Rigorous bounds for posterior inference in universal probabilistic programming

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Logic of Probabilistic Programming @ CIRM 2022

A random walk as a probabilistic program

```
start = sample uniform(0,3)
position = start; distance = 0
while position > 0:
    step = sample uniform(-1, 1)
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What is $p(\texttt{start} \mid \text{observation})$? $\rightarrow$ Bayesian inference

- continuous distributions
- unbounded loops
- unbounded number of **`sample`**s

Existing inference methods

1. **Approximate:** posterior $\approx X$

- Monte Carlo (particle filter, MCMC)
- or optimization-based (variational inference)

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PYRO

2. Exact: posterior $= X$

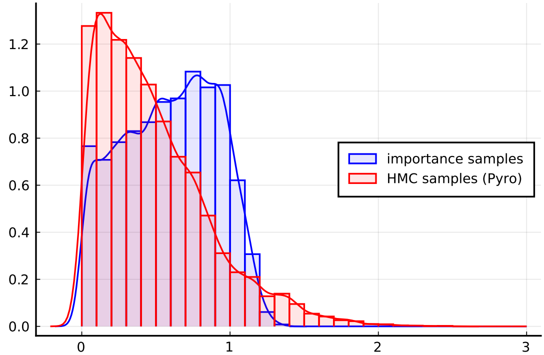
- symbolic expression

PSI SOLVER

HAKARU

ΣΠPL

Issues with existing methods



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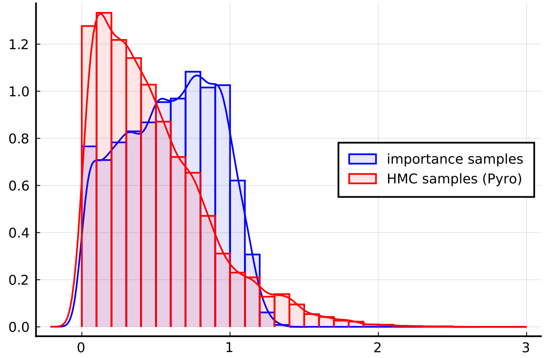

- **approximate methods:** convergence (e.g. for multimodal models)
- **exact methods:** restricted models (e.g. no recursion)

Rigorous Bounds on the Posterior: $\mathsf{posterior}(E) \in [a, b]$

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. . . for

- a universal PPL (including branching & recursion)
- with continuous distributions
- and conditioning (**`observe`**)

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- construct ground truth for inference problems
- to debug approximate inference

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How?

1. interval traces & interval arithmetic (basic idea)
2. interval type system (overapproximation)
3. symbolic execution (optimization of special case)

Semantics of a probabilistic program

Let $P : \mathbb{R}$ a probabilistic program.

- trace space: $\mathbb{T} := \bigcup_{n \in \mathbb{N}} \mathbb{R}^n$
- value function: $\mathsf{val}_P : \mathbb{T} \to \mathbb{R}$
- weight function: $\mathsf{wt}_P : \mathbb{T} \to [0, \infty)$

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Unnormalized posterior of an event E:

$$[\![P]\!](E) := \int_{\mathsf{val}_P^{-1}(E)} \mathsf{wt}_P(\boldsymbol{t}) \, \mathrm{d}\boldsymbol{t} = \text{“} \mathbb{P}(\mathtt{start} \in E \wedge \textsf{obs}) \text{”}$$

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Bayes' rule:

$$\mathbb{P}(\texttt{start} \in E \mid \textsf{obs}) = \frac{1}{Z} \mathbb{P}(\texttt{start} \in E \wedge \textsf{obs}) \quad \text{where } Z := \mathbb{P}(\textsf{obs})$$

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Normalized posterior:

$$\mathsf{posterior}_P(E) := \frac{1}{Z}[\![P]\!](E) \qquad \text{where } Z := [\![P]\!](\mathbb{R}).$$

Method 1: Interval traces

	standard semantics
traces	$\langle 0.2, 0.8 \rangle$
	$\mathbb{T} := \bigcup_{n \in \mathbb{N}} \mathbb{R}^n$
value	$\mathsf{val}_P : \mathbb{T} \to \mathbb{R}$
weight	$\mathsf{wt}_P : \mathbb{T} \to [0, \infty)$
posterior	$[\![P]\!](E)$
	integral over $\mathbb{T}$

Method 1: Interval traces

Idea: summarize traces using intervals

	standard semantics	interval semantics
traces	$\langle 0.2, 0.8 \rangle$	$\langle [0.2, 0.3], [0.7, 0.8] \rangle$
