Amortized Rejection Sampling in Universal Probabilistic Programming

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TL;DR

- Rejection sampling is widely used in implementing complex generative models.
- Inference in probabilistic programs including unbounded loops (e.g. rejection sampling) is hard.
- We address the problem of efficient amortized importance-sampling-based inference, in particular Inference Compilation (IC) [4], in such models.
- We show naive application of IC can produce importance weights with unbounded variance.
- We propose Amortized Rejection Sampling (ARS), an importance sampling procedure that produces finite variance weights and unbiased expectations for programs that include rejection sampling loops.
- We implement ARS in pyprob [1; 2] in a way that requires minimal modifications to user code.

(a) Original program

$x \sim p(x)$
for $k \in \mathbb{N}^+$ **do**
  $\boldsymbol{z}^k \sim p(\boldsymbol{z}|x)$
  if $c(x, \boldsymbol{z}^k)$ **then**
    $\boldsymbol{z} = \boldsymbol{z}^k$
    break
observe$(y, p(y|\boldsymbol{z}, x))$

(b) Inference compilation

$x \sim q(x|y)$
$w \leftarrow \frac{p(x)}{q(x|y)}$
for $k \in \mathbb{N}^+$ **do**
  $\boldsymbol{z}^k \sim q(\boldsymbol{z}|x, y)$
  $w^k \leftarrow \frac{p(\boldsymbol{z}^k|x)}{q(\boldsymbol{z}^k|x,y)}$
  $w \leftarrow w\, w^k$
  if $c(x, \boldsymbol{z}^k)$ **then**
    $\boldsymbol{z} = \boldsymbol{z}^k$
    break
$w_{IC} \leftarrow wp(y|\boldsymbol{z}, x)$

(c) Equivalent to above

$x \sim p(x)$
$\boldsymbol{z} \sim p(\boldsymbol{z}|x, c(x, z))$
observe$(y, p(y|\boldsymbol{z}, x))$

(d) ARS

$x \sim q(x|y)$
$w \leftarrow \frac{p(x)}{q(x|y)}$
$\boldsymbol{z} \sim q(\boldsymbol{z}|x, y, c(x, z))$
$w \leftarrow w\, \frac{p(\boldsymbol{z}|x,c(x,z))}{q(\boldsymbol{z}|x,y,c(x,z))}$
$w_C \leftarrow w\, p(y|\boldsymbol{z}, x)$

IC weights

$$w_{IC} = \frac{p(x)}{q(x|y)} p(y|x, z) \Pi_{k=1}^{L} w^k$$

Theorem: Under some mild conditions if the following holds then the variance of w_{IC} is infinite.

$$\mathbb{E}_{\boldsymbol{z} \sim q(\boldsymbol{z}|x,y)} \left[\frac{p(\boldsymbol{z}|x)^2}{q(\boldsymbol{z}|x, y)^2} (1 - p(A|x, \boldsymbol{z})) \right] \geq 1$$

where A is the event of $c(x, \boldsymbol{z})$ being satisfied.

Collapsed weights

$$w_C = \frac{p(x)}{q(x|y)} \frac{p(\boldsymbol{z}|x, A)}{q(\boldsymbol{z}|x, y, A)} p(y|x, \boldsymbol{z})$$

- $\mathbb{E}[w_{IC}] = \mathbb{E}[w_C]$ but these weights do not cause infinite variance importance sampling estimates.
- Unfortunately, we cannot directly compute w_C

