Markovian Score Climbing: Variational Inference with KL(p∥q)

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Abstract

Modern variational inference (VI) uses stochastic gradients to avoid intractable expectations, enabling large-scale probabilistic inference in complex models. VI posits a family of approximating distributions \( q \) and then finds the member of that family that is closest to the exact posterior \( p \). Traditionally, VI algorithms minimize the “exclusive Kullback-Leibler (KL)” \( KL(q \parallel p) \) (Jordan et al., 1999; Blei et al., 2017), which leads to a computationally convenient optimization. For a restricted class of models, it leads to coordinate-ascent algorithms (Robert and Casella, 2004). For a wider class, it leads to efficient computation of unbiased gradients for stochastic optimization (Paisley et al., 2012; Salimans and Knowles, 2013; Ranganath et al., 2014). However, optimizing the inclusive KL results in an approximation that underestimates the posterior uncertainty (Minka, 2005).

To address this limitation, VI researchers have considered alternative divergences (Li and Turner, 2016; Dieng et al., 2017). One candidate is the “inclusive KL” \( KL(p \parallel q) \) (Gu et al., 2015; Bornschein and Bengio, 2015; Finke and Thiery, 2019). This divergence more accurately captures posterior uncertainty, but results in a challenging optimization problem.

In this paper, we develop Markovian score climbing (MSC), a simple algorithm for reliably minimizing the inclusive KL. Consider a valid Markov chain Monte Carlo (MCMC) method, a Markov chain whose stationary distribution is \( p \). The algorithm we develop iteratively samples the chain \( z[k] \), and then uses those samples to follow the score function of the variational approximation, \( \nabla \log q(z[k]) \), with a Robbins-Monro step-size schedule. This method, which we call Markovian score climbing (MSC), converges to a local optimum of the inclusive KL. It does not suffer from the systematic errors inherent in existing methods, such as Reweighted Wake-Sleep and Neural Adaptive Sequential Monte Carlo, which lead to bias in their final estimates. In a variant that ties the variational approximation directly to the Markov chain, MSC further provides a new algorithm that melds VI and MCMC. We illustrate convergence on a toy model and demonstrate the utility of MSC on Bayesian probit regression for classification as well as a stochastic volatility model for financial data.

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portance sampling (CIS) and conditional sequential Monte Carlo (CSMC) (Andrieu et al., 2010) kernels, examples of MCMC methods that tie in well with MSC. This melding of VI and MCMC maintains its convergence properties.

In several empirical studies, we demonstrate the convergence properties and advantages of MSC. First, we illustrate the systematic errors of the biased methods and how MSC differs on a simple toy skew-normal model. Then we compare MSC with expectation propagation (EP) and importance sampling (IS)-based optimization (Bornschein and Bengio, 2015; Finke and Thiery, 2019) on a Bayesian probit classification example with benchmark data. Finally, we apply MSC and SMC-based optimization (Gu et al., 2015) to fit a stochastic volatility model on exchange rate data.

Contributions. The contributions of this paper are (i) developing Markovian score climbing, a simple algorithm that provably minimizes \( KL(p \| q) \); (ii) identifying systematic errors in existing methods that lead to bias in their variational approximation; and (iii) empirical studies that confirm convergence and illustrates the utility of MSC.

Related Work. Much recent effort in VI has focused on optimizing cost functions that are not the exclusive KL divergence. Li and Turner (2016) and Dieng et al. (2017) study Rényi divergences and \( \chi \) divergences, respectively. The most similar to our work are the methods by Bornschein and Bengio (2015); Gu et al. (2015); Finke and Thiery (2019), using IS or SMC to optimize the inclusive KL divergence. The RWS algorithm by Bornschein and Bengio (2015) uses IS both to optimize model parameters and the variational approximation. Neural adaptive SMC by Gu et al. (2015) jointly learn an approximation to the posterior and optimize the marginal likelihood of time series with gradients estimated by SMC. Finke and Thiery (2019) draw connections between important weighted autoencoders (Burda et al., 2016), adaptive IS and methods like the RWS. These three works all rely on IS or SMC to estimate expectations with respect to the posterior. This introduces a systematic bias in the gradients that leads to a solution which is not a local optimum to the inclusive KL divergence.

Another line of work studies the combination of VI with Monte Carlo (MC) methods. Salimans et al. (2015) take inspiration from the MCMC literature to define their variational approximation. The method by Hoffman et al. (2019) uses the variational approximation to improve Hamiltonian MC. Variational SMC as proposed by Naesseth et al. (2018); Le et al. (2018); Maddison et al. (2017) uses the SMC sample process itself to define an approximation to the posterior. Follow up work by Lawson et al. (2018); Moretti et al. (2019) improve on variational SMC in various ways by using twisting (Guarniero et al., 2017; Heng et al., 2017; Lindsten et al., 2018).

Domke and Sheldon (2019) show that it is possible to take a MC estimator of the marginal likelihood and turn it into a posterior approximation. The method by Habib and Barber (2019) uses auxiliary variables to define a more flexible approximation to the posterior, then subsequently at test time apply MCMC. These methods all optimize a variational approximation based on MC methods to minimize the exclusive KL divergence. On the contrary, the method proposed in this paper minimizes the inclusive KL divergence. The method by Hoffman (2017) optimizes an initial approximation to the posterior in exclusive KL, then refines this with a few iterations of MCMC to estimate gradients with respect to the model parameters. Ruiz and Titsias (2019) define the variational approximation as an initial distribution to which a few steps of MCMC is applied, and then optimize a new contrastive divergence. This divergence is different from the inclusive KL and MCMC is used as a part of the variational approximation rather than gradient estimation.

Using MCMC together with stochastic optimization, for e.g. maximum likelihood estimation of latent variable models, is studied by (Gu and Kong, 1998; Kuhn and Lavielle, 2004; Andrieu and Vihola, 2014). In contrast the method proposed uses it for VI.

2. Background

Let \( p(z, x) \) be a probabilistic model for the latent (unobserved) variables \( z \) and data \( x \). In Bayesian inference the main concern is computing the posterior distribution \( p(z | x) \), the conditional distribution of the latent variables given the observed data. The posterior is

\[
p(z | x) = \frac{p(z, x)}{p(x)}. \tag{1}
\]

The normalization constant is the marginal likelihood \( p(x) \), computed by integrating (or summing) the joint model \( p(z, x) \) over all values of \( z \). For most models of interest, however, exactly computing the posterior is intractable, and we must approximate it.

