Quantifying the probable approximation error of probabilistic inference programs

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Abstract

This paper introduces a new technique for quantifying the approximation error of a broad class of probabilistic inference programs, including ones based on both variational and Monte Carlo approaches. The key idea is to derive a subjective bound on the symmetrized KL divergence between the distribution achieved by an approximate inference program and its true target distribution. The bound’s validity (and subjectivity) rests on the accuracy of two auxiliary probabilistic programs: (i) a “reference” inference program that defines a gold standard of accuracy and (ii) a “meta-inference” program that answers the question “what internal random choices did the original approximate inference program probably make given that it produced a particular result?” The paper includes empirical results on inference problems drawn from linear regression, Dirichlet process mixture modeling, HMMs, and Bayesian networks. The experiments show that the technique is robust to the quality of the reference inference program and that it can detect implementation bugs that are not apparent from predictive performance.

1 Introduction

A key challenge for practitioners of probabilistic modeling is the approximation error introduced by variational and Monte Carlo inference techniques. The Kullback-Leibler (KL) divergence [6] between the result of approximate inference — i.e. the variational approximation, or the distribution induced by one run of the sampler — and the true target distribution is typically unknown. Predictive performance on a held-out test set is sometimes used as a proxy, but this need not track posterior convergence.

This paper introduces a new technique for quantifying the approximation error of a broad class of probabilistic inference programs, including variational and Monte Carlo approaches. The key idea is to derive a “subjective” bound on the symmetrized KL divergence between the distribution achieved by an approximate inference program and its true target distribution. The bound’s validity (and subjectivity) rests on beliefs about the accuracy of auxiliary probabilistic program(s). The first is a “reference” inference program that defines a gold standard of accuracy but that might be difficult to compute. When the original approximate inference program has a tractable output probability density, this is sufficient. If the output density of the approximate inference program is not available, then the technique also depends on the accuracy of a “meta-inference” program that answers the question “what internal random choices did the approximate inference program of interest probably make, assuming that it produced a particular result that was actually produced by the reference?” In Section 3.3 we relate this technique to some recent work.

The technique is implemented as a probabilistic meta-program for the Venture probabilistic programming platform [12], written in the VentureScript language. The paper includes empirical results on inference problems drawn from linear regression, Dirichlet process mixture modeling, HMMs, and Bayesian networks. The experiments show that the technique is robust to the quality of the reference inference program and that it can detect implementation bugs that are not apparent from predictive performance.
Figure 1: Estimating subjective divergences for probabilistic inference programs. (a) relates subjective divergence and Kullback-Leibler (KL) divergence. (b) and (c) show estimated subjective divergence profiles for sampling-based and optimization-based inference respectively on a small Bayesian linear regression problem using an oracle reference program (vertical error bars show bootstrap 90% confidence intervals, horizontal error bars show interquartile ranges, and \( N = M = 500 \) runs were used for each point). (d) shows a model program implemented in VentureScript, and (e), (f), and (g) show VentureScript programs used to estimate subjective divergences for a sampling importance resampling (LW-SIR) inference program. (h) shows a schematic of the probabilistic programs and process used in Algorithm 1 to estimate subjective divergence.
2 Estimating subjective divergences

Kullback-Leibler (KL) divergences between an inference program’s approximating distribution and
its target distribution are objective model-independent measures of the approximation error. How-
ever, tractable techniques for estimating KL divergences for approximate inference are lacking. This
paper defines a quantity, subjective divergence, in terms of the following elements:

1. Model program $z, x \sim p(z, x)$: Samples latent variables $z \sim p(z)$ and data $x | z \sim p(x | z)$ for
probabilistic model $p(z, x)$.

2. Data $x^*$: A specific dataset which induces the posterior distribution $p(z | x^*)$.

3. Approximate inference program $y, z \sim q(y, z; x^*)$: Samples output $z$ from $q(z; x^*)$, which approxi-
imates $p(z; x^*)$, and also returns the history $y$ of the inference program execution that generated
$z$. An approximate inference program induces a weight function $w(z) := p(z; x^*) / q(z; x^*)$.

4. Reference inference program $z \sim r(z; x^*)$: A gold standard sampler that approximates the post-
erior $p(z | x^*)$. If the reference inference program $r(z; x^*)$ is exact, so that $r(z; x^*) = p(z | x^*)$ for
all $z$, or equivalently $D_{KL}(r(z; x^*) || p(z; x^*)) = 0$, we call it an oracle.

5. Inference output marginal density estimators $\hat{q}_{\text{IS}}(z; x^*)$ and $\hat{q}_{\text{HM}}(z; x^*)$: Estimators of marginal
density $q(z; x^*) = \int q(y; z; x^*) dy$ for inference program output $z$ such that $E[\hat{q}_{\text{IS}}(z; x^*)] =
q(z; x^*)$ and $E[1/\hat{q}_{\text{HM}}(z; x^*)] = 1/q(z; x^*)$ for all $z$ and $x^*$. $\hat{q}_{\text{IS}}(z; x^*)$ and $\hat{q}_{\text{HM}}(z; x^*)$ denote
random variables. A realized estimate of $q(z; x^*)$ induces a realized weight estimate. In all
cases, expectations without a subscript are with respect to $\hat{q}_{\text{IS}}(z; x^*)$ or $\hat{q}_{\text{HM}}(z; x^*)$.

Definition 1 (Subjective Divergence).

$$D_{\text{SBJ}}(q(z; x^*) || p(z; x^*)) := E_{z \sim r(z; x^*)} \left[ E \left[ \log \frac{p(z; x^*)}{\hat{q}_{\text{IS}}(z; x^*)} \right] \right] - E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z; x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right]$$

Proposition 1. If an oracle reference program is used (where $r(z; x^*) = p(z; x^*)$ for all $z$), then
$D_{\text{SBJ}}(q(z; x^*) || p(z; x^*)) \geq D_{\text{KL}}(q(z; x^*) || p(z; x^*)) + D_{\text{KL}}(p(z; x^*) || q(z; x^*))$

This proposition is proven in Section 3. To construct inference output marginal density estima-
tors $\hat{q}_{\text{IS}}(z; x^*)$ and $\hat{q}_{\text{HM}}(z; x^*)$, we make use of a meta-inference program $y \sim m(y; z, x^*)$, which
samples inference program execution history $y$ from an approximation to the condi-
tional distribution $q(y; z; x^*)$ given inference program output $z$, such that the ratio of densities
$q(y; z, x^*) / m(y; z, x^*)$ can be efficiently computed given $y, z$, and $x^*$. The baseline $\hat{q}_{\text{IS}}(z; x^*)$ esti-
mator samples $y \sim m(y; z, x^*)$ and produces a single sample importance sampling estimate:
$q(y; z, x^*) / m(y; z, x^*)$. The baseline $\hat{q}_{\text{HM}}(z; x^*)$ estimator obtains $y \sim q(y; z, x^*)$ from the his-
tory of the inference program execution that generated $z$, and produces a single sample harmonic mean
estimate: $q(y; z, x^*) / m(y; z, x^*)$. A procedure for estimating subjective divergence using these
baseline meta-inference based estimators is shown in Algorithm 1.

Algorithm 1 Subjective divergence estimation for general inference programs

Require: Elements 1–4, meta-inference program $y \sim m(y; z, x^*)$, number of reference replicates
$N$, number of inference replicates $M$

1: for $i \leftarrow 1$ to $N$ do
2: $z_i^* \sim r(z; x^*)$ \hspace{1cm} \text{\triangleright} N$ independent replicates using reference inference program $r(z; x^*)$
3: $y_i^* \sim m(y; z_i^*, x^*)$ \hspace{1cm} \text{\triangleright} Plausible inference program execution history producing $z_i^*$
4: $\hat{q}_i^* \leftarrow q(y_i^*; z_i^*, x^*) \ \ m(y_i^*; z_i^*, x^*)$ \hspace{1cm} \text{\triangleright} Estimate of marginal output density $q(z_i^*; x^*)$
5: $\hat{w}_i^* \leftarrow \frac{p(z_i^*; x^*)}{\hat{q}_i^*}$ \hspace{1cm} \text{\triangleright} Estimate of weight
6: end for

7: for $j \leftarrow 1$ to $M$ do
8: $y_j^* \sim q(y_i^*; z_i^*, x^*)$ \hspace{1cm} \text{\triangleright} $M$ independent replicates using inference program $q(z; x^*)$
9: $\hat{q}_j^* \leftarrow \frac{q(y_j^*; z_j^*, x^*)}{m(y_j^*; z_j^*, x^*)}$ \hspace{1cm} \text{\triangleright} Output $z_j^*$ and execution history $y_j^*$ from inference program
10: $\hat{w}_j^* \leftarrow \frac{p(z_j^*; x^*)}{\hat{q}_j^*}$ \hspace{1cm} \text{\triangleright} Estimate of weight
11: end for
12: return $\frac{1}{N} \sum_{i=1}^{N} \log \hat{w}_i^* - \frac{1}{M} \sum_{j=1}^{M} \log \hat{w}_j^*$
Figure 2: Raw log estimated weight data (a) and timing data (b) for individual runs of the VentureScript implementation of Algorithm 1 on a black box variational inference program. Weights are colored by the source of z (inference or reference program), and timing data is broken down into stages of the estimation procedure. (c) shows a schematic illustration of the relationship between key KL divergences and subjective divergence estimated by Algorithm 1 in the case when the reference program is an exact inference oracle.

We have produced a VentureScript inference programming library that implements Algorithm 1. In our applications, the weight estimate computation can be performed incrementally within the inference program and meta-inference program, obviating the need for an explicit representation of inference program execution history and the separate weight computation illustrated in Figure 1. The subjective divergence is based on estimating the symmetrized KL divergence in order to handle the fact that the posterior density is only available in unnormalized form (the symmetrized KL can be expressed purely in terms of unnormalized densities). We use a reference sampler as a proxy for a posterior sampler (accepting subjectivity) to address the challenge of Monte Carlo estimation with respect to the posterior \( p(z|x^*) \) for the term \( \text{DKL}(p(z|x^*)||q(z|x^*)) \) in the symmetrized KL. For inference programs with an output density \( q(z;x^*) \) that can be computed efficiently, such as mean-field variational families, the weight estimate in Algorithm 1 can be replaced with the true weight \( p(z,x^*)/q(z|x^*) \), and the subjective divergence is equivalent to the symmetrized KL divergence when an oracle reference is used. For inference programs with a large number of internal random choices \( y \), the densities on outputs \( q(z;x^*) \) are intractable to compute, and Algorithm 1 uses meta-inference to construct marginal density estimators \( \hat{q}_S(z;x^*) \) and \( \hat{q}_{HM}(z;x^*) \) such that Proposition 1 holds. Subjective divergence can be interpreted as approximately comparing samples from the inference program of interest to gold standard samples through the lens of the log-weight function \( \log w(\cdot) \).

