Guaranteed Bounds for Posterior Inference in Universal Probabilistic Programming

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(Joint work with Raven Beutner and Fabian Zaiser)

What is (Bayesian Statistical) Probabilistic Programming?

Bayes' Rule

$$\mathbb{P}[\theta \mid \mathcal{D}] = \frac{\mathbb{P}[\mathcal{D} \mid \theta] \mathbb{P}[\theta]}{\mathbb{P}[\mathcal{D}]}$$
Posterior \propto Likelihood × Prior



Thomas Bayes (1701-1761)

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Probabilistic Programming

- a general-purpose means of expressing probabilistic models as programs, and automatically performing Bayesian inference.

- Probabilistic programming offers an elegant way of generalising graphical models, allowing a much richer representation of models, compositionally.
- Probabilistic programming systems are equipped with implementations of general-purpose inference algorithms.

Vision of Probabilistic Programming

- Expressing probabilistic models as programs: elegant, unifying, potentially benefiting from PL research (semantics and program analysis).
- Availability of general-purpose Bayesian inference engines for arbitrary programs of a universal PPL promotes democratic access to ML algorithms.

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What is the Reality?

Unfortunately existing inference algorithms

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 angle have few guarantees on the result, and / or
- only work on a restricted class of programs (models).



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Our Contributions

Guaranteed (nonstochastic and sound) bounds on the posterior distributions.

- ✓ Diagnostics / (partial) correctness specification: can identify errors in inference results
- ✓ General applicability: works for a very broad class of probabilistic programs
- ✓ Basis for a new general-purpose inference algorithm (ongoing work).