2.1. Variational Inference with KL(p∥q)

One approach to approximating the posterior is with VI. VI turns the intractable problem of computing the posterior into an optimization problem that can be solved numerically. The idea is to first posit a variational family of approximating distributions \( q(z; \lambda) \), parametrized by \( \lambda \). Then minimize a metric or divergence so that the vari-
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The most common VI objective is to minimize the exclusive KL, KL(q ∥ p). This objective is an expectation with respect to the approximating distribution q that is convenient to optimize. But this convenience comes at a cost—the q optimized to minimize KL(q ∥ p) will underestimate the variance of the posterior (Dieng et al., 2017; Blei et al., 2017; Turner and Sahani, 2011).

One way to mitigate this issue is to instead optimize the inclusive KL,

$$\text{KL}(p(z|x) \parallel q(z; \lambda)) := \int p(z|x) \log \frac{p(z|x)}{q(z; \lambda)} \, dz. \quad (2)$$

This objective, though more difficult to work with, does not lead to underdispersed approximations. In the context of VI, it has motivated neural adaptive SMC (Gu et al., 2015), RWS (Bornschein and Bengio, 2015), and EP (Minka, 2001). This paper develops MSC, a new algorithm to minimize the inclusive KL divergence.

Minimizing eq. (2) is equivalent to minimizing the cross entropy LKL(λ),

$$\min_{\lambda} L_{KL}(\lambda) := \min_{\lambda} -\int p(z|x) \log q(z; \lambda) \, dz. \quad (3)$$

The gradient w.r.t. the variational parameters is

$$g_{KL}(\lambda) := \nabla_{\lambda} L_{KL}(\lambda) = -\int p(z|x)s(z; \lambda) \, dz, \quad (4)$$

where we define $$s(z; \lambda)$$ to be the score function,

$$s(z; \lambda) := \nabla_{\lambda} \log q(z; \lambda). \quad (5)$$

Because the cross entropy is an expectation with respect to the (intractable) posterior, computing its gradient pointwise is intractable. Recent algorithms for solving eq. (3) focus on stochastic gradient descent (Bornschein and Bengio, 2015; Gu et al., 2015; Finke and Thiery, 2019).

2.2. Stochastic Gradient Descent with IS

We use stochastic gradient descent (SGD) in VI when the gradients of the objective are intractable. The SGD updates

$$\lambda_k = \lambda_{k-1} - \varepsilon_k g_{KL}(\lambda_{k-1}), \quad (6)$$

converges to a local optimum of eq. (3) if the gradient estimate $$\hat{g}_{KL}$$ is unbiased, $$E[\hat{g}_{KL}(\lambda)] = g_{KL}(\lambda)$$, and the step sizes satisfy $$\sum_{k} \varepsilon_k^2 < \infty$$, $$\sum_{k} \varepsilon_k = \infty$$ (Robbins and Monro, 1951; Kushner and Yin, 2003).

When the objective is the exclusive KL(q ∥ p), we can use score-function gradient estimators (Paisley et al., 2012; Salimans and Knowles, 2013; Ranganath et al., 2014), reparameterization gradient estimators (Rezende et al., 2014; Kingma and Welling, 2014), or combinations of the two (Ruiz et al., 2016; Naesseth et al., 2017). These methods provide unbiased stochastic gradients that can help find a local optimum of the exclusive KL.

But consider minimizing the inclusive KL(p ∥ q) eq. (2). For inclusive KL gradient estimation is difficult; it requires an expectation with respect to the posterior p.

One strategy is to use IS (Robert and Casella, 2004) to rewrite the gradient as an expectation with respect to q. Specifically, the gradient of the inclusive KL is proportional to

$$\nabla_{\lambda} KL_{KL}(\lambda) \approx -\mathbb{E}_{q(z; \lambda)} \left[ \frac{p(z|x)}{q(z; \lambda)} s(z; \lambda) \right], \quad (7)$$

where the constant of proportionality $$1/p(x)$$ is independent of the variational parameters and will not affect the solution of the corresponding fixed point equation. This gradient is unbiased, but estimating it using standard MC methods can lead to high variance and poor convergence.

Gu et al. (2015) and Bornschein and Bengio (2015) instead propose the following self-normalized IS (or corresponding SMC) estimate

$$\nabla_{\lambda} KL_{KL}(\lambda) \approx -\sum_{s=1}^{S} \sum_{r=1}^{W} W_r s(z^r; \lambda), \quad (8)$$

where $$W_s = \frac{p(x|x)}{q(x|z_s)}$$, $$z^r \sim q(z^r; \lambda)$$, and $$s(z; \lambda) = \nabla_{\lambda} \log q(z; \lambda)$$. However, eq. (8) is not unbiased. The estimator suffers from systematic error and, consequently, the fitted variational parameters are no longer optimal with respect to the original minimization problem in eq. (3). (See Naesseth et al. (2019); Owen (2013); Robert and Casella (2004) for details about IS and SMC methods)

MSC addresses this shortcoming, introducing an algorithm that provably converges to a solution of eq. (3).

3. Markovian Score Climbing

The key idea in MSC is to use MCMC methods to estimate the intractable gradient. Under suitable conditions on the algorithm, MSC is guaranteed to converge to a local optimum of KL(p ∥ q). The extra computational cost is negligible compared to the biased approaches discussed in section 2.2.

First, we discuss generic MCMC methods to estimate gradients in a SGD algorithm. Then, we discuss CIS, an example Markov kernel that is a simple modification of IS. The
corresponding extension to SMC, i.e. the CSMC kernel, is discussed in the supplement. Next, we discuss learning model parameters. Then, we show that the resulting MSC algorithm is exact in the sense that it converges asymptotically to a local optima of the inclusive KL divergence. Finally, we discuss the large-scale data issue.

3.1. Stochastic Gradient Descent using MCMC

When using gradient descent to optimize the inclusive KL we must compute an expectation of the score function \( s(z; \lambda) \) eq. (5) with respect to the true posterior. To avoid this intractable expectation we propose to use stochastic gradients estimated using samples generated from a MCMC algorithm, with the posterior as its stationary distribution. The key step to ensure convergence, without having to run an infinite inner loop of MCMC updates, is to not re-initialize the Markov chain at each step. Instead, the sample \( z[k−1] \) used to estimate the gradient at step \( k−1 \) is passed to a Markov kernel \( z[k] \sim M(\cdot | z[k−1]) \), with the posterior as its stationary distribution, to get an updated \( z[k] \) that is then used to estimate the current gradient, i.e. the score \( s(z[k]; \lambda) \). This leads to a Markovian stochastic approximation algorithm (Gu and Kong, 1998), where the noise in the gradient estimate is Markovian. Because we are moving in an ascent direction of the score function at each iteration and using MCMC, we refer to the method developed in this paper as Markovian score climbing.

It is not a requirement that the Markov kernel \( M \) is independent of the variational parameters \( \lambda \). In fact MSC allows for tying the variational approximation directly to the Markov chain. We detail MSC in algorithm 1.