3 Analyzing subjective divergences

Having defined subjective divergence and a procedure for estimating it, we now prove Prop. 1 using bounds on the expected log estimated weight taken under the inference program of interest \( E_{z \sim q(z|x^*)} [\log p(z,x^*)/\hat{q}_{HM}(z;x^*)] \) and the expected log estimated weight taken under the reference program \( E_{z \sim p(z|x^*)} [\log p(z,x^*)/\hat{q}_{IS}(z;x^*)] \). The expectation under the inference program of interest is less than the log normalizing constant \( \log p(x^*) \) by at least \( \text{DKL}(q(z;x^*)||p(z|x^*)) \):

**Lemma 1.** \( E_{z \sim q(z|x^*)} [\log p(z,x^*)/\hat{q}_{HM}(z;x^*)] \leq \log p(x^*) - \text{DKL}(q(z;x^*)||p(z|x^*)) \)

(derivation based on Jensen’s inequality in Appendix C). Note that this constitutes a lower bound on the “ELBO” variational objective. The expectation under an oracle reference program is greater
than the log normalizing constant by at least $D_{\text{KL}}(p(z|x^*)||q(z;x^*))$:

Lemma 2. $E_{z \sim p(z|x^*)} \left[ \log \frac{p(z;x^*)}{q(z;x^*)} \right] \geq \log p(x^*) + D_{\text{KL}}(p(z|x^*)||q(z;x^*))$

(derivation based on Jensen’s inequality in Appendix C). The subjective divergence is the difference between the expectation under the reference program (bounded in Lemma 2) and the expectation under the inference program of interest (bounded in Lemma 3). Taking the difference of the bounds cancels the log $p(x^*)$ terms and proves Proposition 1. Relationships between key quantities in the proof are illustrated in Figure 2. By Proposition 1 if an oracle reference program is available, we can estimate an upper bound on the symmetrized KL divergence by estimating a subjective divergence.

### 3.1 Effect of quality of reference inference program

If the reference inference program $r(z;x^*)$ is not an oracle, it is still possible to retain the validity of subjective divergence as an upper bound, depending on the accuracy of the reference program:

Proposition 2. If $D_{\text{KL}}(r(z;x^*)|p(z|x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*)) - D_{\text{KL}}(p(z|x^*)||q(z;x^*))$ then $D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq D_{\text{KL}}(q(z;x^*)||p(z|x^*)) + D_{\text{KL}}(p(z|x^*)||q(z;x^*))$

Proposition 3. If $D_{\text{KL}}(r(z;x^*)|p(z|x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*))$ then

$$E_{z \sim r(z;x^*)} \left[ \log \frac{p(z;x^*)}{q(z;x^*)} \right] \geq \log p(x^*)$$

$$D_{\text{SBJ}}(q(z;x^*)|p(z|x^*)) \geq D_{\text{KL}}(q(z;x^*)||p(z|x^*))$$

(derivations in Appendix C). When the density $q(z;x^*)$ is available, we use $\hat{q}_{\text{BSJ}}(z;x^*) = \hat{q}_{\text{HM}}(z;x^*) = q(z;x^*)$, and $D_{\text{SBJ}}$ replaces the $D_{\text{KL}}(p(z|x^*)||q(z;x^*))$ term in the symmetrized KL divergence with $D_{\text{KL}}(r(z;x^*)|q(z;x^*)) = D_{\text{KL}}(r(z;x^*)|p(z|x^*))$. Figure 3 compares subjective divergence profiles obtained using oracle reference and approximate inference references of varying quality.

### 3.2 Effect of quality of meta-inference program

In the setting of an oracle reference program and the baseline marginal density estimators $\hat{q}_{\text{BSJ}}(z;x^*)$ and $\hat{q}_{\text{HM}}(z;x^*)$ used in Algorithm 1, the quality of the meta-inference $m(y;z,x^*)$ determines the tightness of the upper bound of Proposition 1. In particular, the gap between the true symmetrized KL divergence and the subjective divergence is the symmetrized conditional relative entropy $\delta$

(derivation in Appendix D)

$$E_{z \sim \hat{q}(z|x^*)} \left[ D_{\text{KL}}(q(y;z,x^*)|m(y;z,x^*)) \right] + E_{z \sim p(z|x^*)} \left[ D_{\text{KL}}(m(y;z,x^*)||q(y;z,x^*)) \right]$$

which measures how closely the meta-inference approximates $q(y;z,x^*)$, the conditional distribution on inference execution histories given inference output $z$. Note that if we had exact meta-inference and could compute its density, the weight estimate simplifies to $w(z) := p(z,x^*)/q(z,x^*)$, and
we could remove this gap. More generally, the gap is due to the biases of the estimators for \( \log q(z; x^*) \) that are induced by taking the \( \log(\cdot) \) of the estimates of \( q(z; x^*) \) produced by \( \hat{q}_{BS}(z; x^*) \) and \( \hat{q}_{HM}(z; x^*) \), which are related to the variances of \( \hat{q}_{BS}(z; x^*) \) and \( 1/\hat{q}_{HM}(z; x^*) \). For example, compare the variance of the baseline \( \hat{q}_{BS}(z; x^*) \) with the bias of the induced estimator of \( \log q(z; x^*) \):

\[
\text{Var} \left( \frac{\hat{q}_{BS}(z; x^*)}{q(z; x^*)} \right) = E \left[ \left( \frac{\hat{q}_{BS}(z; x^*)}{q(z; x^*)} \right)^2 - 1 \right] = \chi^2_P(m(y; z, x^*)|q(y|z; x^*)) \tag{2}
\]

\[
\log q(z; x^*) - E[\log \hat{q}_{BS}(z; x^*)] = E[\log \frac{q(z; x^*)}{\hat{q}_{BS}(z; x^*)}] = D_{KL}(m(y; z, x^*)|q(y|z; x^*)) \tag{3}
\]

where \( \chi^2_P(m(y; z, x^*)|q(y|z; x^*)) \) is the Pearson chi-square divergence [10]. The bias of the estimator of \( \log q(z; x^*) \) manifests in the second term in Equation (3).

See Appendix 15 for details.

### 3.3 Related work

In [10] the authors point out that unbiased estimators like \( \hat{q}_{BS}(z; x^*) \) and unbiased reciprocal estimators like \( \hat{q}_{HM}(z; x^*) \) estimate lower and upper bounds of the log-estimand respectively, which they use to estimate lower and upper bounds on \( \log p(x^*) \). [10] also suggests combining stochastic upper bounds on \( \log p(x^*) \), obtained by running reversed versions of sequential Monte Carlo (SMC) algorithms starting with an exact sample obtained when simulating data \( x^* \) from the model, with lower bounds on the ELBO, to upper bound KL divergences. The authors of [21] introduce a general auxiliary variable formalism for estimating lower bounds on the ELBO of Markov chain inference, which is equivalent to estimation of our expected log estimated weight under the inference program for the baseline \( \hat{q}_{HM} \) estimator applied to Markov chains.

### 4 Applications

We used the VentureScript implementation of Algorithm 1 to estimate subjective divergence profiles for diverse approximate inference programs applied to several probabilistic models.

In addition to applying the technique to mean-field variational inference, where the output density \( q(z; x^*) \) is available, we derived meta-inference programs for two classes of inference programs whose density is generally intractable: sequential inference utilizing a Markov chain of detailed-balance transition operators and particle filtering in state space models. For sequential inference, we use a coarse-grained representation of the inference execution history that suppresses internal random choices made within segments of the Markov chain that satisfy detailed balance with respect to a single distribution. The meta-inference program is also sequential detailed-balance inference, but with the order of the transition operators reversed. This reversed Markov chain is an instance of the formalism of [21], was used to construct annealed importance sampling (AIS) [15], and was sampled from in [4] and [10]. The weight estimate corresponds to the AIS marginal likelihood estimate. The subjective divergence for standard non-sequential MCMC can be analyzed using this construction, but results in a trivial upper bound on the KL divergence due to the failure of the approximating assumptions used to derive the meta-inference program. For particle filtering in state space models, we use the conditional SMC (CSMC) update [2] and the weight estimate is the marginal likelihood estimate of the particle filter. It is intuitive that we use CSMC to answer “how might have a particle filter produced a given particle?” A special case of the particle filter is sampling importance resampling, for which the meta-inference program (shown in Figure 14) places the output sample \( z \) in one of \( K \) particles, and samples the remaining \( K - 1 \) particles from the prior. See Appendix 13 for derivations.

### 4.1 Linear regression

We first considered a small Bayesian linear regression problem, with unknown intercept and slope latent variables (model program shown in Figure 14), and generated subjective divergence profiles for sampling-based and variational inference programs (shown in Figure 15 and Figure 16) using an oracle reference. We estimated profiles for two black box mean-field [19] programs which differed in their choice of variational family—each family had a different fixed variance for the latents. We varied the number of iterations of stochastic gradient descent to generate the profiles, which exhibited distinct nonzero asymptotes. We also estimated profiles for two sequential inference

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1 Improving upon the baseline inference output marginal density estimators and reducing the gap between subjective divergence and symmetric KL divergence seems a promising direction for future work.
programs that consist of alternating between observing an additional data point $x^*_t$ and running a transition operator $k_t$ that targets the partial posterior $p(z|x^*_1:t)$ for $t = 1, \ldots, T$ with $T = 11$ data points. One program used repeated application of Metropolis-Hastings (MH) transitions with a resimulation (prior) proposal within each $k_t$ and the other used applications of a random-walk MH transition. We varied the number of applications within each $k_t$ of the primitive MH transition operator. The profile based on resimulation MH converged more rapidly. Finally, we produced a subjective divergence profile for a likelihood-weighting sampling importance resampling (LW-SIR) inference program by varying the number of particles. LW-SIR was the only algorithm applied to this problem whose subjective divergence profile converged to zero.²

### 4.2 Bayesian networks

We estimated subjective divergence profiles for approximate inference programs applied to a noisy-or Bayesian network (subset shown in Figure 4a). The network contained 25 latent causes, and 35 findings, with prior cause probabilities of 0.001, transmission probabilities of 0.9, and spontaneous finding activation probabilities of 0.001, with edges sampled uniformly with probability 0.7 of presence. All findings were active. We compared four sequential inference programs that all advanced through the same sequence of target distributions defined by gradually lowering the finding spontaneous activation probability from 0.99 to the true model value 0.001 across 10 equal-length steps, but applied distinct types of transition operators $k_t$ at each step. We compared the use of a single-site resimulation MH operator, a block resimulation MH operator, single-site Gibbs operator, and block Gibbs operator as primitive operators within each $k_t$ for $t = 1, \ldots, 10$, and varied the number of applications of each primitive operator within each $k_t$ to generate the profiles, shown in Figure 4c. For the reference program we used sequential inference with four applications of block Gibbs between each target distribution step. Inference for this problem is hard for single-site Gibbs operators due to explaining away effects, and hard for resimulation-based operators due to the low probability of the data under the prior. The resimulation MH based profiles exhibited much slower convergence than those of the Gibbs operators.