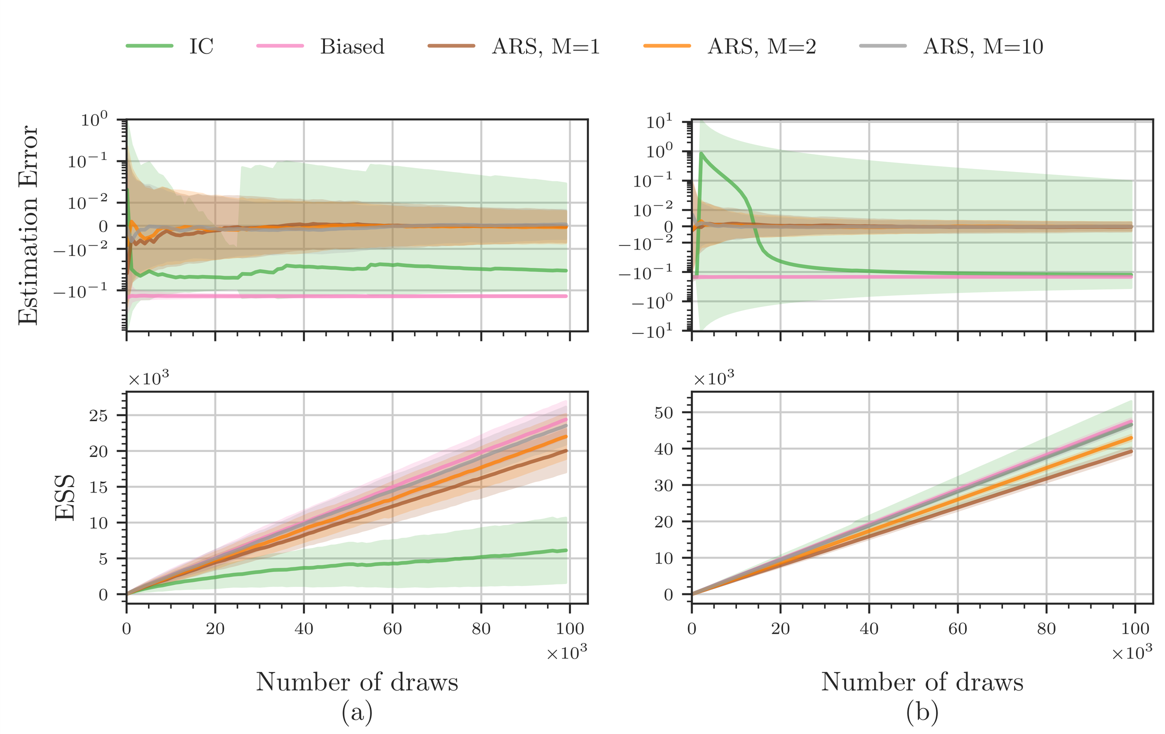
Amortized Rejection Sampling (ARS)

$$w_C = \frac{p(x)}{q(x|y)} \frac{p(\boldsymbol{z}|x)}{q(\boldsymbol{z}|x, y)} p(y|x, \boldsymbol{z}) \frac{q(A|x, y)}{p(A|x)}$$

- $q(A|x, y)$ is the probability of exiting the rejection sampling loop under the proposal.
- $p(A|x)$ is the probability of exiting the rejection sampling loop in the original probabilistic program.
- We use Monte Carlo to get unbiased estimates of $q(A|x, y)$ and $\frac{1}{p(A|x)}$.

Marsaglia [5; 6]

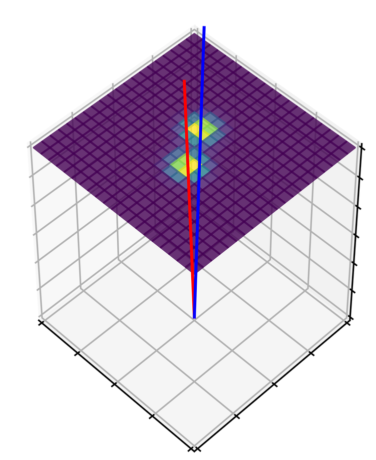
for $k \in \mathbb{N}^+$ **do**
  $a_k \sim \text{Uniform}(-1, 1)$
  $b_k \sim \text{Uniform}(-1, 1)$
  $s = a_k^2 + b_k^2$
  if $s < 1$ **then**
    $a = a_k$
    $b = b_k$
    break
$\mu = a\sqrt{\frac{-2\log(s)}{s}}$
observe$(y_1, \mathcal{N}(\mu, \sigma^2))$
observe$(y_2, \mathcal{N}(\mu, \sigma^2))$