**Algorithm 1 Markovian Score Climbing**

**Input:** Markov kernel \( M(z' | z; \lambda) \) with stationary distribution \( p(z|x) \), variational family \( q(z; \lambda) \), initial \( \lambda_0 \), initial \( z[0] \), step size sequence \( \epsilon_k \), and number of iterations \( K \).

**Output:** \( \lambda_K \approx \lambda^* \).

1. for \( k = 1, \ldots, K \) do
2. Sample \( z[k] \sim M(\cdot | z[k−1]; \lambda_{k−1}) \)
3. Compute \( s(z[k]; \lambda_{k−1}) = \nabla_\lambda \log q(z[k]; \lambda_{k−1}) \)
4. Set \( \lambda_k = \lambda_{k−1} + \epsilon_k s(z[k]; \lambda_{k−1}) \)
5. end

Next, we discuss CIS (Andrieu et al., 2010; Naesseth et al., 2019), an example Markov kernel with adaptation that is a simple modifications of its namesake IS. The corresponding extension to SMC, the CSMC kernel (Andrieu et al., 2010; Naesseth et al., 2019), is discussed in the supplement. Using these Markov kernels to estimate gradients, rather than IS and SMC (Gu et al., 2015; Bornschein and Bengio, 2015), lead to algorithms that provably converge to a local optimum of the inclusive KL divergence.

3.2. Conditional Importance Sampling

CIS is an IS-based Markov kernel with \( p(z|x) \) as its stationary distribution (Andrieu et al., 2010; Naesseth et al., 2019). It modifies the classical IS algorithm by retaining one of the samples from the previous iteration, the so-called conditional sample. Each iteration consists of three steps: generate new samples from a proposal, compute weights, and then update the conditional sample for the next iteration. We explain in detail below.

First, set the first proposed sample to be equal to the conditional sample from the previous iteration, i.e. \( z^1 = z[k−1] \), and propose the remaining \( S−1 \) samples from a proposal distribution \( q \)

\[
z^i \sim q(z; \lambda), \quad i = 2, \ldots, S.
\]

The proposal does not necessarily need to be equal to the variational approximation, a common option is to use the model prior \( p(z) \). However, we will in the remainder of this paper assume that the variational approximation is used as the proposal.

Then, compute the importance weights for all \( S \) samples, including the conditional sample. The importance weights for \( i = 1, \ldots, S \) are

\[
w^i = \frac{p(z^i, x)}{q(z^i; \lambda)}, \quad \tilde{w}^i = \frac{w^i}{\sum_{j=1}^S w^j}.
\]

Finally, generate an updated conditional sample by picking one of the proposed values with probability proportional to its (normalized) weight, i.e.,

\[
z[k] = z^j,
\]

where \( J \) is a discrete random variable with probability \( \mathbb{P}(J = j) = \tilde{w}^j \).

Iteratively repeating this procedure constructs a Markov chain with the posterior \( p(z|x) \) as its stationary distribution (Andrieu et al., 2010; Naesseth et al., 2019). With this it is possible to attain an estimate of the (negative) gradient with respect to the variational parameters of eq. (3) as follows:

\[
s(z[k]; \lambda) = \nabla_\lambda \log q(z[k]; \lambda),
\]

where \( z[k] \) is the conditional sample retained at each iteration of the CIS algorithm. Another option is to make use of all the particles at each iteration, i.e. the Rao-Blackwellized estimate,

\[
\bar{g}_{KL}(\lambda) = \sum_{i=1}^S \tilde{w}^i s(z^i; \lambda).
\]
We summarize one full iteration of the CIS algorithm in algorithm 2. This algorithm defines a Markov kernel $M(z[k] | z[k-1]; \lambda)$ with the posterior as its stationary distribution, useful for MSC.

### 3.3. Model Parameters

If the probabilistic model has unknown parameters $\theta$ one solution is to assign them a prior distribution, include them in the latent variable $z$, and apply the method outlined above to approximate the posterior. However, an alternative solution is to use the maximum likelihood (ML) principle and optimize the marginal likelihood, $p(x; \theta)$, jointly with the approximate posterior, $q(z; \lambda)$. We propose to use Markovian score climbing based on the Fisher identity of the gradient

$$
\hat{g}_{\text{ML}}(\theta) = \nabla_{\theta} \log p(x; \theta) = \nabla_{\theta} \log \int p(z,x; \theta) \, dz
$$

$$
= \mathbb{E}_{p(x|z)}[\nabla_{\theta} \log p(z,x; \theta)].
$$

With a Markov kernel $M(z[k] | z[k-1]; \theta, \lambda)$, with the posterior distribution $p(z|x; \theta)$ as its stationary distribution, the approximate gradient is

$$
\hat{g}_{\text{ML}}(\theta) = \nabla_{\theta} \log p(z[k], x; \theta).
$$

The generic MSC algorithm for maximization of the log-marginal likelihood, with respect to $\theta$, and minimization of the inclusive KL divergence, with respect to $\lambda$, is summarized in algorithm 3. Using MSC only for ML estimation of $\theta$, with a fixed Markov kernel $M$ and without the VI steps on lines 13 and 15, is equivalent to the MCMC maximum likelihood method by Gu and Kong (1998).

### 3.4. The Convergence of MSC

One of the main benefits of MSC is that it is possible, under conditions, to ensure that the variational parameter estimate $\lambda_k$ as provided by algorithm 1 converges to a local optima of the inclusive KL divergence as the number of iterations $K$ tend to infinity.

To state the main result we make a few definitions. Let $\lambda^*$ be a minimizer of the inclusive KL divergence in eq. (3). Consider the ordinary differential equation (ODE) defined by

$$
\frac{d}{dt} \hat{\lambda}(t) = \mathbb{E}_{p(x|z)}[-s(z, \lambda(t))],
\quad \hat{\lambda}(0) = \lambda_0,
$$

and its solution $\hat{\lambda}(t), t \geq 0$. If the ODE in eq. (12) admits the unique solution $\hat{\lambda}(t) = \tilde{\lambda}, t \geq 0$ for $\hat{\lambda}(0) = \tilde{\lambda}$, then $\tilde{\lambda}$ is called a stability point. The minimizer $\lambda^*$ is a stability point of eq. (12). A set $\Lambda$ is called the domain of attraction of $\lambda^*$, if the solution to eq. (12) for $\hat{\lambda}(0) \in \Lambda$ remains in $\Lambda$ and converges to $\tilde{\lambda}$.

We formalize the convergence result in proposition 1. The result is an adaptation of Gu and Kong (1998, Theorem 1) and based on Benveniste et al. (1990, Theorem 3.17, page 304).