### 4.3 Hidden Markov models

We next applied the technique to a hidden Markov model (HMM) with discrete state and observation space (40 time steps, 2 hidden states, 3 observation states), and produced subjective divergence profiles for two particle filter inference programs with prior (forward simulation) and conditional proposals. Both particle filters used independent resampling. We used exact forward-filtering backwards sampling for the reference inference program. The profiles with respect to the number of particles are shown in Figure 4d. The conditional proposal profile exhibits faster convergence as expected. Note that for the single particle case there are no latent random choices $y$ in these the particle filters, and the subjective divergence is the symmetrized KL divergence.

²The profiles for the sequential detailed balance inference scheme converge to the sum of symmetrized KL divergences between consecutive partial posteriors $p(z), p(z|x^*_1), p(z|x^*_2), \ldots, p(z|x^*_T)$. See Appendix E.2 for details.
Applications of primitive operator per datum

Subjective Divergence

Seq. Inf. (k=Single-Site Resim. MH)
Seq. Inf. (k=Single-Site MH/Gibbs Cycle, Buggy)
Seq. Inf. (k=Single-Site MH/Gibbs Cycle, Fixed)

(a) Subjective divergence profiles (apparent bug: subjective divergence not improving)

Expected log likelihood

Seq. Inf. (k=Single-Site Resim. MH)
Seq. Inf. (k=Single-Site MH/Gibbs Cycle, Buggy)
Seq. Inf. (k=Single-Site MH/Gibbs Cycle, Fixed)

(b) Expected log likelihood profiles (no apparent bug: Gibbs/MH outperforms vanilla MH)

Figure 5: Comparing the effect of a bug in a MH transition operator implementation on subjective divergence profiles and on profiles of the expected log likelihood.

4.4 Detecting an ergodicity violation in samplers for Dirichlet process mixture modeling

We estimated subjective divergence profiles (Figure 5a) for sequential inference programs in an uncollapsed Dirichlet process mixture model (DPMM) with \( T = 1000 \) data points simulated from the model program, with partial posteriors \( p(z|x^*_t) \) for \( t = 1, \ldots, T \) for the sequence of target distributions. For the reference, we used a relatively trusted sequential inference program based on Venture’s built-in single-site resimulation MH implementation. We estimated subjective divergence profiles for inference based on the single-site resimulation MH operator and for inference based on a cycle operator consisting of single-site Gibbs steps for the latent cluster assignments, and resimulation MH for global parameters. The subjective divergence of the Gibbs/MH operator exhibited anomalous behavior, and degraded with additional inference, quickly becoming worse than the resimulation MH operator. This led us to identify a bug in our Gibbs/MH operator in which no inference was being performed on the within-cluster variance parameter. The profile for the corrected operator exhibited markedly faster convergence than the resimulation MH profile. For comparison, we estimated the expected log likelihood \( E_{z \sim q(z|x^*)} [\log p(x^*_1:T|z)] \) for output samples \( z \) produced at the termination of these inference programs. The expected log likelihood profile (Figure 5b) for the Gibbs/MH operator with a bug was significantly higher (better) than the profile for resimulation MH, despite being significantly poorer than the profile in the corrected version. Note that unlike the subjective divergence profiles, the expected log likelihood profiles for the operator with a bug may not have seemed anomalous.

5 Discussion

This paper introduced a new technique for quantifying the approximation error of a broad class of probabilistic inference programs. The key ideas are (i) to assess error relative to subjective beliefs in the quality of a reference inference program, (ii) to use symmetrized divergences, and (iii) to use a meta-inference program that finds probable executions of the original inference program if its output density cannot be directly assessed. The approach is implemented as a probabilistic meta-program in VentureScript that uses ancillary probabilistic meta-programs for the reference and meta-inference schemes.

Much more empirical and theoretical development is needed. Specific directions include better characterizing the impact of reference and meta-inference quality and identifying the contexts in which the theoretical bounds are predictably tight or loose. Applying the technique to a broad corpus of VentureScript programs seems like a useful first step. Empirically studying the behavior of subjective divergence for a broader sample of buggy inference programs also will be informative.

It also will be important to connect the approach to results from theoretical computer science, including the computability \(^1\) and complexity \(^9\) of probabilistic inference. For example, the asymptotic scaling of probabilistic program runtime can be analyzed using the standard random access memory model \(^5\) under suitable assumptions about the implementation. This includes the model program; the inference program; the reference program; the meta-inference program; and the probabilistic meta-program implementing Algorithm 1. It should thus be possible to align the computational tractability of approximate inference of varying qualities with standard results from algorithmic and computational complexity theory, by combining such an asymptotic analysis with...
a careful treatment of the variances of all internal Monte Carlo estimators.

This technique opens up other new research opportunities. For example, it may be possible to predict the probable performance of approximate inference by building probabilistic models that use characteristics of problem instances to predict subjective divergences. It may also be possible to use the technique to justify inference heuristics such as [17] and [3], and the stochastic Bayesian relaxations from [14], [13]. Finally, it seems fruitful to use the technique to study the query sensitivity of approximate inference [20].

Practitioners of probabilistic modeling and inference are all too familiar with the difficulties that come with dependence on approximation algorithms, especially stochastic ones. Diagnosing the convergence of sampling schemes is known to be difficult in theory [8] and in practice [7]. Many practitioners respond by restricting the class of models and queries they will consider. The definition of “tractable” is sometimes even taken to be synonymous with “admits polynomial time algorithms for exactly calculating marginal probabilities”, as in [18]. Probabilistic programming throws these difficulties into sharp relief, by making it easy to explore an unbounded space of possible models, queries, and inference strategies. Hardly any probabilistic inference programs come with certificates that they give exact answers in polynomial time.

It is understandable that many practitioners are wary of expressive probabilistic languages. The techniques in this paper make it possible to pursue an alternative approach: use expressive languages for modeling and potentially even also stochastic inference strategies, but also build quantitative models of the time-accuracy profiles of approximate inference, in practice, from empirical data. This is an inherently subjective process, involving qualitative and quantitative assumptions at the meta-level. However, we note that probabilistic programming can potentially help manage this meta-modeling process, providing new probabilistic—or in some sense meta-probabilistic—tools for studying the probable convergence profiles of probabilistic inference programs.

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A Basic notation

The notation \( p(z) \) is used to denote the distribution of a random variable, as well as the corresponding probability density function, and we rely on the context to disambiguate between the two. In particular, the KL divergence from probability distribution \( p(z) \) to probability distribution \( q(z) \) is denoted \( D_{\text{KL}}(p(z)||q(z)) \):

\[
D_{\text{KL}}(p(z)||q(z)) = E_{z \sim p(z)} \left[ \log \frac{p(z)}{q(z)} \right]
\]

where the \( p(z) \) and \( q(z) \) inside the expectation are density functions which take values \( z \) as input, and \( z \sim p(z) \) indicates a random variable with distribution \( p(z) \). Throughout, when comparing two distributions \( p(z) \) and \( q(z) \) we assume that they have equal support (\( p(z) = 0 \iff q(z) = 0 \)). The symmetrized KL divergence between \( p(z) \) and \( q(z) \) is

\[
D_{\text{KL}}(p(z)||q(z)) + D_{\text{KL}}(q(z)||p(z))
\]

In this appendix, we use the shorthand \( p \) for \( p(z) \), and \( D_{\text{KL}}(p||q) \) for \( D_{\text{KL}}(p(z)||q(z)) \) when there is no ambiguity as to the distributions represented by \( p \) and \( q \).

B Deriving the subjective divergence

This section provides a pedagogical derivation of subjective divergence. Suppose we seek to estimate the KL divergence between two distributions \( q(z) \) and \( p(z) \) (in this section we do not initially assume these to be approximate inference or posterior distributions in particular). We walk through a motivating derivation of the subjective divergence as an approach to this problem.

B.1 Monte Carlo estimation

Suppose we can sample from \( q \) and \( p \), and that normalized densities of \( q \) and \( p \) are available. Then, we can estimate either direction of KL divergence using simple Monte Carlo, e.g.:

\[
D_{\text{KL}}(q||p) = E_{z \sim q} \left[ \log \frac{q(z)}{p(z)} \right] \approx \frac{1}{N} \sum_{i=1}^{N} \log \frac{q(z_i)}{p(z_i)}
\]

where \( z_i \sim q \). The accuracy of the estimates is determined by the variance in the log weight \((\log \frac{q(z_i)}{p(z_i)})\) and \( N \).

B.2 Symmetrized KL divergence

Suppose now that only unnormalized densities \( \tilde{q}(z) \) and \( \tilde{p}(z) \) can be computed with unknown normalizing constants \( Z_P \) and \( Z_Q \), but that we can still sample from \( q \) and \( p \). Then the two directions of KL divergence are:

\[
D_{\text{KL}}(q||p) = E_{z \sim q} \left[ \log \frac{q(z)}{p(z)} \right] = E_{z \sim q} \left[ \log \frac{\tilde{q}(z)/Z_Q}{\tilde{p}(z)/Z_P} \right] = \log \frac{Z_P}{Z_Q} + E_{z \sim q} \left[ \log \frac{\tilde{q}(z)}{\tilde{p}(z)} \right] \tag{7}
\]

\[
D_{\text{KL}}(p||q) = E_{z \sim p} \left[ \log \frac{p(z)}{q(z)} \right] = E_{z \sim p} \left[ \log \frac{\tilde{p}(z)/Z_P}{\tilde{q}(z)/Z_Q} \right] = \log \frac{Z_Q}{Z_P} + E_{z \sim p} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right] \tag{8}
\]

Suppose we can accurately estimate the expectation terms for both of these quantities using simple Monte Carlo, but that estimating the terms \( \log \frac{Z_Q}{Z_P} \) and \( \log \frac{Z_P}{Z_Q} \) is more difficult.