	$\mathbb{T} := \bigcup_{n \in \mathbb{N}} \mathbb{R}^n$	$\mathbb{T}_{\mathbb{I}} := \bigcup_{n \in \mathbb{N}} \mathbb{I}^n$
value	$\mathsf{val}_P : \mathbb{T} \to \mathbb{R}$	$\mathsf{val}_P^{\mathbb{I}} : \mathbb{T}_{\mathbb{I}} \to \mathbb{I}$
weight	$\mathsf{wt}_P : \mathbb{T} \to [0, \infty)$	$\mathsf{wt}_P^{\mathbb{I}} : \mathbb{T}_{\mathbb{I}} \to \mathbb{I}_{[0,\infty)}$
posterior	$[\![P]\!](E)$	$[\mathsf{lowerBd}_P^{\mathcal{T}}(E), \mathsf{upperBd}_P^{\mathcal{T}}(E)]$
	integral over $\mathbb{T}$	sum over partition $\mathcal{T} \subset \mathbb{T}_{\mathbb{I}}$

Interval trace semantics

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start = sample uniform(0,3)
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	standard	interval semantics
`start`	0.6	$[0.5, 0.6]$
`position`		
`distance`		
trace t	$\langle 0.6, 0.2, -0.8 \rangle$	$\langle [0.5, 0.6], [0.1, 0.2], [-0.9, -0.8] \rangle$
weight $\mathsf{wt}(t)$	1	$[1, 1]$
return value $\mathsf{val}(t)$		

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Bounding the posterior

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$$\mathrm{vol}(\langle [a_1, b_1], \ldots, [a_n, b_n] \rangle) := (b_1 - a_1) \times \cdots \times (b_n - a_n)$$

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Bounding the posterior

$$
\begin{aligned}
&\mathsf{lowerBd}_P^{\mathcal{T}}(I) \\
&:= \sum_{\boldsymbol{t}_{\mathbb{I}} \in \mathcal{T}} \mathrm{vol}(\boldsymbol{t}_{\mathbb{I}}) \cdot (\min \mathsf{wt}_P^{\mathbb{I}}(\boldsymbol{t}_{\mathbb{I}})) \cdot [\mathsf{val}_P^{\mathbb{I}}(\boldsymbol{t}_{\mathbb{I}}) \subseteq I] \\
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&=: \mathsf{upperBd}_P^{\mathcal{T}}(I)
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Soundness

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Completeness

For all intervals I and $\epsilon > 0$, there is a countable set $\mathcal{T} \subseteq \mathbb{T}_{\mathbb{I}}$ s.t.

$$\text{upperBd}_P^{\mathcal{T}}(I) - \epsilon \le [\![P]\!](I) \le \text{lowerBd}_P^{\mathcal{T}}(I) + \epsilon$$

under the assumptions:

- the primitive functions are continuous*
- each **`sample`**d value is used at most once in each condition, **`observe`** statement, and in the return value.

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For all intervals I and $\epsilon > 0$, there is a finite set $\mathcal{T} \subseteq \mathbb{T}_{\mathbb{I}}$ s.t.

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Method 2: Interval type system

$\rightarrow$ to overapproximate recursion and conditionals (not resolvable by intervals)

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- types keep track of the value and weight interval
- $\vdash P : \begin{Bmatrix} [v, v'] \\ [w, w'] \end{Bmatrix}$ means $\mathsf{val}_P(\boldsymbol{t}) \in [v, v']$ and $\mathsf{wt}_P(\boldsymbol{t}) \in [w, w']$.
- efficient type inference
- uses interval arithmetic & widening to approximate fixpoints

Method 3: Symbolic execution

$\rightarrow$ optimization for a common special case

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For each program path,

- α_k: the k-th **`sample`**
- $\mathcal{V}$: result value, e.g. $\alpha_1 + 2\alpha_2$