**Proposition 1.** Assume that $C1$–$C6$, detailed in the supplement, hold. If $\lambda_k$ for $k \geq 1$ defined by algorithm 1 is a bounded sequence and almost surely visits a compact subset of the domain of attraction of $\lambda^*$ infinitely often, then

$$
\lambda_k \to \lambda^* \quad \text{almost surely.}
$$

**Proof.** See the Supplementary Material.

### 3.5. MSC on Large-Scale Data

If the dataset is large it might be impractical to evaluate the full likelihood at each step and it would be preferable to consider only a subset of the data at each iteration. For the exclusive KL divergence this is straightforward; the likelihood enters as a sum of the individual log-likelihood terms for all datapoints, and a simple unbiased estimate can be
constructed by sampling one (or a few) datapoints to evaluate at each iteration. However, for the inclusive KL divergence the likelihood enters as a product and subsampling is difficult in general.

Standard MCMC kernels require evaluation of the complete likelihood at each iteration, which means that the method proposed in this paper likewise must evaluate all the data points at each iteration of algorithm 1. An option is to follow Li and Turner (2016); Dieng et al. (2017) and use subset average likelihoods. In appendix A we prove that this approach leads to systematic errors that are difficult to quantify. It does not minimize the inclusive KL from p to q, rather it minimizes the KL divergence from a perturbed posterior $\bar{p}$ to q. A potential remedy to this issue, that we leave for future work, is to consider approximate MCMC (with theoretical guarantees) such as reviewed in e.g. Bardenet et al. (2017); Angelino et al. (2016).

4. Empirical Evaluation

In the empirical studies we illustrate convergence on a toy model and demonstrate the utility of MSC on Bayesian probit regression for classification as well as a stochastic volatility model for financial data.

The studies show that MSC (i) converges to the true solution whereas the biased methods do not; (ii) achieves similar predictive performance as EP and IS on probit regression while being more robust to the choice of sample size $S$; and (iii) learns superior or as good stochastic volatility models as SMC.

4.1. Skew Normal Distribution

We illustrate the impact of the biased gradients discussed in section 2.2 on a toy example. Let $p(z|x)$ be a scalar skew normal distribution with location, scale and shape parameters $(\xi, \omega, \alpha) = (0.5, 2, 5)$. We let the variational approximation be a family of normal distributions $q(z; \lambda) = \mathcal{N}(z; \mu, \sigma^2)$. For this choice of posterior and approximating family it is possible to compute the analytical solution for the inclusive KL divergence; it corresponds to matching the moments of the variational approximation and the posterior distribution. In fig. 1 we show the results of SGD using the biased gradients from eq. (8), i.e. using self-normalized IS to estimate the gradients, and MSC (this paper) as described in section 3. We set the number of samples to $S = 2$. We can see how the biased gradient leads to systematic errors when estimating the variational parameters, whereas MSC obtains the true solution. Increasing the number of samples for the estimator in eq. (8) will lower the bias, and in the limit of infinite samples $S$ it is exact. However, MSC provides consistent estimates of the variational parameters even with small number of samples.

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Figure 1. MSC converges to the true solution, while the biased IS approach does not. Example of learnt variational parameters for IS- and MSC-based gradients of the inclusive KL, as well as true parameters. The example uses a Gaussian approximation to a skew normal posterior distribution. Iterations in log-scale.

Note that the biased IS-gradients results in an underestimation of the variance. One of the main motivations for using inclusive KL as optimization objective is to avoid such underestimation of uncertainty. This example shows that when the inclusive KL is optimized with biased gradients the solution can no longer be trusted in this respect.

The gradients for Rényi- and $\chi$ divergences used in e.g. Li and Turner (2016); Dieng et al. (2017) suffer from a similar bias. The supplement provides a $\chi$ divergence analogue to fig. 1.

4.2. Bayesian Probit Regression

Probit regression is commonly used for binary classification in machine learning and statistics. The Bayesian probit regression model assigns a Gaussian prior to the parameters. The prior and likelihood are

$$p(z) = \mathcal{N}(z; 0, I),$$

$$P(y_i = y | z, x_i) = \Phi(x_i^\top z)^y (1 - \Phi(x_i^\top z))^{1-y},$$

where $y \in \{0, 1\}$ and $\Phi(\cdot)$ is the cumulative distribution function of the normal distribution. We apply the model for prediction in several UCI datasets (Dua and Graff, 2017). We let the variational approximation be a Gaussian distri-
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Figure 2. MSC is more robust to the number of samples $S$. The fitted mean parameter $\mu^*$, for three representative dimensions of $z$, of MSC (this paper) and IS (cf. (Bornschein and Bengio, 2015)) on the Ionos and Heart datasets. The error bars corresponds to 100 random initializations.

Table 1 illustrates the predictive performance of the fitted model on held-out test data. The results where generated by splitting each dataset 100 times into 90% training and 10% test data, then computing average prediction error and its standard deviation. MSC performs as well as EP which is particularly well suited to this problem. However, EP requires more model-specific derivations and can be difficult to implement when the moment matching subproblem cannot be solved in closed form. In these experiments the bias introduced by IS does not impact the predictive performance compared to MSC.

We compare how the approximations based on MSC and IS are affected by the number of samples $S$ at each iteration. In fig. 2 we plot the mean value $\mu^*$ based on 100 random initializations for several values of $S$ on the Heart and Ionos datasets. The MSC is more robust to the choice of $S$, converging to similar mean values for all the choices of $S$ in this example. For the Heart dataset, IS clearly struggles with a bias for low values of the number of samples $S$.

### 4.3. Stochastic Volatility

The stochastic volatility model is commonly used in financial econometrics (Chib et al., 2009). The model is

$$p(z_0 ; \theta) = \mathcal{N}(z_0 ; 0, \frac{\sigma^2}{1 - \phi^2}),$$

$$p(z_i | z_{i-1} ; \theta) = \mathcal{N}(z_i ; \mu + \phi(z_{i-1} - \mu), \sigma^2),$$

$$p(x_i | z_i ; \theta) = \mathcal{N}(x_i ; 0, \beta \exp(z_i)),$$

where the parameters are constrained as follows $\theta = (\sigma^2, \phi, \mu, \beta) \in \mathbb{R}_+ \times (-1, 1) \times \mathbb{R} \times \mathbb{R}_+$. Both the poste-

| Dataset      | EP (Minka, 2001) | IS (B.B. 2015) | MSC (this paper) |
|--------------|-----------------|----------------|------------------|
| Pima         | 0.227 ± 0.048   | 0.229 ± 0.047  | 0.227 ± 0.046    |
| Ionos        | 0.115 ± 0.053   | 0.115 ± 0.054  | 0.117 ± 0.053    |
| Heart        | 0.161 ± 0.066   | 0.163 ± 0.066  | 0.160 ± 0.063    |