Consider the direction \( D_{\text{KL}}(q||p) \). Estimating only the expectation term allows us to estimate differences in KL divergence \( D_{\text{KL}}(q_1||p) \) or \( D_{\text{KL}}(q_2||p) \) if the normalizing constants \( Z_Q1 \) and \( Z_Q2 \) are the same. The ‘evidence lower bound’ (ELBO) optimized in variational inference is such an expectation, in which often \( Z_Q1 = Z_Q2 = 1 \). The ELBO is used to guide a search or optimization process over a space of \( q \in \mathcal{Q} \) to minimize \( D_{\text{KL}}(q||p) \). However, not knowing the normalizing constant \( Z_P \) prevents us from estimating the KL divergence itself.
Note that in the symmetrized KL divergence, the terms containing the normalizing constants cancel, and we are left with:

\[
D_{KL}(q||p) + D_{KL}(p||q) = E_{z \sim q} \left[ \log \frac{\tilde{q}(z)}{\tilde{p}(z)} \right] + E_{z \sim p} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right] = E_{z \sim p} \log \tilde{p}(z) - E_{z \sim q} \log \tilde{q}(z) = E_{z \sim p} \left[ \log w(z) \right] - E_{z \sim q} \left[ \log w(z) \right]
\]

where we define the unnormalized weight function as \( w(z) := \frac{\tilde{p}(z)}{\tilde{q}(z)} \). Suppose we use a simple Monte Carlo estimator for each of the two expectations in the above expression of the symmetric KL divergence by sampling from \( q \) and \( p \) respectively, and take the difference in estimates. This can be interpreted as comparing samples from \( q \) against samples from \( p \) by projecting them through the log-weight function \( \log w(z) \) onto \( \mathbb{R} \).

### B.3 Non-oracle reference inference program

We now refine the setting to more closely match the approximate inference setting, in which it is relatively easy to sample from \( q \), and difficult to sample from \( p \). Specifically, we assume that the term \( E_{z \sim q} \left[ \log w(z) \right] \) is relatively easier to estimate than \( E_{z \sim p} \left[ \log w(z) \right] \). This is often the case, for example, if \( p \) is a posterior distribution and \( q \) is the approximating distribution of a typical inference program. We consider using samples from a proxy \( r(z) \) instead of samples from \( p(z) \), for which \( r \) is more efficient to sample from than \( p \) itself, but otherwise using the original weight function \( w(z) \) which is defined in terms of \( p \) and \( q \). Instead of the symmetric KL divergence between \( q \) and \( p \) we are then estimating:

\[
E_{z \sim r} \log w(z) = E_{z \sim q} \log w(z) = E_{z \sim r} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right] - E_{z \sim q} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right]
\]

The difference between our expectation and the true symmetrized KL is:

\[
D_{KL}(r||q) - D_{KL}(r||p) - D_{KL}(p||q)
\]

For \( D_{KL}(r||p) = 0 \) the difference is zero. Assuming certain conditions on \( r \), we still estimate an upper bound on the symmetrized KL divergence (see Proposition 3) and the KL divergence from \( q(z; x^*) \) to \( p(z|x^*) \) (see Proposition 3).

### B.4 Inference program output marginal density estimators

We now handle the setting in which the density \( q(z) \) is not available, even up to a normalizing constant, due to the presence of internal random choices \( y \) involved in sampling from \( q(z) \):

\[
q(z) = \int q(y, z) dy
\]

where \( y \) is high-dimensional. We take \( q(y, z) \) to be an inference program, and we refer to \( y \) as an inference execution history. Note that unlike in the main text, the dependence on the data set \( x^* \) is omitted in the notation of this section. When \( y \) and \( z \) are jointly sampled from \( q(y, z) \) by first sampling \( y \sim q(y) \) followed by \( z|y \sim q(z|y) \), \( y \) is the history of the inference program execution that generated \( z \). Consider the symmetrized KL divergence:

\[
D_{KL}(q(z)||p(z)) + D_{KL}(p(z)||q(z)) = E_{z \sim p(z)} \left[ \log w(z) \right] - E_{z \sim q(z)} \left[ \log w(z) \right]
\]

\[
E_{z \sim p(z)} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right] - E_{z \sim q(z)} \left[ \log \frac{\tilde{p}(z)}{\tilde{q}(z)} \right]
\]
We will construct a Monte Carlo estimate of the symmetrized KL divergence that uses estimators \( \hat{q}(z) \), which are potentially stochastic given \( z \), instead of the true densities \( q(z) \):

\[
\frac{1}{N} \sum_{i=1}^{N} \log \frac{\hat{p}(z_i^p)}{\hat{q}(z_i^p)} = \frac{1}{M} \sum_{j=1}^{M} \log \frac{\hat{p}(z_j^q)}{\hat{q}(z_j^q)}
\]  

(19)

for \( z_i^p \sim p(z) \) for \( i = 1, \ldots, N \) and \( z_j^q \sim q(z) \) for \( j = 1, \ldots, M \). The expectation of the estimate is:

\[
E_{z \sim p(z)} \left[ E \left[ \log \frac{\hat{p}(z)}{\hat{q}(z)} \right] \right] - E_{z \sim q(z)} \left[ E \left[ \log \frac{\hat{p}(z)}{\hat{q}(z)} \right] \right]
\]

(20)

where the inner expectations are with respect to the distributions of the random variables \( \hat{q}(z) \) conditioned on \( z \). We want the expectation of our estimate to be an upper bound on the true symmetrized KL divergence. To enforce this, we choose distinct estimators for \( \hat{q}(z) \), denoted \( \hat{q}_{\text{IS}}(z) \) and \( \hat{q}_{\text{HM}}(z) \) respectively, for use with the samples \( z \sim p(z) \) and for use with the samples \( z \sim q(z) \) such that the following two conditions hold:

\[
E_{z \sim p(z)} \left[ E \left[ \log \frac{\hat{p}(z)}{\hat{q}_{\text{IS}}(z)} \right] \right] \geq E_{z \sim p(z)} \left[ \log \frac{\hat{p}(z)}{q(z)} \right]
\]

(21)

\[
E_{z \sim q(z)} \left[ E \left[ \log \frac{\hat{p}(z)}{\hat{q}_{\text{HM}}(z)} \right] \right] \leq E_{z \sim q(z)} \left[ \log \frac{\hat{p}(z)}{q(z)} \right]
\]

(22)

This will ensure that the expectation of our estimate is greater than the symmetrized KL divergence. To achieve this, we require that:

\[
E \left[ \log \frac{\hat{p}(z)}{\hat{q}_{\text{IS}}(z)} \right] \geq \log \frac{\hat{p}(z)}{q(z)} \quad \forall z
\]

(23)

\[
E \left[ \log \frac{\hat{p}(z)}{\hat{q}_{\text{HM}}(z)} \right] \leq \log \frac{\hat{p}(z)}{q(z)} \quad \forall z
\]

(24)

This is equivalent to the requirement that:

\[
E [\log \hat{q}_{\text{IS}}(z)] \leq \log q(z) \quad \forall z
\]

(25)

\[
E [\log \hat{q}_{\text{HM}}(z)] \geq \log q(z) \quad \forall z
\]

(26)

As pointed out in [10] (see Lemma 3 and Lemma 4 in Appendix C), these requirements are met if:

\[
E [\hat{q}_{\text{IS}}(z)] = q(z) \quad \forall z
\]

(27)

\[
E \left[ (\hat{q}_{\text{HM}}(z))^{-1} \right] = (q(z))^{-1} \quad \forall z
\]

(28)

There are potentially many choices for \( \hat{q}_{\text{IS}}(z) \) and \( \hat{q}_{\text{HM}}(z) \) that satisfy these conditions. To construct the baseline estimators we assume that we can efficiently compute the joint density \( q(y, z) \). For the estimator \( \hat{q}_{\text{IS}}(z) \) we use an importance sampling estimator with importance distribution \( m(y; z) \) where

\[
E_{y \sim m(y; z)} \left[ \frac{q(y, z)}{m(y; z)} \right] = q(z) \quad \forall z
\]

(29)

Defining:

\[
\hat{q}_{\text{IS}}(z) = 1 \frac{1}{L} \sum_{i=1}^{L} q(y_i; z) \quad \text{for} \quad y_i \sim m(y; z)
\]

(30)

satisfies the unbiasedness condition of Equation 27 for \( \hat{q}_{\text{IS}}(z) \). To construct the estimator \( \hat{q}_{\text{HM}}(z) \) we note that

\[
E_{y \sim q(y; z)} \left[ \frac{m(y; z)}{q(y; z)} \right] = \frac{1}{q(z)} \quad \forall z
\]

(31)
We define $\hat{q}_{\text{HM}}(z)$ as a harmonic mean estimator:

$$\hat{q}_{\text{HM}}(z) = \frac{L}{\sum_{l=1}^{L} \frac{m(y_{l}; z)}{q(y_{l}; z)}} \quad \text{for} \quad y_{l} \sim q(y|z) \quad (32)$$

which satisfies the unbiased reciprocal condition of Equation 28 for $\hat{q}_{\text{HM}}(z)$. Algorithm 1 uses $L = 1$ for both $\hat{q}_{\text{IS}}(z)$ and $\hat{q}_{\text{HM}}(z)$, and obtains the sample of inference program execution history $y \sim q(y|z)$ from the joint sample that generated $z$. Note that only one such sample is immediately available for each $z$, although we could conceivably start a Markov chain at the exact sample $y$ with $q(y|z)$ as its stationary distribution to obtain more samples $y$ marginally distributed according to $q(y|z)$. Using more sophisticated versions of $\hat{q}_{\text{HM}}(z)$ and $\hat{q}_{\text{IS}}(z)$ is left for future work. Note that for the single-particle baseline estimators and an oracle reference, the sole determiner of the gap between the subjective divergence and the symmetrized KL is the quality of the distribution $m(y; z)$ as an approximation to $q(y|z)$. We refer to $m(y; z)$ as the meta-inference distribution.

**C Proofs**

**Lemma 1.** For $\hat{q}_{\text{HM}}(z; x^*)$ such that $E \left[ \left( \hat{q}_{\text{HM}}(z; x^*) \right)^{-1} \right] = q(z; x^*)^{-1}$ for all $z$,

$$E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right] \leq \log p(x^*) - D_{\text{KL}}(q(z; x^*) || p(z|x^*))$$

**Proof.**

Factoring out the normalizing constant $p(x^*)$ using $p(z, x^*) = p(z|x^*)p(x^*)$:

$$E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right] = E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] + \log p(x^*) \right]$$

$$= E_{z \sim q(z; x^*)} \left[ E \left[ \log p(x^*) \right] \right] + E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right]$$

Linearity of expectation:

$$= E_{z \sim q(z; x^*)} \left[ E \left[ \log p(x^*) \right] \right] + E_{z \sim q(z; x^*)} \left[ E \left[ \frac{p(z|x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right]$$

The normalizing constant $p(x^*)$ is a constant:

$$= \log p(x^*) + E_{z \sim q(z; x^*)} \left[ E \left[ \frac{p(z|x^*)}{\hat{q}_{\text{HM}}(z; x^*)} \right] \right]$$

Linearity of expectation:

$$= \log p(x^*) + E_{z \sim q(z; x^*)} \left[ E \left[ \log p(z|x^*) \right] - E \left[ \log \hat{q}_{\text{HM}}(z; x^*) \right] \right]$$

Conditioned on $z$, $p(z|x^*)$ is a constant:

$$= \log p(x^*) + E_{z \sim q(z; x^*)} \left[ \log p(z|x^*) - E \left[ \log \hat{q}_{\text{HM}}(z; x^*) \right] \right]$$

