\)

- Density function of a program \(M\) (w.r.t. stock measure on traces):
  \[
P_M(s) = \begin{cases} 
  w & \text{if } M \Downarrow_s^w G \text{ for some } G \\
  0 & \text{otherwise}
  \end{cases}
  \]

- Outcome of evaluation of \(M\) as a function of trace \(s\):
  \[
  O_M(s) = \begin{cases} 
  G & \text{if } M \Downarrow_s^w G \text{ for some } w \\
  \text{fail} & \text{otherwise}
  \end{cases}
  \]

- A subprobability measure on program traces:
  \[
  \llbracket M \rrbracket_S(A) = \int_A P_M(s) \mu(ds)
  \]

- Can obtain measure on values by transformation: \(\llbracket M \rrbracket_S = \llbracket M \rrbracket_S O_M^{-1}\)

**Theorem**

\[
\llbracket M \rrbracket_S = \llbracket M \rrbracket_{\downarrow} = \llbracket M \rrbracket_{\Rightarrow}
\]

Recall: \(\llbracket M \rrbracket_{\Rightarrow}\) - Small-step distributional semantics
\(\llbracket M \rrbracket_{\downarrow}\) - Big step distributional semantics
Let $(\Omega, \Sigma)$ be an arbitrary measurable space. Suppose we want to sample from some distribution $\pi$ on $\Sigma$.

Define a proposal kernel $Q(x, A) : \Omega \times \Sigma \to \mathbb{R}$ and a measurable acceptance function $\alpha(x, y) : \Omega \times \Omega \to [0, 1]$ such that the resulting Metropolis-Hastings transition kernel:

$$P(x, A) = \int_A \alpha(x, y)Q(x, dy) + \delta(x)(A) \int_\Omega (1 - \alpha(x, t))Q(s, dt)$$

is reversible with respect to $\pi$:

$$\int_A P(x, B)\pi(dx) = \int_B P(y, A)\pi(dy)$$

for all $A, B \in \Sigma$.

Then $\pi$ is the stationary distribution of the Markov chain with transition kernel $P$.

If $Q(x, A) = \int_A q(x, y)\mu(dy)$ and $\pi(A) = \int_A \pi(x)\mu(dx)$, detailed balance equation simplifies.
Idea: formalize the algorithm used by Church (or slightly simplified version thereof):

- Given trace $s = [s_1, \ldots, s_n]$ in program $M$, choose $k$ s.t. $k \geq 0$, $k \leq n$ at random.
- Partially evaluate $M$ under the trace $[s_1, \ldots, s_k]$, yielding $M'$.
- Evaluate $M'$, sampling values $[t_{k+1}, \ldots, t_m]$ from target distributions on the way.
- Set $t = [s_1, \ldots, s_n t_{n+1}, \ldots, t_m]$, accept with probability $\alpha(s, t) = \min\{1, \frac{|t|}{|s|}\}$

Problem: the proposal kernel corresponding to this algorithm has no density! Fixing a prefix would immediately set the integral to 0. The lack of density makes the proof much harder. We have decided to leave it as further work and start with a kernel which has density.
Solution: update all elements of the trace, following the approach of (Hur, Nori et al, 2015).

Let $s = [s_1, \ldots, s_n]$ be the previous trace. For each $i$-th random choice:

- If $i < n$, draw $t_i = \text{Gaussian}(s_1, \sigma^2)$.
- Otherwise, draw $t_i$ from target distribution.

Repeat until we get a generalized value and return trace $t$. Accept with probability

$$\alpha(s, t) = \begin{cases} 0 & \text{if } P_M(t) = 0 \\ 1 & \text{if } P_M(s)q(s, t) = 0 \\ \min\{1, \frac{P_M(t)q(t, s)}{P_M(s)q(s, t)}\} & \text{otherwise} \end{cases}$$
Inference- Take 2

This algorithm has the following transition kernel $P$:

$$
\text{peval}(M, s) = \begin{cases} 
M & \text{if } s = [] \\
M' & \text{if }(M, 1, []) \Rightarrow (M_k, w_k, s_k) \rightarrow (M', w', s) \\
\text{fail} & \text{otherwise}
\end{cases}
$$

for some $M_k, w_k, s_k, w'$ such that $s_k \neq s$

$$
q(s, t) = (\prod_{i=1}^{k} \text{pdf}_{\text{Gaussian}}(s_i, \sigma^2, t_i)) \cdot P_N(t_{k+1..|t|}) \text{ if } |t| \neq 0
$$

where $k = \min\{|s|, |t|\}$ and $N = \text{peval}(M, t_1..k)$

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

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

$$
P(s, A) = \int_A \alpha(s, t) Q(s, dt) + \delta(s)(A) \cdot \int (1 - \alpha(s, t)) Q(s, dt)
$$

Stationary distribution: $\pi(A) = [M]_S(A)/[M]_S(S)$ (normalized distribution on traces)
Definition of correctness

Define $P^n(x, A)$ to be the probability of reaching $A$ from $x$ in $n$ steps:

$$P^0(s, A) = \delta(s)(A)$$
$$P^{n+1}(s, A) = \int P(t, A)P^n(s, dt)$$

The variational norm is a measure of “closeness” of probability measures:

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

Let $T^n(s, A) = P^n(s, O_M^{-1}(A))$ and $[M]_{G\mathcal{V}}(A) = [M](A)/[M]_{G\mathcal{V}}$.

The algorithm can be considered correct if for every trace $s$ with $P_M(s) \neq 0$,

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

Theorem (Tierney 1994)

Let $P$ be a Metropolis kernel (as given earlier). If $\pi$ is the stationary distribution of $P$ and $P$ is $\pi$-irreducible and aperiodic, then

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

Lemma (Strong Irreducibility, implies $\pi$-irreducibility)

If $P_M(s) > 0$ and $[M]^S_{\downarrow}(A) > 0$ then $P(s, A) > 0$.

Lemma (Aperiodicity)

$P$ is $\pi$-aperiodic.

Then the above theorem from gives: $\lim_{n \to \infty} \| P^n(x, \cdot) - \pi \| = 0$

Theorem (Main Result)

For every trace $s$ with $P_M(s) \neq 0$, $\lim_{n \to \infty} \| T^n(s, \cdot) - [M]_{SV} \| = 0$. 
Further work

- Finish proofs of two remaining technical lemmas (in second part)
- Translation of Church to the calculus
- Trial implementation
- Understanding conditioning
- Alternative inference algorithm, similar to Church
- Program MCMC in calculus itself