Test error for Bayesian probit regression; lower is better. Estimated using EP (Minka, 2001), IS (cf. Bornschein and Bengio (2015)), and MSC (this paper) for 3 UCI datasets. Predictive performance is comparable between the methods.

\[
q(z_0 ; \phi) = \mathcal{N}(z_0 ; 0, \frac{\sigma^2}{1 - \phi^2}),
\]

where $\Sigma$ is a diagonal covariance matrix. We compare MSC (this paper) with the biased IS-based approach (cf. eq. (8) and Bornschein and Bengio (2015)) and EP (Minka, 2001) that minimizes the inclusive KL locally. For SGD methods we make use of the adaptive step-size by Kingma and Ba (2014).
The benefit of using the inclusive KL is to obtain a more “robust” approximation that does not underestimate the uncertainty. However, in this paper we have argued, and illustrated numerically, that such underestimation of uncertainty can still be an issue, if the optimization is based on biased gradient estimates, as is the case for previously proposed VI algorithms. As a remedy, we introduced Markovian score climbing, a new way to reliably learn a variational approximation that minimizes the inclusive KL. This results in a method that melds VI and MCMC. We have illustrated its convergence properties on a simple toy example, and studied its performance on Bayesian probit regression for classification as well as a stochastic volatility model for financial data.

A. Subset Average Likelihood

Li and Turner (2016); Dieng et al. (2017), who study different classes of divergences where the likelihood also enters as a product, propose to replace the true likelihood at each iteration with a “subset average likelihood”. The subset average likelihood approach makes the following approximation

$$p(x | z) = \prod_{i=1}^{n} p(x_i | z) \approx p(x_M | z)^2 := \prod_{j \in M} p(x_j | z)^2,$$

where $M \subset \{1, \ldots, n\}$ is a set of indices corresponding to a mini-batch of size $m = |M|$ data points sampled uniformly from $\{x_1, \ldots, x_n\}$ with or without replacement. Considering the same approach for the inclusive KL case the unbiased stochastic gradient obtained is

$$\frac{1}{S} \sum_{s=1}^{S} \frac{p(z^s)p(x_M | z^s)^2}{q(z^s | \lambda)} \nabla_\lambda \log q(z^s | \lambda), \; z^s \sim q(z | \lambda).$$

This approximation also leads to a systematic error in the SGD algorithm. It is no longer minimizing the KL divergence from the posterior $p$ to the variational approximation $q$. In fact, it is possible to show that it is actually minimizing the KL divergence from a perturbed posterior $\bar{p}$, where the likelihood is replaced by a mixture of all potential subset average likelihoods, to the variational approximation $q$. This result is formalized by proposition 2.

Proposition 2. Using the stochastic gradient defined by eq. (13) and an iterative SGD algorithm according to eq. (6) the fixed points $\lambda^*$ are identical to the solution to

$$\nabla_\lambda \text{KL}(\bar{p}(z | x) || q(z | \lambda)) = 0,$$

where the perturbed posterior $\bar{p}$, if it exists, is given by

$$\bar{p}(z | x) \propto p(z) \sum_{M \in \#} p(x_M | z)^2.$$
and $\mathcal{M}$ is the set of all possible combinations of minibatches $M$ of size $m$.

**Proof.** See the Supplementary Material.

In the supplement we provide illustrations on a simulated example. It is in general difficult to determine the magnitude of the error introduced by the subset average likelihood in practical applications. The subset average likelihood approach for Rényi and $\chi^2$ divergences (Li and Turner, 2016; Dieng et al., 2017) likewise leads to a systematic error in the stochastic gradient. Furthermore, the fixed points of the resulting stochastic systems for these divergences are difficult to quantify, making it even harder to understand the effect of the approximation.

**References**

C. Andrieu and M. Vihola. Markovian stochastic approximation with expanding projections. *Bernoulli*, 20(2), Nov. 2014.

C. Andrieu, A. Doucet, and R. Holenstein. Particle Markov chain Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 72(3):269–342, 2010.

E. Angelino, M. J. Johnson, R. P. Adams, et al. Patterns of scalable bayesian inference. *Foundations and Trends® in Machine Learning*, 9(2-3):119–247, 2016.

R. Bardenet, A. Doucet, and C. Holmes. On Markov chain Monte Carlo methods for tall data. *Journal of Machine Learning Research*, 18(47):1–43, 2017.

A. Benveniste, M. Métivier, and P. Priouret. *Adaptive algorithms and stochastic approximations*, volume 22. Springer Science & Business Media, 1990.

D. Blei, A. Kucukelbir, and J. D. McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.

B. Bornschein and Y. Bengio. Reweighted wake-sleep. In *International Conference on Learning Representations*, 2015.

Y. Burda, R. Grosse, and R. Salakhutdinov. Importance weighted autoencoders. In *International Conference on Learning Representations*, 2016.

S. Chib, Y. Omori, and M. Asai. *Multivariate Stochastic Volatility*, pages 365–400. Springer Berlin Heidelberg, Berlin, Heidelberg, 2009.

A. B. Dieng, D. Tran, R. Ranganath, J. Paisley, and D. Blei. Variational inference via chi upper bound minimization. In *Advances in Neural Information Processing Systems 30*, pages 2732–2741. Curran Associates, Inc., 2017.

J. Domke and D. R. Sheldon. Divide and couple: Using monte carlo variational objectives for posterior approximation. In *Advances in Neural Information Processing Systems*, pages 338–347, 2019.

D. Dua and C. Graff. UCI machine learning repository, 2017. URL http://archive.ics.uci.edu/ml.

A. Finke and A. H. Thiery. On importance-weighted autoencoders. *arXiv:1907.10477*, 2019.

Z. Ghahramani and M. J. Beal. Propagation algorithms for variational Bayesian learning. In *Advances in neural information processing systems*, pages 507–513, 2001.

M. G. Gu and F. H. Kong. A stochastic approximation algorithm with Markov chain Monte-Carlo method for incomplete data estimation problems. *Proceedings of the National Academy of Sciences*, 95(13):7270–7274, 1998.

S. S. Gu, Z. Ghahramani, and R. E. Turner. Neural adaptive sequential Monte Carlo. In *Advances in Neural Information Processing Systems 28*, pages 2629–2637. Curran Associates, Inc., 2015.

P. Guarniero, A. M. Johansen, and A. Lee. The iterated auxiliary particle filter. *Journal of the American Statistical Association*, 112(520):1636–1647, 2017.