Using Lemma 4 (see below) with the given condition $E \left[ \left( \hat{q}_{\text{HM}}(z; x^*) \right)^{-1} \right] = q(z; x^*)^{-1}$ for all $z$:

$$\leq \log p(x^*) + E_{z \sim q(z; x^*)} \left[ \log p(z|x^*) - \log q(z; x^*) \right]$$

$$= \log p(x^*) + E_{z \sim q(z; x^*)} \left[ \log \frac{p(z|x^*)}{q(z; x^*)} \right]$$

Using the definition of Kullback-Leibler (KL) divergence 6:

$$= \log p(x^*) - D_{\text{KL}}(q(z; x^*) || p(z|x^*))$$

**Lemma 2.** For $\hat{q}_{\text{IS}}(z; x^*)$ such that $E[\hat{q}_{\text{IS}}(z; x^*)] = q(z; x^*)$ for all $z$,

$$E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{\hat{q}_{\text{IS}}(z; x^*)} \right] \right] \geq \log p(x^*) + D_{\text{KL}}(p(z|x^*) || q(z; x^*))$$

**Lemma 4.** For $\hat{q}_{\text{IS}}(z; x^*)$ such that $E[\hat{q}_{\text{IS}}(z; x^*)] = q(z; x^*)$ for all $z$,

$$E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{\hat{q}_{\text{IS}}(z; x^*)} \right] \right] \geq \log p(x^*) + D_{\text{KL}}(p(z|x^*) || q(z; x^*))$$
Lemma 5. Linearity of expectation: Factoring out the normalizing constant \( p(x^*) \) using \( p(z, x^*) = p(z|x^*)p(x^*) \):

\[
E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{q_{\text{IS}}(z; x^*)} \right] \right] = E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z|x^*)p(x^*)}{q_{\text{IS}}(z; x^*)} \right] \right]
\]

(44)

Linearity of expectation:

\[
= E_{z \sim p(z|x^*)} \left[ E \left[ \log p(x^*) + \log \frac{p(z|x^*)}{q_{\text{IS}}(z; x^*)} \right] \right]
\]

(45)

The normalizing constant \( p(x^*) \) is a constant:

\[
= \log p(x^*) + E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{q_{\text{IS}}(z; x^*)} \right] \right]
\]

(46)

Linearity of expectation:

\[
= \log p(x^*) + E_{z \sim p(z|x^*)} \left[ E \left[ \log p(z|x^*) - \log q_{\text{IS}}(z; x^*) \right] \right]
\]

(47)

Conditioned on \( z \), \( p(z|x^*) \) is a constant:

\[
= \log p(x^*) + E_{z \sim p(z|x^*)} \left[ \log p(z|x^*) - E \left[ \log q_{\text{IS}}(z; x^*) \right] \right]
\]

(48)

Using Lemma 3 (see below) with the given condition \( E[q_{\text{IS}}(z; x^*)] = q(z; x^*) \) for all \( z \):

\[
\geq \log p(x^*) + E_{z \sim p(z|x^*)} \left[ \log p(z|x^*) - \log q(z; x^*) \right]
\]

(49)

\[
= \log p(x^*) + E_{z \sim p(z|x^*)} \left[ \log \frac{p(z|x^*)}{q(z; x^*)} \right]
\]

(50)

Using the definition of Kullback-Leibler (KL) divergence \( D \):

\[
= \log p(x^*) + D_{KL}(p(z|x^*)||q(z; x^*))
\]

(51)

Lemma 3 (Unbiased estimators are lower bound log estimators [10]). For any \( \hat{x} \) such that \( E[\hat{x}] = x \), \( E[\log \hat{x}] \leq \log x \)

Proof.

By Jensen’s inequality, since \( \log(\cdot) \) is concave:

\[
E[\log \hat{x}] \leq \log E[\hat{x}]
\]

(52)

By given condition \( E[\hat{x}] = x \):

\[
= \log x
\]

(53)

Lemma 4 (Unbiased reciprocal estimators are upper bound log estimators [10]). For any \( \hat{x} \) such that \( E[\hat{x}^{-1}] = x^{-1} \), \( E[\log \hat{x}] \geq \log x \)

Proof.

\[
E[\log \hat{x}] = E \left[ - \log \left( \frac{1}{\hat{x}} \right) \right]
\]

(54)

By Jensen’s inequality, since \( - \log(\cdot) \) is convex:

\[
\geq - \log \left( E \left[ \frac{1}{\hat{x}} \right] \right)
\]

(55)

By given condition \( E[\hat{x}^{-1}] = x^{-1} \):

\[
= - \log \left( \frac{1}{x} \right)
\]

(56)

\[
= \log x
\]

(57)

\[
= \log x
\]

(58)

\[
= \log x
\]

(59)

Lemma 5. For \( q_{\text{IS}}(z) \) such that \( E[q_{\text{IS}}(z; x^*)] = q(z; x^*) \),

\[
E_{z \sim r(z|x^*)} \left[ E \left[ \log \frac{p(z|x^*)}{q_{\text{IS}}(z; x^*)} \right] \right] \geq \log p(x^*) - D_{KL}(r(z; x^*)||p(z|x^*)) + D_{KL}(r(z; x^*)||q(z; x^*))
\]

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Proposition 1. If an oracle reference program is used then
\[ D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq D_{\text{KL}}(q(z;x^*)||p(z|x^*)) + D_{\text{KL}}(p(z|x^*)||q(z;x^*)) \]

Proof. The definition of subjective divergence:
\[ D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) := E_{z \sim r(z;x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{IS}}(z;x^*)} \right] - E_{z \sim q(z;x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{HM}}(z;x^*)} \right] \right] \right] \]

Using an oracle reference inference program \( r(z;x^*) = p(z|x^*) \) \( \forall z \):
\[ = E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{IS}}(z;x^*)} \right] - E_{z \sim q(z;x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{HM}}(z;x^*)} \right] \right] \right] \]

Using Lemma 1 to bound the second expectation:
\[ \geq E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{IS}}(z;x^*)} \right] - (\log p(x^*) - D_{\text{KL}}(q(z;x^*)||p(z|x^*))) \right] \]

Using Lemma 2 to bound the first expectation:
\[ \geq (\log p(x^*) + D_{\text{KL}}(p(z|x^*)||q(z;x^*))) - (\log p(x^*) - D_{\text{KL}}(q(z;x^*)||p(z|x^*))) \]

The log normalizing constant \( \log p(x^*) \) cancels:
\[ = D_{\text{KL}}(p(z|x^*)||q(z;x^*)) + D_{\text{KL}}(q(z;x^*)||p(z|x^*)) \]

Proposition 2. If \( D_{\text{KL}}(r(z;x^*)||p(z|x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*)) - D_{\text{KL}}(p(z|x^*)||q(z;x^*)) \) then \( D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq D_{\text{KL}}(q(z;x^*)||p(z|x^*)) + D_{\text{KL}}(p(z|x^*)||q(z;x^*)) \)

Proof. Taking the definition of subjective divergence and the difference of the bounds of Lemma 5 and Lemma 1 gives
\[ D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq -D_{\text{KL}}(r(z;x^*)||p(z|x^*)) + D_{\text{KL}}(r(z;x^*)||q(z;x^*)) + D_{\text{KL}}(q(z;x^*)||p(z|x^*)) \]

If \( D_{\text{KL}}(r(z;x^*)||p(z|x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*)) - D_{\text{KL}}(p(z|x^*)||q(z;x^*)) \) then
\[ D_{\text{KL}}(p(z|x^*)||q(z;x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*)) - D_{\text{KL}}(r(z;x^*)||p(z|x^*)) \]
\[ D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq D_{\text{KL}}(p(z|x^*)||q(z;x^*)) + D_{\text{KL}}(q(z;x^*)||p(z|x^*)) \]

Proposition 3. If \( D_{\text{KL}}(r(z;x^*)||p(z|x^*)) \leq D_{\text{KL}}(r(z;x^*)||q(z;x^*)) \) then
\[ E_{z \sim r(z;x^*)} \left[ E \left[ \log \frac{p(z,x^*)}{q_{\text{IS}}(z;x^*)} \right] \right] \geq \log p(x^*) \]
\[ D_{\text{SBJ}}(q(z;x^*)||p(z|x^*)) \geq D_{\text{KL}}(q(z;x^*)||p(z|x^*)) \]

Proof. The first result follows from Lemma 5. The second result follows from the definition of subjective divergence and the difference in the bounds of the first result and Lemma 1.
D Effect of quality of meta-inference program

This section analyzes the difference between subjective divergence and the symmetrized KL divergence for the procedure of Algorithm 1 in the oracle reference setting. In this case, the gap between the subjective divergence and the true KL divergence is the symmetrized conditional relative entropy between the meta-inference distribution and the conditional distribution on execution histories given inference program output. To see this, first consider the expected log estimated weight under the inference program:

\[
E_{z \sim q(z;x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{q_{HM}(z; x^*)} \right] \right]
\]

(75)

\[
E_{z \sim q(z;x^*)} \left[ E_{y \sim q(y|z;x^*)} \left[ \log \frac{p(z|x^*)m(y; z, x^*)}{q(y, z; x^*)} \right] \right] + \log p(x^*)
\]

(76)

\[
= \log p(x^*) - D_{KL}(q(y, z; x^*)|p(z|x^*)m(y; z, x^*))
\]

(77)

Using the chain rule for joint KL divergence [6]:

\[
= \log p(x^*) - D_{KL}(q(z; x^*)|p(z|x^*)) - E_{z \sim q(z;x^*)} \left[ D_{KL}(q(y|z; x^*)|m(y; z, x^*)) \right]
\]

(78)

Next, consider the expected log estimated weight under the oracle reference program:

\[
E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{q_{IS}(z; x^*)} \right] \right]
\]

(79)

\[
E_{z \sim p(z|x^*)} \left[ E_{y \sim m(y;z,x^*)} \left[ \log \frac{p(z|x^*)m(y; z, x^*)}{q(y, z; x^*)} \right] \right] + \log p(x^*)
\]

(80)

\[
= \log p(x^*) + D_{KL}(p(z|x^*)|q(z;x^*)) + E_{z \sim p(z|x^*)} \left[ D_{KL}(m(y; z, x^*)|q(y|z;x^*)) \right]
\]

(81)

Using the chain rule for joint KL divergence [6]:

\[
= \log p(x^*) + D_{KL}(p(z|x^*)|q(z;x^*)) + E_{z \sim p(z|x^*)} \left[ D_{KL}(m(y; z, x^*)|q(y|z;x^*)) \right]
\]

(82)

The difference in these expectations is the subjective divergence \(D_{SBJ}\):

\[
D_{SBJ}(q(z; x^*)|p(z|x^*))
\]

(83)

\[
= E_{z \sim p(z|x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{q_{IS}(z; x^*)} \right] \right] - E_{z \sim q(z;x^*)} \left[ E \left[ \log \frac{p(z, x^*)}{q_{HM}(z; x^*)} \right] \right]
\]