- Δ: guards, e.g. $\{\alpha_1 \leq 0, \alpha_1 + \alpha_2 > 1\}$
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$$[\![P]\!](I) = \sum_{\text{paths}} \int_{\Delta \cup \{\mathcal{V} \in I\}} \left(\prod \Xi\right) \mathrm{d}\alpha$$

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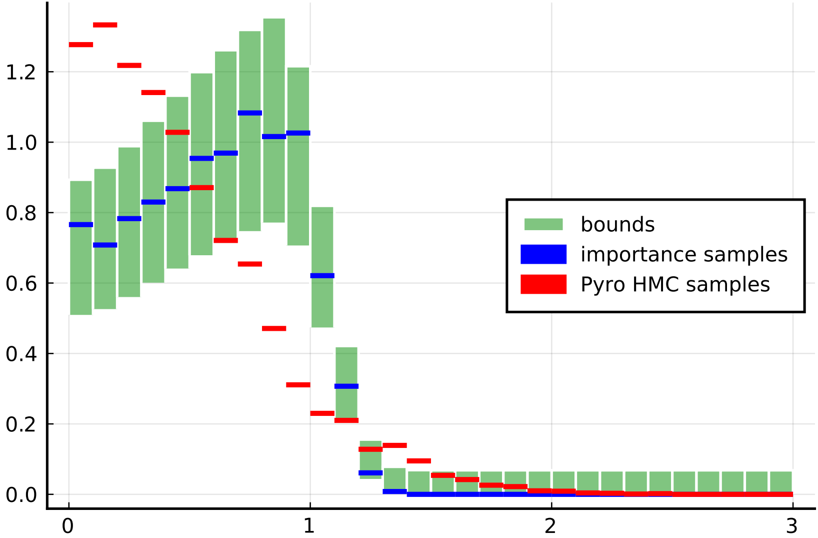
If Δ and $\mathcal{V}$ are affine then use

- polytope volume computation ($\rightarrow$ Vinci tool)
- linear optimization & interval arithmetic

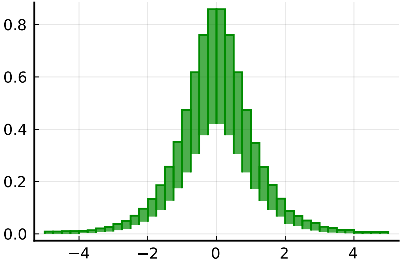
Empirical evaluation

Empirical evaluation

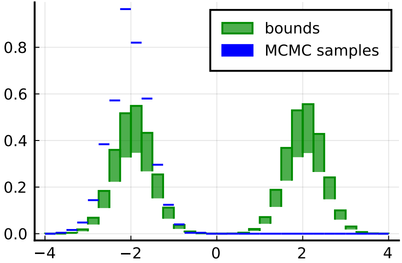


(time: 50 minutes)

Examples that are hard for MCMC



(a) Neal's funnel (5 seconds)



(b) Binary Gaussian mixture model (90 seconds)

Comparison with previous work

Sankaranarayanan et al. (PLDI13)

- bounding probabilities (but no `observe`)
- ours is usually slower, but often better bounds

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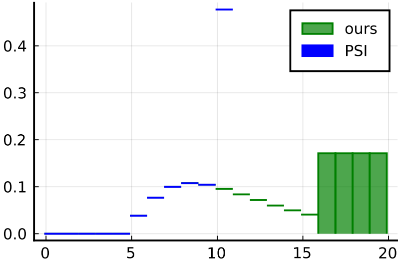
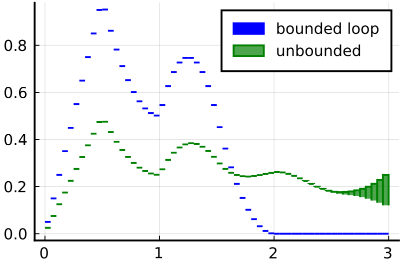
PSI solver

- consistency check: benchmarks from the PSI repository
- we can handle unbounded loops, contrary to PSI



(a) $\approx$ 2 minutes



(b) $\approx$ 20 seconds

Limitations

- lots of branching
- high-dimensional models (many `sample`s)

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Future work

- better heuristics for finding a "good" $\mathcal{T}$
- can this be refined into an approximate inference algorithm?

Rigorous Bounds on the Posterior: posterior$(E) \in [a, b]$

…for a universal PPL with continuous distributions and conditioning (`observe`)

Why?

- construct ground truth
- debug approximate inference

How?

1. interval trace semantics
2. interval type system
3. symbolic execution

Backup slides

Trace partitioning heuristics

Option 1: split equidistantly in each dimension

Option 2:

- start with the full interval trace $\langle[-\infty, \infty], \dots\rangle$
- pick the next interval $\boldsymbol{t}_{\mathbb{I}}$ trace or, depending on the input program, select it with a mix of the following criteria
  - high weight $\mathsf{wt}^{\mathbb{I}}_{P}(\boldsymbol{t}_{\mathbb{I}})$
  - wide value interval $\mathsf{val}^{\mathbb{I}}_{P}(\boldsymbol{t}_{\mathbb{I}})$
  - large volume $\mathrm{vol}(\boldsymbol{t}_{\mathbb{I}})$
- split that box in half along the dimension that reduces the width of the interval of the posterior expected value the most
- repeat.

Interval type system

Types:

- unweighted: $\sigma ::= [v, v'] \mid \sigma \to \mathcal{A}$
- weighted: $\mathcal{A} ::= \left\{ \begin{matrix} \sigma \\ [w, w'] \end{matrix} \right\}$

Selected typing rules:

$$\frac{\Gamma; \varphi : \sigma \to \mathcal{A}; x : \sigma \vdash M : \mathcal{A}}{\Gamma \vdash \mu_x^{\varphi}.M : \left\{ \begin{matrix} \sigma \to \mathcal{A} \\ [1, 1] \end{matrix} \right\}}$$

$$\frac{\Gamma \vdash M : \left\{ \begin{matrix} \sigma_1 \to \left\{ \begin{matrix} \sigma_2 \\ [e, f] \end{matrix} \right\} \\ [a, b] \end{matrix} \right\} \quad \Gamma \vdash N : \left\{ \begin{matrix} \sigma_1 \\ [c, d] \end{matrix} \right\}}{\Gamma \vdash MN : \left\{ \begin{matrix} \sigma_2 \\ [a, b] \times^{\mathbb{I}} [c, d] \times^{\mathbb{I}} [e, f] \end{matrix} \right\}}$$