R. Habib and D. Barber. Auxiliary variational MCMC. In *International Conference on Learning Representations*, 2019.

J. Heng, A. N. Bishop, G. Deligiannidis, and A. Doucet. Controlled sequential Monte Carlo. *arXiv:1708.08396*, 2017.

M. Hoffman, P. Sountsov, J. V. Dillon, I. Langmore, D. Tran, and S. Vasudevan. Neutra-lizing bad geometry in Hamiltonian Monte Carlo using neural transport. *arXiv:1903.03704*, 2019.

M. D. Hoffman. Learning deep latent Gaussian models with Markov chain Monte Carlo. In *Proceedings of the 34th International Conference on Machine Learning*, pages 1510–1519, 2017.

M. I. Jordan, Z. Ghahramani, T. S. Jaakkola, and L. K. Saul. An introduction to variational methods for graphical models. *Machine Learning*, 37(2):183–233, Nov. 1999.

D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
D. P. Kingma and M. Welling. Auto-encoding variational Bayes. In *International Conference on Learning Representations*, 2014.

E. Kuhn and M. Lavielle. Coupling a stochastic approximation version of EM with an MCMC procedure. *ESAIM: Probability and Statistics*, 8:115–131, 2004.

H. Kushner and G. G. Yin. *Stochastic approximation and recursive algorithms and applications*, volume 35. Springer Science & Business Media, 2003.

D. Lawson, G. Tucker, C. A. Naesseth, C. Maddison, and Y. Whye Teh. Twisted variational sequential Monte Carlo. *Third workshop on Bayesian Deep Learning (NeurIPS)*, 2018.

T. A. Le, M. Igl, T. Rainforth, T. Jin, and F. Wood. Auto-encoding sequential Monte Carlo. In *International Conference on Learning Representations*, 2018.

Y. Li and R. E. Turner. Rényi divergence variational inference. In *Advances in Neural Information Processing Systems* 29, pages 1073–1081. Curran Associates, Inc., 2016.

F. Lindsten, M. I. Jordan, and T. B. Schön. Particle Gibbs with ancestor sampling. *The Journal of Machine Learning Research*, 15(1):2145–2184, 2014.

F. Lindsten, J. Helske, and M. Vihola. Graphical model inference: Sequential Monte Carlo meets deterministic approximations. In *Advances in Neural Information Processing Systems* 31, pages 8201–8211. Curran Associates, Inc., 2018.

C. J. Maddison, D. Lawson, G. Tucker, N. Heess, M. Norouzi, A. Mnih, A. Doucet, and Y. Whye Teh. Filtering variational objectives. In *Advances in Neural Information Processing Systems*, 2017.

T. Minka. Divergence measures and message passing. Technical report, Technical report, Microsoft Research, 2005.

T. P. Minka. Expectation propagation for approximate Bayesian inference. In *Proceedings of the Seventeenth conference on Uncertainty in artificial intelligence*, pages 362–369. Morgan Kaufmann Publishers Inc., 2001.

A. K. Moretti, Z. Wang, L. Wu, I. Drori, and I. Pe’er. Particle smoothing variational objectives. *arXiv:1909.09734*, 2019.

C. A. Naesseth, F. J. Ruiz, S. W. Linderman, and D. Blei. Reparameterization gradients through acceptance-rejection sampling algorithms. In *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, 2017.

C. A. Naesseth, S. Linderman, R. Ranganath, and D. Blei. Variational sequential Monte Carlo. In *International Conference on Artificial Intelligence and Statistics*, volume 84, pages 968–977. PMLR, 2018.

C. A. Naesseth, F. Lindsten, and T. B. Schön. Elements of sequential Monte Carlo. *Foundations and Trends® in Machine Learning*, 12(3):307–392, 2019.

A. B. Owen. *Monte Carlo theory, methods and examples*. 2013.

J. W. Paisley, D. Blei, and M. I. Jordan. Variational Bayesian inference with stochastic search. In *International Conference on Machine Learning*, 2012.

R. Ranganath, S. Gerrish, and D. Blei. Black box variational inference. In *Artificial Intelligence and Statistics*, 2014.

D. J. Rezende, S. Mohamed, and D. Wierstra. Stochastic backpropagation and approximate inference in deep generative models. In *International Conference on Machine Learning*, 2014.

H. Robbins and S. Monro. A stochastic approximation method. *The Annals of Mathematical Statistics*, pages 400–407, 1951.

C. Robert and G. Casella. *Monte Carlo statistical methods*. Springer Science & Business Media, 2004.

F. J. R. Ruiz and M. K. Titsias. A contrastive divergence for combining variational inference and MCMC. In *Proceedings of the 36th International Conference on Machine Learning*, pages 5537–5545, 2019.

F. J. R. Ruiz, M. K. Titsias, and D. Blei. The generalized reparameterization gradient. In *Advances in Neural Information Processing Systems*, 2016.

T. Salimans and D. A. Knowles. Fixed-form variational posterior approximation through stochastic linear regression. *Bayesian Analysis*, 8(4):837–882, 2013.

T. Salimans, D. Kingma, and M. Welling. Markov chain Monte Carlo and variational inference: Bridging the gap. In *International Conference on Machine Learning*, pages 1218–1226, 2015.

R. E. Turner and M. Sahani. Two problems with variational expectation maximisation for time-series models. In D. Barber, A. T. Cemgil, and S. Chiappa, editors, *Bayesian time series models*, chapter 5, pages 109–130. Cambridge University Press, 2011.
B. Supplementary Material

Conditional Sequential Monte Carlo

Just like CIS is a straightforward modification of IS, so is CSMC a straightforward modification of SMC. We make use of CSMC with ancestor sampling as proposed by Lindsten et al. (2014) combined with twisted SMC (Guarniero et al., 2017; Heng et al., 2017; Naesseth et al., 2019). While SMC can be adapted to perform inference for almost any probabilistic model (Naesseth et al., 2019), we here focus on the state space model

\[ p(z_{1:T}, x_{1:T}) = p(z_1)p(x_1 | z_1)\prod_{t=1}^{T} p(z_t | z_{t-1})p(x_t | z_t), \]

where we assume that the prior \( p(z_1) \) and transition \( p(z_t | z_{t-1}) \) are conditionally Gaussian. Because the prior and transition distributions are Gaussian it is convenient to define the full approximation to the posterior \( p(z_{1:T} | x_{1:T}) \) to be the multivariate normal

\[ q(z_{1:T}; \lambda) = q(z_1; \lambda_1)\prod_{t=2}^{T} q(z_t | z_{t-1}; \lambda_t), \tag{15} \]

\[ q(z_t | z_{t-1}; \lambda_t) \propto p(z_t)\psi(z_t; \lambda_t), \]

\[ q(z_t; \lambda_t) \propto p(z_t)\psi(z_t; \lambda_t), \]

where \( \psi \) are twisting potentials

\[ \psi(z_t; \lambda_t) = \exp\left(-\frac{1}{2}z_t^\top\Lambda_t z_t + v_t^\top z_t\right), \]

with \( \lambda_t = (\Lambda_t, v_t) \). We are now equipped to explain the CSMC kernel that updates a conditional trajectory \( z_{1:T}[k-1] = (z_1[k-1], \ldots, z_T[k-1]) \). Each iteration of CSMC consists of three steps: initialization for \( t = 1 \), running a modified SMC algorithm for \( t > 1 \), and then updating the conditional sample for the next iteration. We explain in detail below.