(84)

\[
= (D_{KL}(p(z|x^*)|q(z;x^*)) + D_{KL}(q(z;x^*)|p(z|x^*)) + E_{z \sim p(z|x^*)} \left[ D_{KL}(m(y; z, x^*)|q(y|z;x^*)) \right] + E_{z \sim q(z;x^*)} \left[ D_{KL}(q(y|z;x^*)|m(y; z, x^*)) \right]
\]

(85)

(86)

Therefore the looseness of the bound on the actual symmetric KL divergence is:

\[
E_{z \sim p(z|x^*)} \left[ D_{KL}(m(y; z, x^*)|q(y|z;x^*)) \right] + E_{z \sim q(z;x^*)} \left[ D_{KL}(q(y|z;x^*)|m(y; z, x^*)) \right]
\]

(87)

To gain intuition about how the gap is related to the accuracy of inference output marginal density estimation, consider the variance of \(q_{IS}(z; x^*)\) and the bias of the induced estimator of \(\log q(z; x^*)\):

\[
\text{Var} \left( \frac{q_{IS}(z; x^*)}{q(z; x^*)} \right) = E \left[ \left( \frac{q_{IS}(z; x^*)}{q(z; x^*)} \right)^2 - \left( E \left[ \frac{q_{IS}(z; x^*)}{q(z; x^*)} \right] \right)^2 \right]
\]

(88)

\[
E_{y \sim m(y;z,x^*)} \left[ \frac{q(y,z,x^*)}{q(z; x^*)m(y; z, x^*)} \right]^2 - 1
\]

(89)

\[
E_{y \sim m(y;z,x^*)} \left[ \frac{q(y,z,x^*)}{m(y; z, x^*)} \right]^2 - 1
\]

(90)

\[
\chi^2(m(y; z, x^*)|q(y|z;x^*))
\]

(91)

\[
\log q(z; x^*) - E \left[ \log q_{IS}(z; x^*) \right] = E \left[ \log \frac{q(z; x^*)}{q_{IS}(z; x^*)} \right]
\]

(92)

\[
E_{y \sim m(y;z,x^*)} \left[ \log \frac{q(z; x^*)m(y; z, x^*)}{q(y, z; x^*)} \right]
\]

(93)

\[
E_{y \sim m(y;z,x^*)} \left[ \log \frac{m(y; z, x^*)}{q(y|z;x^*)} \right]
\]

(94)

\[
D_{KL}(m(y; z, x^*)|q(y|z;x^*))
\]

(95)
Also consider the variance of \((\hat{q}_{HM}(z; x^*))^{-1}\) and the bias of the induced estimator for \(\log q(z; x^*)\):

\[
\text{Var}\left(\frac{q(z; x^*)}{\hat{q}_{HM}(z; x^*)}\right) = E\left[\left(\frac{q(z; x^*)}{\hat{q}_{HM}(z; x^*)}\right)^2 - \left(E\left[\frac{q(z; x^*)}{\hat{q}_{HM}(z; x^*)}\right]\right)^2\right]
\]

(96)

\[
= E_{y|z \sim q(y|z; x^*)}\left[\left(\frac{q(z; x^*)m(y; z, x^*)}{q(y; z; x^*)}\right)^2 - 1\right]
\]

(97)

\[
= E_{y|z \sim q(y|z; x^*)}\left[\left(\frac{m(y; z, x^*)}{q(y|z; x^*)}\right)^2 - 1\right]
\]

(98)

\[
E[\log \hat{q}_{HM}(z; x^*)] - \log q(z; x^*) = E\left[\log \frac{\hat{q}_{HM}(z; x^*)}{q(z; x^*)}\right]
\]

(100)

\[
= E_{y|z \sim q(y|z; x^*)}\left[\log \frac{q(y; z; x^*)}{\hat{q}_{HM}(z; x^*)m(y; z, x^*)}\right]
\]

(101)

\[
= E_{y|z \sim q(y|z; x^*)}\left[\log \frac{q(y|z; x^*)}{m(y; z, x^*)}\right]
\]

(102)

\[
= D_{KL}(q(y|z; x^*)||m(y; z, x^*))
\]

(103)

Above, \(\chi^2_p\) is the Pearson chi-square divergence [16]:

\[
\chi^2_p(p(y)||q(y)) := \int \left(\frac{q(y) - p(y)}{p(y)}\right)^2 dy
\]

(104)

\[
= \int \frac{(q(y) - p(y))^2}{p(y)^2} dy
\]

(105)

\[
= \int \frac{q(y)^2 + p(y)^2 - 2p(y)q(y)}{p(y)^2} dy
\]

(106)

\[
= \int \frac{(q(y))^2 - 1}{p(y)} dy
\]

(107)

E Derivations for specific inference programs

We now show how Algorithm [1] can be applied to estimate subjective divergences for three large classes of approximate inference programs: “assessable” inference, sequential stochastic approximate inference, and particle filtering in state space models.

For convenience, we first introduce new notation specific to the baseline inference output marginal density estimators \(\hat{q}_{IS}\) and \(\hat{q}_{HM}\) that are used in Algorithm [1]. Since in this setting, both \(\hat{q}_{IS}\) and \(\hat{q}_{HM}\) involve sampling a single inference execution history \(y\), and returning an estimate \(q(y; z; x^*)/m(y; z, x^*)\), we denote the estimated weight for a latent sample \(z\), conditioned on a sampled inference execution history \(y\), as:

\[
\hat{w}_y(z) := \frac{p(z, x^*)}{\hat{q}_{IS}(y; z, x^*)} = \frac{p(z, x^*)m(y; z, x^*)}{q(y; z, x^*)}
\]

(108)

In order to use Algorithm [1] we must be able to efficiently compute the function \(\hat{w}_y(z)\) and sample from the meta-inference program \(m(y; z, x^*)\). This section lists constructions of \(q(y; z; x^*)\) and \(m(y; z, x^*)\) that satisfy these properties.

E.1 Assessable inference

If the density \(q(z; x^*)\) can be efficiently computed exactly, we consider \(q(z; x^*)\) an assessable inference program. Inference output marginal density estimators and meta-inference are not required to estimate subjective divergence for assessable inference programs, and the procedure of Algorithm [1] can be simplified to Algorithm [2]. Examples of assessable inference include simple variational families for which the density of the variational approximation, \(q_\theta(z; x^*)\) where \(\theta\) are the variational parameters, can be efficiently computed.
Algorithm 2 Subjective divergence estimation for assessable inference programs

Require: Assessable inference program $z|x \sim q(z;x^*)$, reference inference program $z|x \sim r(z;x^*)$, number of reference replicates $N$, number of inference replicates $M$

1: for $i \leftarrow 1$ to $N$ do
2: $z_i^t \sim r(z;x^*)$
3: $w_i^t \leftarrow \frac{p(z_i^t|x^*)}{q(z_i^t|x^*)}$
4: end for
5: for $j \leftarrow 1$ to $M$ do
6: $z_j^t \sim q(z;x^*)$
7: $w_j^t \leftarrow \frac{p(z_j^t|x^*)}{q(z_j^t|x^*)}$
8: end for
9: return $\frac{1}{N} \sum_{i=1}^{N} \log w_i^t - \frac{1}{M} \sum_{j=1}^{M} \log w_j^t$

E.2 Sequential stochastic approximate inference programs

Consider a sequential stochastic inference program that proceeds through a series of steps with intermediate internal states $y_t \in \mathcal{Y}_1, \ldots, y_T \in \mathcal{Y}_T$ and returns a final state $z \in Z$, such that the joint distribution of the inference program at this level of representation factorizes into a Markov chain:

$$q(y, z; x^*) = q(y_1; x^*) \prod_{t=1}^{T-1} q(y_{t+1} | y_t; x^*) q(z | y_T; x^*)$$  (109)

In general the intermediate steps $y_t$ need not share common state spaces $\mathcal{Y}_t$. The approximating distribution of the inference program is defined as the marginal distribution of its output: $q(z; x^*)$. Note that evaluating the density $q(z; x^*)$ is generally computationally intractable. The optimal meta-inference distribution for this representation also factorizes into a Markov chain:

$$m^*(y; z, x^*) = q(y_1; x^*) \prod_{t=1}^{T-1} q(y_{t+1} | y_t; x^*) q(y_T | z; x^*)$$  (110)

Although it may be difficult to construct efficient programs which sample from the optimal meta-inference distribution, Equation (110) suggests that we can start by designing meta-inference programs that sample states $y_t$ in reverse according to a Markov chain:

$$m(y; z, x^*) = \prod_{t=1}^{T-1} m(y_t | y_{t+1}; z, x^*) m(y_T; z, x^*)$$  (111)

This mirrors the construction used in [21] to estimate variational lower bounds for Markov chain Monte Carlo. The variational lower bound of [21] corresponds to the inference program term in subjective divergence with the baseline meta-inference estimator $\hat{q}_{HM}$:

$$E_{z \sim q(z; x^*)} \left[ E \left[ \log \frac{p(z; x^*)}{\hat{q}_{HM}(z; x^*)} \right] \right] = E_{z \sim q(z; x^*)} \left[ E_{y \sim q(y; z; x^*)} \left[ \log \frac{p(z; x^*) m(y; z, x^*)}{q(y; z; x^*)} \right] \right]$$  (112)

We next derive and analyze meta-inference programs for two instances of sequential stochastic approximate inference.

E.2.1 Detailed balance transitions with state extensions

The derivation of this section uses an inference program corresponding to the single particle version of Algorithm 2 of [10] and a meta-inference program corresponding to the single particle version of Algorithm 3 of [10].