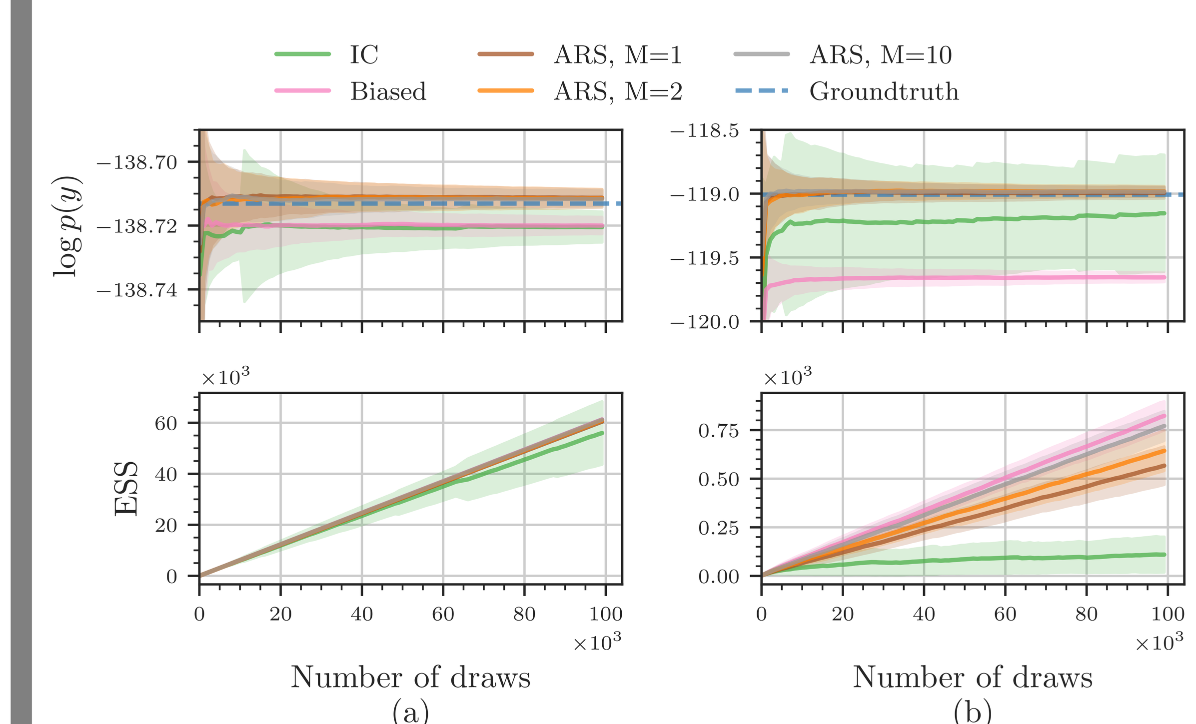


(a) $y_1 = y_2 = 0$ (b) $y_1 = y_2 = -1$

Mini-SHERPA

Mini-SHERPA is a simplified model of high-energy reactions of particles [3]. It uses rejection sampling extensively to simulate a particle decay event and the energy deposited by the resulting particles in a simplified detector.





Algorithm

$x \sim q(x|y)$
$w \leftarrow \frac{p(x)}{q(x|y)}$
for $k \in \mathbb{N}^+$ **do**
  $\boldsymbol{z}^k \sim q(\boldsymbol{z}|x, y)$
  if $c(x, \boldsymbol{z}^k)$ **then**
    $\boldsymbol{z} = \boldsymbol{z}^k$
    break
$w \leftarrow w\, \frac{p(\boldsymbol{z}|x)}{q(\boldsymbol{z}|x,y)}$
$K \leftarrow 0$
for $i \in 1, \dots N$ **do**
  $\boldsymbol{z}'_i \leftarrow q(\boldsymbol{z}|x, y)$
  $K \leftarrow K + c(\boldsymbol{z}, x)$
for $j \in 1, \dots M$ **do**
  for $l \in \mathbb{N}^+$ **do**
    $\boldsymbol{z}''_{j,l} \leftarrow q(\boldsymbol{z}|x, y)$
    if $c(x, \boldsymbol{z}''_{j,l})$ **then**
      $T_j \leftarrow l$
      break
$T \leftarrow \frac{1}{M} \Sigma_{j=1}^{M} T_j$
$w \leftarrow w\, \frac{KT}{N}$
$w \leftarrow w\, p(y|\boldsymbol{z}, x)$

Implementation

We introduce two new functions to tag the beginning and end of rejection sampling loops.

Original

```
x = sample(P_x)
while True:

    z = sample(P_z(x))
    if c(x, z):

        break
observe(P_y(x,z), y)
return x, z
```

Annotated

```
x = sample(P_x)
while True:
    rs_start()
    z = sample(P_z(x))
    if c(x, z):
        rs_end()
        break
observe(P_y(x,z), y)
return x, z
```

References

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