First, perform (conditional) IS for the first step where \( t = 1 \). Set \( z_1^1 = z_1[k-1] \) and propose the remaining \( S - 1 \) samples from a proposal distribution \( q \)

\[ z_i^1 \sim q(z_i; \lambda_1), \quad i = 2, \ldots, S \]

and compute the importance weights for \( i = 1, \ldots, S \)

\[ w_i^1 = \frac{p(z_i^1)\psi(z_i^1; \lambda_1)}{q(z_i; \lambda_1)}, \quad \bar{w}_1^i = \frac{w_1^i}{\sum_{j=1}^{S} w_j^i}. \]

Then, for each step \( t > 1 \) in turn perform resampling, ancestor sampling, propagation and weighting. Resampling picks the most promising earlier sample to propagate, i.e. for \( i = 2, \ldots, S \) simulate ancestor variables \( a_{t-1}^i \) with probability

\[ P\left(a_{t-1}^i = j\right) = \bar{w}_{t-1}^j. \]

For \( i = 1 \) instead, simulate the corresponding ancestor variable \( a_{t-1}^1 \) with probability

\[ P\left(a_{t-1}^1 = j\right) \propto \bar{w}_{t-1}^j q(z_t[k-1] | z_{t-1}^1; \lambda_1), \]

where \( z_t[k-1] \) is the corresponding element of the conditional trajectory \( z_{1:T} \) from the previous iteration. This is known as ancestor sampling (Lindsten et al., 2014).

When propagating for \( i = 1 \) simply set \( z_i^1 = z_i[k-1] \), and simulate the remainder from the proposal distribution

\[ z_i^i \sim q(z_i | z_{i-1}^i; \lambda), \quad i = 2, \ldots, S \]
Set \( z_{1:t}^i = (z_{1:t-1}^i, z_t^i) \) and compute the weights for all \( i = 1, \ldots, S \)

\[
 w_i^t = \frac{p(z_t^i \mid z_{1:t-1}^i)p(x_{t-1} \mid z_{1:t-1}^i)}{q(z_t^i \mid z_{1:t-1}^i; \lambda_t)} \frac{\lambda^t}{\psi(z_t^i \mid z_{1:t-1}^i; \lambda_t)},
\]

(16)

\[
 \hat{w}_i^t = \frac{w_i^t}{\sum_{j=1}^S w_j^t}.
\]

For the final step \( t = T \) the (unnormalized) weights are instead

\[
 w_T^i = \frac{p(z_T^i \mid z_{1:T-1}^i)p(x_{T-1} \mid z_{1:T-1}^i)}{q(z_T^i \mid z_{T-1}^i; \lambda_T)} \frac{p(x_T \mid z_T^i)}{\psi(z_T^i \mid z_{1:T-1}^i; \lambda_T)}. 
\]

(17)

Finally, an updated conditional sample is generated by picking one of the proposed trajectories with probability proportional to its (normalized) weight, i.e.

\[
 z_{1:T}[k] = z_{1:T}^j,
\]

where \( J \) is a discrete random variable with probability \( \mathbb{P}(J = j) = \hat{w}_T^j \).

Repeating this procedure iteratively constructs a Markov chain with the posterior \( p(z_{1:T} \mid x_{1:T}) \) as its stationary distribution (Andrieu et al., 2010; Lindsten et al., 2014; Naesseth et al., 2019). With this it is possible to attain an estimate of the integral to its (normalized) weight, i.e.

\[
 \int \cdots \int M(z_\Lambda, dz') \leq C_1 \binom{1 + |z|^q}.
\]

Proof of Proposition 1

This result is an adaptation of Gu and Kong (1998, Theorem 1) based on Benveniste et al. (1990, Theorem 3.17, page 304). Suppose that \( \lambda_k \in \mathbb{R}^d \) and that \( \Lambda \) is an open set in \( \mathbb{R}^d \). Furthermore, suppose \( z[k] \in \mathbb{R}^d \) and that \( Z \) is an open set in \( \mathbb{R}^d \). Denote the Markov kernel in MSC, algorithm 1, by \( M_\Lambda(z, dz') \) and repeated application of it by \( M_\Lambda(z, dz') = \int \cdots \int M_\Lambda(z, dz_1)M_\Lambda(z_1, dz_2) \cdots M_\Lambda(z_{k-1}, dz') \). \(|z|\) denotes the length of the vector \( z \). Let \( Q \) be any compact subset of \( \Lambda \), and \( q > 1 \) a sufficiently large real number such that the following assumptions hold. We follow Gu and Kong (1998) and assume:

C 1. Assume that the step size sequence satisfies \( \sum_{k=1}^\infty \epsilon_k = \infty \) and \( \sum_{k=1}^\infty \epsilon_k^2 < \infty \).

C 2 (Integrability). There exists a constant \( C_1 \) such that for any \( \lambda \in \Lambda, z \in Z \) and \( k \geq 1 \),

\[
 \int \left( 1 + |z|^q \right) M_\Lambda(z, dz') \leq C_1 \left( 1 + |z|^q \right)
\]

C 3 (Convergence of the Markov Chain). Let \( p(z \mid x) \) be the unique invariant measure for \( M_\lambda \). For each \( \lambda \in \Lambda \),

\[
 \lim_{k \to \infty} \sup_{z \in Z} \frac{1}{1 + |z|^q} \int \left( 1 + |z'|^q \right) |M_\lambda(z, dz') - p(dz' \mid x)| = 0.
\]

C 4 (Continuity in \( \lambda \)). There exists a constant \( C_2 \), such that for all \( \lambda, \lambda' \in Q \)

\[
 \left| \int \left( 1 + |z'|^q \right) (M_\lambda(z, dz') - M_{\lambda'}(z, dz')) \right| \leq C_2 |\lambda - \lambda'| \left( 1 + |z|^q \right).
\]
Markovian Score Climbing

Algorithm 4 Conditional Sequential Monte Carlo

Input: Model \( p(z_{1:T}, x_{1:T}) \), proposal \( q(z_{1:T}; \lambda) \), conditional sample \( z_{1:T}[k−1] \), and total number of internal samples \( S \).
Output: \( z_{1:T}[k] \sim M(\cdot | z_{1:T}[k−1]; \lambda) \), updated conditional sample.