Suppose that the internal states $y_t$ are defined on state spaces of increasing dimension. In particular, suppose each intermediate state $y_t$ for $t = 2, \ldots, T$ decomposes into two components $y_t = (u_{t-1}, v_t)$, and $y_1 = v_1$, where $v_t \in \mathcal{V}_t$ for $t = 1, \ldots, T$ and $u_t \in \mathcal{U}_t = \mathcal{U}_{t-1} \times \mathcal{V}_t$ for $t = 2, \ldots, T-1$ and $\mathcal{U}_1 = \mathcal{V}_1$, and $z = u_T \in Z = \mathcal{U}_T = \mathcal{U}_{T-1} \times \mathcal{V}_T$. The inference program is composed of a sequence of extension steps $q(v_t | u_{t-1}; x^*)$ and transition steps $q(u_t | u_{t-1}, v_t; x^*) = k_t(u_t; u_{t-1}, v_t)$ and the joint density is:

$$q(y, z; x^*) = q(v_1; x^*) k_1(u_1; v_1) \prod_{t=2}^{T-1} q(v_t | u_{t-1}; x^*) k_t(u_t; u_{t-1}, v_t) q(v_T | u_{T-1}; x^*) k_T(z; u_{T-1}, v_T)$$  (113)
We assume that each transition operator $k_t$ satisfies the detailed balance condition for some target distribution $p_t$ defined on $\mathcal{U}_t$ such that the final target distribution is the posterior ($p_T(z) = p(z|x^*)$):

$$p_t(u)k_t(u';u) = p_t(u')k_t(u;u') \quad \forall u, u' \in \mathcal{U}_t, t = 1, \ldots, T$$  \hspace{1cm} (114)

Consider the conditional distributions that comprise the optimal meta-inference Markov chain of Equation [10] for this setting:

$$m^*(y_t|y_{t+1}; z, x^*) = q(y_t|y_{t+1}; x^*) = q(u_{t-1}, v_t|u_t, v_{t+1}; x^*)$$  \hspace{1cm} (115)

$$= q(u_{t-1}, v_t|u_t; x^*)$$  \hspace{1cm} (116)

$$= \frac{q(u_{t-1}, v_t, u_t; x^*)}{q(u_t; x^*)}$$  \hspace{1cm} (117)

$$= \frac{q(u_{t-1}, v_t; x^*)}{q(u_t; x^*)}k_t(u_t; u_{t-1}, v_t)$$  \hspace{1cm} (118)

To derive a meta-inference program we approximate the optimal conditionals with:

$$m(y_t|y_{t+1}; z, x^*) = q(y_t|y_{t+1}; x^*) = \frac{p_t(u_{t-1}, v_t)}{p_t(u_t)}k_t(u_t; u_{t-1}, v_t) = k_t(u_t; u_{t-1}, v_t)$$  \hspace{1cm} (119)

Assuming that $q(u_t; x^*) = p_t(u_t)$ amounts to assuming that the operator $k_t$ converges to $p_t$ and assuming that $q(u_{t-1}, v_t; x^*) = p_t(u_{t-1}, v_t)$ amounts to assuming that the operator $k_{t-1}$ converges to $p_{t-1}$ and that $p_{t-1}(u_{t-1})q(v_t|u_{t-1}; x^*) = p_t(u_{t-1}, v_t)$. Composing these conditional distributions, the full meta-inference program consists of running the transition operators $k_t$ in reverse order:

$$m(y; z, x^*) = k_1(v_1; u_1) \prod_{t=2}^{T-1} k_t(u_{t-1}, v_t; u_t) k_T(u_{T-1}, v_T; z)$$  \hspace{1cm} (120)

We define $\tilde{p}_t$ as an unnormalized density for target distribution $p_t$ with arbitrary normalizing constant for $t = 1, \ldots, T - 1$, except for $p_T$, for which the unnormalized density is defined as $\tilde{p}_T(z) := p(z, x^*)$ with normalizing constant $p(x^*)$. The weight estimate for the meta-inference program is then:

$$\tilde{w}_y(z) = \frac{p(z, x^*)m(y; z, x^*)}{q(y; z, x^*)}$$  \hspace{1cm} (121)

$$= \frac{p(z, x^*)k_1(v_1; u_1) \prod_{t=2}^{T-1} k_t(u_{t-1}, v_t; u_t)}{q(v_1; x^*)k_1(v_1; u_1) \prod_{t=2}^{T-1} q(v_t|u_{t-1}; x^*)k_t(u_{t-1}, v_t; u_t)} k_T(u_{T-1}, v_T; z)$$  \hspace{1cm} (122)

$$= \frac{p(z, x^*)}{q(v_1; x^*)} k_1(v_1; u_1) \prod_{t=2}^{T} q(v_t|u_{t-1}; x^*)k_t(u_{t-1}, v_t; u_t) k_T(u_{T-1}, v_T; z)$$  \hspace{1cm} (123)

$$= \frac{\tilde{p}_T(z)p(x^*)}{q(v_1; x^*)} \prod_{t=2}^{T} \tilde{p}_t(u_{t-1}, v_t) \frac{k_t(u_{t-1}, v_t; u_t)}{k_T(u_{T-1}, v_T; z)}$$  \hspace{1cm} (124)

$$= \frac{\tilde{p}_T(z)}{q(v_1; x^*)} \prod_{t=2}^{T} \tilde{p}_t(u_{t-1}, v_t)$$  \hspace{1cm} (125)

$$= \frac{1}{q(v_1; x^*)} \prod_{t=2}^{T} \tilde{p}_t(u_{t-1}, v_t)$$  \hspace{1cm} (126)

$$= \frac{1}{q(v_1; x^*)} \prod_{t=2}^{T} \tilde{p}_t(u_{t-1}, v_t)$$  \hspace{1cm} (127)

$$= \frac{\tilde{p}_1(v_1)}{q(v_1; x^*)} \prod_{t=1}^{T-1} \frac{\tilde{p}_{t+1}(u_{t+1}, v_{t+1})}{\tilde{p}_t(u_t)}$$  \hspace{1cm} (128)

E.2.2 Coarse representation of inference programs

Significantly, each of the operators $k_t$ may be composition of a large number of steps of primitive transition operators satisfying detailed balance (e.g. Metropolis Hastings kernels) for target distribution $p_t$. Also, each MH operator may contain additional random choices such as accept and reject decisions. The execution histories $y$ of $q(y, z; x^*)$ in Equation [113] do not represent these finer-grained states of the inference program.
**E.2.3 Detailed balance transitions with fixed state space**

If we let \( \mathcal{V}_t = \emptyset \) for \( t = 2, \ldots, T \), we recover a Markov chain with fixed state space \( \mathcal{V}_1 = \mathcal{U}_1 = \cdots = \mathcal{U}_{T-1} = \mathcal{Z} \), and the inference program is the annealed importance sampling algorithm \[15\]. In this case, the estimated weight simplifies to

\[
\hat{w}_y(z) = \frac{\tilde{p}_t(v_1)}{q(v_1; x)} \prod_{t=1}^{T-1} \frac{\tilde{p}_{t+1}(u_t)}{p_t(u_t)}
\]

(129)

Defining \( u_0 := v_1 \) and defining \( p_0(u_0) := q(u_0; x^*) \), the estimated weight is:

\[
\hat{w}_y(z) = \prod_{t=0}^{T-1} \frac{\hat{p}_{t+1}(u_t)}{p_t(u_t)}
\]

(130)

Note that in this simplified setting, the approximating assumptions used to derive the meta-inference distribution of Equation [120] are \( k_t(u'; u) = p_t(u') \) for all \( u, u' \) and \( p_{t-1}(u) = p_t(u) \) for all \( u \), for all \( t = 1, \ldots, T \). The inference and meta-inference programs for this formulation are shown in Algorithms 3 and Algorithm 4.

**Algorithm 3 Inference program for Section E.2.3**

**Require:** Model program \( p(z, x) \), dataset \( x^* \), transition operators \( k_1, \ldots, k_T \) satisfying detailed balance with respect to \( p_t \) where \( p_T(z) = p(z|x^*) \), initializing distribution \( p_0(z) \).

1: \( u_0 \sim p_0(z) \)
2: for \( t \leftarrow 1 \) to \( T - 1 \) do
3: \( u_t \sim k_t(u; u_{t-1}) \)
4: end for
5: \( z \sim k_T(z; u_{T-1}) \)
6: return \((u_{0:T-1}, z)\)

**Algorithm 4 Meta-inference program for Section E.2.3**

**Require:** Model program \( p(z, x) \), dataset \( x^* \), transition operators \( k_1, \ldots, k_T \) satisfying detailed balance with respect to \( p_t \) where \( p_T(z) = p(z|x^*) \), initializing sample \( z^* \).

1: \( u_{T-1} \sim k_T(u; z^*) \)
2: for \( t \leftarrow T - 2 \) to 0 do
3: \( u_t \sim k_{t+1}(u; u_{t+1}) \)
4: end for
5: return \( u_{0:T-1} \)

**E.2.4 Asymptotic gap between subjective divergence and symmetrized KL**

We now discuss how the quality of meta-inference is manifested in the subjective divergence bounds for the sequential inference program defined in Section E.2.3 and an oracle reference program. If we suppose that all transition operators \( k_t \) converge to their target distributions \( (k_t(u'; u) = p_t(u')\forall u' \) for \( t = 1, \ldots, T \), then the expected log estimated weight under the inference program is:

\[
E_{z \sim q(z;x^*)} \left[ E_{y|z \sim q(y|z;x^*)} \left[ \log \hat{w}_y(z) \right] \right] = E_{z \sim q(z;x^*)} \left[ \sum_{t=0}^{T-1} \log \frac{\tilde{p}_{t+1}(u_t)}{p_t(u_t)} \right]
\]

(131)

\[
= \log p(x^*) + \sum_{t=0}^{T-1} E_{u_t \sim p_t} \left[ \log \frac{p_{t+1}(u_t)}{p_t(u_t)} \right]
\]

(132)

\[
= \log p(x^*) - \sum_{t=0}^{T-1} D_{KL}(p_t(z)||p_{t+1}(z))
\]

(133)

where we have used the fact that the normalizing constant of \( \tilde{p}_T \) is \( p(x^*) \), that the normalizing constants of \( \tilde{p}_1, \ldots, \tilde{p}_{T-1} \) were arbitrary (and can be one), and that \( \tilde{p}_0 \) is normalized. The expected
log estimated weight under the reference program is:

$$E_{z \sim p(z|x^*)} \left[ E_{y \sim m(y;z,x^*)} \left[ \log \tilde{w}_y(z) \right] \right] = E_{z \sim p(z|x^*)} \left[ E_{y \sim m(y;z,x^*)} \left[ \sum_{t=0}^{T-1} \log \frac{\hat{p}_{t+1}(u_t)}{\hat{p}_t(u_t)} \right] \right]$$  \hspace{1cm} (134)

$$= \log p(x^*) + \sum_{t=0}^{T-1} E_{u_t \sim p_{t+1}} \left[ \log \frac{p_{t+1}(u_t)}{p_t(u_t)} \right]$$ \hspace{1cm} (135)

$$= \log p(x^*) + \sum_{t=0}^{T-1} D_{KL}(p_{t+1}(z)||p_t(z))$$ \hspace{1cm} (136)

The subjective divergence with an oracle reference is the difference between these two expectations, which is the sum of symmetrized KL divergences between successive distributions in the sequence $p_0(z), \ldots, p_T(z)$, where $p_T(z)$ is the posterior $p(z|x^*)$:

$$D_{SBJ}(q(z;x^*)||p(z|x^*)) = \sum_{t=0}^{T-1} D_{KL}(p_t(z)||p_{t+1}(z)) + D_{KL}(p_{t+1}(z)||p_t(z))$$  \hspace{1cm} (137)

For inference programs for which the initialization distribution $p_0(u_0)$ is the prior $p(z)$, this is the sum of symmetrized KL divergences between the prior and the posterior of the inference problem. Note that in the limit of convergence for each $k_t$ in the inference program, including $k_T$, the approximating distribution equals the posterior ($q(z;x^*) = p(z|x^*)$) and the true symmetrized KL divergence is zero. The gap between the asymptotic subjective divergence of Equation 137 and the actual divergence of zero is a instance of the quantity defined in Equation 1 which quantifies the quality of meta-inference. In this case, the asymptotic gap can be attributed to the approximating assumption $p_{t-1}(z) = p_t(z)$ that was made when deriving the meta-inference distribution.