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return start
Posterior distribution: p(start | observation)?
```

Existing Inference Methods

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- 1. Approximate methods: posterior $\approx X$
- Monte Carlo (particle filter; Metropolis-Hastings, Gibbs sampling, HMC, etc.): "Through the use of random processes, Metropolis algorithm [Monte Carlo method] offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly." (IEEE Computing award citation)
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2. Exact methods: posterior = X

- Computing a closed-form solution of the posterior inference problem using computer algebra and other forms of symbolic calculations.



Issues with Existing Methods

- exact methods: only work on restricted models (e.g. loop free)
- > approximate methods: implicit assumptions, slow convergence

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A (Real) Conundrum: Pedestrian Example



The two distributions are clearly different: at least one is wrong, but which? (This problem actually sparked and drove the present project.)

Desiderata

- A middle ground between exact and approximate methods.
- ► Given arbitrary program P of a universal PPL with continuous distributions and observe, and error tolerance, infer guaranteed (nonstochastic and sound) bounds of the posterior: a ≤ posterior_P(E) ≤ b

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- Construct (useful aspects of) ground truth for inference problems.
- Debug (implementations of) approximate inference algorithms.

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- 2. constraint-based interval type system: over-approximation of recursive terms
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- value function: val(s) for trace s
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Unnormalized posterior of E (joint distribution of latent and observed variables):

$$\llbracket P \rrbracket(E) := \int_{\{\boldsymbol{s} | \mathsf{val}(\boldsymbol{s}) \in E\}} \mathsf{weight}(\boldsymbol{s}) \, \mathrm{d}\boldsymbol{s} = ``\mathbb{P}(\texttt{start} \in E, \mathsf{obs})'$$

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By Bayes' rule, normalized posterior (conditional probability):

$$\mathbb{P}(\texttt{start} \in E \mid \texttt{obs}) = \frac{\mathbb{P}(\texttt{start} \in E, \texttt{obs})}{\mathbb{P}(\texttt{obs})} = \frac{\llbracket P \rrbracket(E)}{\llbracket P \rrbracket(\mathbb{R})}$$

N.B. Normalising constant, $\mathbb{P}(obs)$, is a special case of unnormalised posterior.

Want to derive bounds of $[\![P]\!](E) \mathrel{\mathop:}= \int_{\{\boldsymbol{s} | \mathsf{val}(\boldsymbol{s}) \in E\}} \mathsf{weight}(\boldsymbol{s}) \, \mathrm{d} \boldsymbol{s}.$

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An interval trace is just a sequence of intervals of the reals; e.g. $\langle [0.1, 0.3], [0.7, 1] \rangle$.

So a set of interval traces summarises a set of traces. E.g. interval trace $\langle [0.1, 0.3], [0.7, 1] \rangle$ contains (or is refined by) traces $\langle 0.2, 0.9 \rangle$ and $\langle 0.23, 0.75 \rangle$.

Idea behind upper bounding $\llbracket P \rrbracket(E)$:

Given event E, find a summary (i.e. covering set) T of interval traces: every s s.t. val(s) ∈ E is contained in some interval trace in T.

Want to derive bounds of $\llbracket P \rrbracket(E) := \int_{\{s | val(s) \in E\}} weight(s) ds.$

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Idea behind upper bounding [[P]](E):
Given event E, find a summary (i.e. covering set) T of interval traces: every s s.t. val(s) ∈ E is contained in some interval trace in T.
Then
[[P]](E) ≤ ∑(max weight(t)) vol(t)

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position = start; distance = 0
while position > 0:
    step = sample uniform(-1, 1)
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    distance += abs(step)
observe 1.1 from normal(distance, 0.1<sup>2</sup>)
return start
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	standard	interval semantics
start		
position		
distance		
trace s	$\langle 0.6,0.2,-0.8 angle$	$\langle [0.5, 0.6], [0.1, 0.2], [-0.9, -0.8] \rangle$
$\mathbf{weight} \ weight(s)$	1	[1, 1]
return value $val(s)$		

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position	0.6	[0.5, 0.6]
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start	0.6	[0.5, 0.6]
position	0.8	[0.6, 0.8]
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$\textbf{weight} \hspace{0.1 cm} \texttt{weight}(\boldsymbol{s})$	≈ 2.4	[0.53, 3.99]
return value $val(s)$	0.6	[0.5, 0.6]

Soundness

For all non-overlapping and exhaustive set of interval traces \mathcal{T} :

 $\mathsf{lowerBd}_P^{\mathcal{T}} \leq [\![P]\!] \leq \mathsf{upperBd}_P^{\mathcal{T}}.$

lowerBd $_P^{\mathcal{T}}$ and upperBd $_P^{\mathcal{T}}$ are super-/sub-additive measures.

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Completeness

For all intervals I and $\epsilon > 0$, there is a countable set \mathcal{T} of (non-overlapping and exhaustive) interval traces s.t.

$$\mathsf{upperBd}_P^{\mathcal{T}}(I) - \epsilon \leq \llbracket P \rrbracket(I) \leq \mathsf{lowerBd}_P^{\mathcal{T}}(I) + \epsilon$$

under the assumptions:

- the primitive functions are continuous*
- each sampled value is used at most once in each conditional, observe statement, and in the return value.

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Empirical Evaluation

Implementation: GuBPI (Guaranteed Bounds for Posterior inference) gubpi-tool.github.io

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Examples that Trip Up MCMC!



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- framework for bounding probabilities of events definable by score-free programs
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PSI solver (CAV2016)

- consistency check: benchmarks from the PSI repository
- we can handle unbounded loops, contrary to PSI. Warning: Artificially bounding recursive programs can yield different (hence wrong) posterior distribution!



Also in our PLDI22 paper¹

- Constraint-based interval type system: approximates unbounded loops and recursion soundly
- **Symbolic execution & linear programming:** optimization for linear guards
- Comparison with statistical validation methods: simulation-based calibration

¹Raven Beutner, C.-H. Luke Ong, Fabian Zaiser: Guaranteed bounds for posterior inference in universal probabilistic programming. PLDI 2022: 536-551

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Limitations: GuBPi struggles if

- program has lots of branching: path explosion problem
- model is high-dimensional (i.e. has many samples)

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Guaranteed Bounds for Posterior Inference in Universal Probabilistic Programming



... are a **middle ground** between *approximate* and *exact*:

- guaranteed correct (vs. approximate inference)
- supports many language features (vs. exact inference)

Theory: soundness & completeness

Practice:

- detect issues with inference results
- competitive on existing benchmarks
- guaranteed partial correctness specifications for programs that other tools cannot handle

Future work

- \blacktriangleright better heuristics for finding a "good" set of interval traces ${\cal T}$
- basis for a new approximate inference algorithm.