18 Set \( z_1^i = z_1[k] \)
19 Sample \( z_1^i \sim q(z_1; \lambda_1) \) for \( i = 2, \ldots, S \)
20 Compute \( w_1^i = \frac{p(z_1^i)q(z_1^i; \lambda_1)}{q(z_1^i; \lambda_1)} \) for \( i = 1, \ldots, S \)

21 for \( t = 2, \ldots, T \) do
22 for \( i = 2, \ldots, S \) do
23 Sample \( a_{t−1}^i \) w.p. \( P(a_{t−1}^i = j) = \tilde{w}_{t−1}^j \)
24 Sample \( z_t^i \sim q(z_t | z_{t−1}^i; \lambda_t) \)
25 end
26 Sample \( a_t^1 \) w.p. \( P(a_t^1 = j) \propto \tilde{w}_{t}^j q(z_t[k]; z_{t−1}^j; \lambda_t) \)
27 Set \( z_t^1 = z_t[k] \)
28 for \( i = 1, \ldots, S \) do
29 Compute \( w_t^i \) in eq. (16) or eq. (17)
30 Set \( z_{1:t}^i = \left( z_{1:t−1}^i, z_t^i \right) \)
31 end
32 end
33 Sample \( J \) with probability \( P(J = j) \propto \tilde{w}_T^j \)
34 Set \( z_{1:T}[k] = z_{1:T}^i \)

C 5 (Continuity in \( z \)). There exists a constant \( C_3 \), such that for all \( z_1, z_2 \in \mathbb{Z} \)

\[
\sup_{\lambda \in \Lambda} \left| \int (1 + |z|^{q+1})(M_\lambda(z_1, dz') - M_\lambda(z_2, dz')) \right| \leq C_3 |z_1 - z_2| (1 + |z_1|^p + |z_2|^p).
\]

C 6 (Conditions on the Score Function). For any compact subset \( Q \subset \Lambda \), there exist positive constants \( p, K_1, K_2, K_3 \) and \( \nu > 1/2 \) such that for all \( \lambda, \lambda' \in \Lambda \) and \( z, z_1, z_2 \in \mathbb{Z}, \)

\[
|\nabla_\lambda \log q(z; \lambda)| \leq K_1 (1 + |z|^{p+1}),
\]

\[
|\nabla_\lambda \log q(z_1; \lambda) - \nabla_\lambda \log q(z_2; \lambda)| \leq K_2 |z_1 - z_2| (1 + |z_1|^p + |z_2|^p),
\]

\[
|\nabla_\lambda \log q(z; \lambda) - \nabla_\lambda \log q(z; \lambda')| \leq K_3 |\lambda - \lambda'|^{\nu} (1 + |z|^{p+1}).
\]

The constants \( C_1, \ldots, C_3 \) and \( \nu \) may depend on the compact set \( Q \) and the real number \( q \).

With the above assumptions the result follows from Gu and Kong (1998, Theorem 1) where (left - their notation, right - our notation)

\[
\theta = \lambda,
\]

\[
x = z,
\]

\[
\Pi_\theta = M_\lambda,
\]

\[
H(\theta, x) = \nabla_\lambda \log q(z; \lambda),
\]

and \( I(\theta, x) = 0, \Gamma_k = 0 \).
Figure 4. The difference in log-standard deviation of the variational approximation, \( \log \sigma^{*}_{MSC} - \log \sigma^{*}_{IS} \), between parameters learnt using MSC (this paper) and IS (cf. (Bornschein and Bengio, 2015)). The dimension of the latent variable is plotted versus the parameters learnt from 100 random splits.

Proof of Proposition 2

The fixed points of the iterative algorithm are the solutions to the equation when we set the expectation of eq. (13) equal to zero. The equation is given by

\[
\mathbb{E} \left[ \frac{1}{S} \sum_{s=1}^{S} p(z') p(x_M | z') \nabla_{\lambda} \log q(z' ; \lambda) \right] = \mathbb{E} \left[ -\frac{p(z) p(x_M | z)}{q(z ; \lambda)} \nabla_{\lambda} \log q(z ; \lambda) \right]
\]

\[
\mathbb{E} \left[ p(z) \frac{1}{|M|} \sum_{M \in M} p(x_M | z)^{n} \nabla_{\lambda} \log q(z ; \lambda) \right] = 0
\]

\[
\iff \mathbb{E}_{p(z|x)} \left[ -\nabla_{\lambda} \log q(z ; \lambda) \right] = 0
\]

\[
\iff \nabla_{\lambda} \text{KL} (p(z | x) || q(z ; \lambda)) = 0,
\]

where the first equality follows because the samples \( z' \) are independent and identically distributed. The second equality follows by the distribution of the mini-batches. The first equivalence follows because \( z \sim q(z ; \lambda) \) and we multiply both sides by a constant independent of \( \lambda \). The final equivalence follows because \( p(z | x) \) does not depend on \( \lambda \). This concludes the proof.

Additional Results Bayesian Probit Regression

We also compare the posterior uncertainty learnt using MSC and IS. Figure 4 shows difference in the log-standard deviation between the posterior approximation learnt using MSC and that using IS, i.e. \( \log \sigma^{*}_{MSC} - \log \sigma^{*}_{IS} \). The figure contains one boxplot for each dimension of the latent variable and is based on data from 100 random train-test splits. We can see that for two of the datasets, Heart and Ionos, MSC on average learns a posterior approximation with higher uncertainty. However, for the Pima dataset the IS-based method tends to learn higher variance approximations.

Additional Results Subset Average Likelihoods

We illustrate the difference between the true and perturbed posteriors in fig. 5 for a toy example where the two distributions can be computed exactly. The model is an unknown mean measured in Gaussian noise with a conjugate prior, i.e. \( z \sim \mathcal{N}(0, 1) \), \( x_i \sim \mathcal{N}(z, 1) \). To be able to exactly compute the perturbed posterior we keep the number of data points small \( n = 10 \). The figure shows the true and perturbed posteriors for two randomly generated datasets with \( m = 2, 5, 9 \).

Bias in \( \chi \)-divergence variational inference (CHIVI)

Figure 6 illustrates the systematic error introduced in the optimal parameters of CHIVI when using biased gradients.
Figure 5. Example of perturbed and true posterior when using subset average likelihoods. The data used is simulated from the model defined by \( z \sim \mathcal{N}(0, 1) \), \( x_i \sim \mathcal{N}(z, 1) \), \( n = 10 \) for two different random seeds. The subset sizes where chosen to be \( m = 2 \) (top row), \( m = 5 \) (top row) and \( m = 9 \) (bottom row).
Figure 6. Example of learnt variational parameters for CHIVI, as well as true parameters when using a Gaussian approximation to a skew normal posterior distribution.