### E.2.5 Choice of target distribution sequence

The asymptotic gap described in the previous section illustrates that the subjective divergence profiles for this class of algorithms depends heavily on the sequence of target distributions $p_t$. One generic sequence of target distributions is the sequential observation sequence: $p_t(z) = p(z|y_1:t)$. The asymptotic subjective divergence bounds (Equation 137) for this sequence depend on the data order.

### E.2.6 Standard non-sequential MCMC

We can represent the standard Markov chain Monte Carlo (MCMC) setting in which a single target distribution $p(z|x^*)$ is targeted by a single kernel $k_1$ which satisfies detailed balance with respect to $p_1(z) = p(z|x^*)$ and is composed of repeated application of primitive transition operators which themselves satisfy detailed balance. In this case, the divergence bound of Equation 137 degenerates to the symmetrized KL divergence between the initializing distribution $p_0(z)$ of the Markov chain and the posterior, and no ‘credit’ is given for running the transition operator. The assumption $p_{t-1}(z) = p_t(z)$ used in deriving the meta-inference program degenerates to $p_0(z) = p_1(z) = p(z|x^*)$, so the meta-inference program is of low quality and the gap between the subjective divergence and the true symmetrized KL divergence (given for the general case in Equation 1) is large.

### E.2.7 Comparing convergence rates of transition operators

Algorithm 3 and Algorithm 4 combined with the subjective divergence estimation procedure of Algorithm 1 can be used as a test-bench for subjectively comparing the convergence rates of transition operators. Specifically, we instantiate sequential detailed balance inference programs that utilize the same sequence of target distributions $p_t$, where we vary the type of primitive transition operator used, and the number of consecutive applications of the primitive transition operator within each of the $k_t$. Note that the asymptotic subjective divergence (Equation 137) is the same regardless of the type of transition operators used within the $k_t$.

### E.3 Particle filtering

Consider a state space model of the form

$$p(z,x) = p(z_1:T, x_1:T) = \left( p(z_1) \prod_{t=2}^{T} p(z_t|z_{t-1}) \left( \prod_{t=1}^{T} p(x_t|z_t) \right) \right)$$ \hspace{1cm} (138)
We apply the particle filter inference program as defined in [11], Algorithm 2.3, with independent resampling, and derive a meta-inference program that permits Algorithm 4 to be used to estimate subjective divergences of this inference program with respect to the smoothing problem, with posterior \( p(z_1:T | x_1:T) \).

To simplify notation, we assume that a fixed number of particles \( K \) is used at each step of the particle filter. We denote the internal states of the particle filter as \( u_i^t \) for \( i = 1, \ldots, K \) and \( t = 1, \ldots, T \) and the internal ancestor choices by \( a_i^t \) for \( i = 1, \ldots, K \) and \( t = 1, \ldots, T - 1 \), where \( a_i^t \) is the index of the parent of state \( u_i^{t+1} \), denoted \( a_i^{t+1} \). The full set of internal states is denoted \( u_{1:T}^1 \) and the full set of internal ancestor choices is denoted \( a_{1:T}^{1:K} \). The proposal densities are denoted \( M_1(u_1) \) and \( M_t(u_t; u_{t-1}) \) for \( t = 2, \ldots, T \). An unnormalized weight is assigned to each particle at each time step, for \( i = 1, \ldots, K \):

\[
w_i^t := \frac{p(u_i^t | u_{i-1}^{t-1}) p(x_t | u_i^t)}{M_t(u_i^t; u_{i-1}^{t-1})}
\]

for \( t = 2, \ldots, T \), and

\[
w_i^1 := \frac{p(u_i^1 | x_1)}{M_1(u_i^1)}
\]

Note that these are not the same type of weight as the \( w(z) \) used directly in the subjective divergence definition. We assume that parent indices are sampled independently from a categorical distribution given the normalized weights. Conditioned on \( u_{1:T}^1 \) and \( a_{1:T-1}^{1:K} \), a single final particle index \( k \) is sampled according to the normalized weights at the final time step. A final hidden sequence \( z_{1:T} \) is then generated deterministically given \( u_{1:T}^1 \), \( a_{1:T-1}^{1:K} \), and \( k \) by selecting \( z_t = u_i^t \) for \( t = 1, \ldots, T \) where \( I_t \) is the ancestor index of state \( u_i^t \) at time \( t \), defined recursively as \( I_T := k \) and \( I_t := a_{I_{t+1}}^{I_t+1} \) for \( t = 1, \ldots, T - 1 \). We define the inference execution history of the particle filter by \( y = (u_{1:T}^1, a_{1:T-1}^{1:K}, k) \), and:

\[
q(y, z; x^*) = \left( \prod_{i=1}^{K} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i \neq I_t}^{K} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right) \left( \frac{w^T_k}{\sum_{j=1}^{K} w_j^T} \right) \left( \prod_{t=1}^{T} \delta(u_i^t, z_t) \right)
\]

For the meta-inference program \( m(y, z; x^*) \), we use the conditional SMC (CSMC) update ([11], Algorithm 3.3), which begins with a hidden state sequence \( z_{1:T} \) and its ancestry \( I = (I_1, \ldots, I_T) \) and runs the particle filter forward with this ancestry and particle states \( u_i^t \) for \( t = 1, \ldots, T \) fixed. Specifically, we first sample the ancestry \( I \) uniformly at random: \( \text{Prob}(I) = \frac{1}{K^T} \), and then proceed with the CSMC update. The density of the meta-inference program is, assuming independent resampling in the particle filter:

\[
m(y; z, x^*) = \frac{1}{K^T} \left( \prod_{i \neq I_t} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i \neq I_t} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right) \left( \prod_{t=1}^{T} \delta(u_i^t, z_t) \right)
\]

The estimated weight then simplifies to:

\[
\hat{w}_y(z) = \frac{p(z, x^*) m(y; z, x^*)}{q(y, z; x^*)}
\]

\[
p(z, x^*) \frac{1}{K^T} \left( \prod_{i \neq I_t} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i \neq I_t} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right) \left( \prod_{t=1}^{T} \delta(u_i^t, z_t) \right)
\]

\[
\left( \prod_{i=1}^{K} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i=1}^{K} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right) \left( \frac{w^T_k}{\sum_{j=1}^{K} w_j^T} \right) \left( \prod_{t=1}^{T} \delta(u_i^t, z_t) \right)
\]

Ignoring \((y, z)\) for which \( \prod_{t=1}^{T} \delta(u_i^t, z_t) = 0 \) because these are not sampled under either \( q(y, z; x^*) \) or \( m(y; z, x^*) \):

\[
p(z, x^*) \frac{1}{K^T} \left( \prod_{i \neq I_t} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i \neq I_t} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right)
\]

\[
\left( \prod_{i=1}^{K} M_1(u_i^1) \right) \left( \prod_{t=2}^{T} \prod_{i=1}^{K} \frac{u_i^{t-1}}{\sum_{j=1}^{K} u_j^{t-1}} M_t(u_i^t; u_{i-1}^{t-1}) \right) \left( \frac{w^T_k}{\sum_{j=1}^{K} w_j^T} \right)
\]
Canceling factors:

\[
\frac{1}{K^T} \left( \prod_{t=2}^{T} \frac{w_{t-1}^{u_{t-1}^{I_t}}}{w_{t-1}^{u_{t-1}^{I_t}}} M_t(u_t^{I_t}; u_{t-1}^{I_t}) \right) \left( \frac{w_y}{\sum_{j=1}^{K} w_j} \right)
\]

(146)

Since \( I_t := a_{t+1} \) for \( t = 1, \ldots, T - 1 \):

\[
\frac{1}{K^T} \left( \prod_{t=2}^{T} \frac{w_{t-1}^{u_{t-1}^{I_t}}}{w_{t-1}^{u_{t-1}^{I_t}}} M_t(u_t^{I_t}; u_{t-1}^{I_t}) \right) \left( \frac{w_y}{\sum_{j=1}^{K} w_j} \right)
\]

(147)

\[
= \left( \prod_{t=1}^{T} \frac{1}{K} \sum_{j=1}^{K} w_j \right) \left( \frac{p(z, x^*)}{M_1(u_1^{I_1}) \prod_{t=2}^{T} M_t(u_t^{I_t}; u_{t-1}^{I_t}) \prod_{t=1}^{T} w_t^{I_t}} \right)
\]

(148)

Using the definition of the particle filter’s marginal likelihood estimate \( \hat{Z} := \prod_{t=1}^{T} \frac{1}{K} \sum_{j=1}^{K} w_j \):

\[
\hat{Z} \left( \frac{p(z, x^*)}{M_1(u_1^{I_1}) \prod_{t=2}^{T} M_t(u_t^{I_t}; u_{t-1}^{I_t}) \prod_{t=1}^{T} w_t^{I_t}} \right)
\]

(149)

Expanding \( p(z, x^*) \) and using the definitions of the weights of Equation 139 and Equation 140:

\[
\hat{Z} \left( \frac{p(z, x^*)}{\prod_{t=2}^{T} M_t(u_t^{I_t}; u_{t-1}^{I_t}) \prod_{t=1}^{T} w_t^{I_t}} \right)
\]

(150)

Using \( z_t = u_t^{I_t} \) for \( t = 1, \ldots, T \):

\[
\hat{Z} \left( \frac{p(z_t)}{\prod_{t=2}^{T} p(z_t | z_{t-1}) \prod_{t=1}^{T} p(x_t^* | u_t^{I_t}) \prod_{t=2}^{T} p(u_t^{I_t}; u_{t-1}^{I_t}) \prod_{t=1}^{T} p(x_t^* | u_t^{I_t})} \right)
\]

(151)

### E.3.1 Special case: sampling importance resampling (SIR)

We can immediately apply the meta-inference program formulation for the particle filter to non-state-space probabilistic models by considering the special case of \( T = 1 \). In this case, the weight estimate is

\[
\hat{w}_y(z) = \frac{1}{K} \sum_{i=1}^{K} w_i = \frac{1}{K} \sum_{i=1}^{K} \frac{p(u_i) p(x_1^* | u_i)}{M_1(u_i)}
\]

(152)

where \( x_1^* \) contains all of the observations, and we recover sampling importance resampling (SIR). The meta-inference program in this case places the output \( z \) into one of \( K \) particles and samples the other \( K - 1 \) particles from the proposal distribution \( M_1 \).