Chain Wielding Strategies for Markov-chain Monte Carlo Estimators in Inclusive Variational Inference

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Abstract

Recently, variational inference methods that minimize the inclusive Kullback-Leibler (KL) divergence using Markov-chain Monte Carlo (MCMC) have been developed. These methods perform stochastic gradient descent by otaining noisy estimates of the gradient using MCMC. So far, multiple ways to operate the Markov-chains have proposed, but it is unclear which results in better VI performance. In this paper, we propose an additional way to operate MCMC-based score estimators for VI, and compare the performance of different schemes. We provide theoretical and empirical analyses of the bias and variance of the three different schemes. Our experiments show that inclusive variational inference using our proposed estimation scheme achieves superior performance, even when compared to evidence lower bound minimization.

1 Introduction

Given an observed data $\mathbf{x}$ and a latent variable $\mathbf{z}$, Bayesian inference aims to analyze $p(\mathbf{z} \mid \mathbf{x})$ given an unnormalized joint density $p(\mathbf{z}, \mathbf{x})$ where the relationship is given by Bayes' rule such that $p(\mathbf{z} \mid \mathbf{x}) = p(\mathbf{z}, \mathbf{x}) / p(\mathbf{x}) \propto p(\mathbf{z}, \mathbf{x})$. Instead of working directly with the target distribution $p(\mathbf{z} \mid \mathbf{x})$, variational inference (VI, Jordan et al. 1999; Blei et al. 2017; Zhang et al. 2019) searches for a variational approximation $q_{\lambda}(\mathbf{z})$ that is similar to $p(\mathbf{z} \mid \mathbf{x})$ according to a discrepancy measure $D(p, q_{\lambda})$.

Naturally, choosing a good discrepancy measure, or objective function, is a critical part of the problem. This fact had lead to a quest for good divergence measures (Li & Turner, 2016; Dieng et al., 2017; Wang et al., 2018; Ruiz & Titsias, 2019). So far, the exclusive KL divergence $D_{\text{KL}}(q_{\lambda} \parallel p)$ (or reverse KL divergence) has been used "exclusively" among various discrepancy measures. This is partly because the exclusive KL is defined as an average over $q_{\lambda}(\mathbf{z})$, which can be estimated efficiently. By contrast, the inclusive KL is defined as

$$D_{\text{KL}}(p \parallel q_{\lambda}) = \int p(\mathbf{z} \mid \mathbf{x}) \log \frac{p(\mathbf{z} \mid \mathbf{x})}{q_{\lambda}(\mathbf{z})} \, d\mathbf{z} = \mathbb{E}_{p(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{z} \mid \mathbf{x})}{q_{\lambda}(\mathbf{z})} \right] \tag{1}$$

where the average is taken over $p(\mathbf{z} \mid \mathbf{x})$. Interestingly, this is a chicken-and-egg problem as our goal is to obtain $p(\mathbf{z} \mid \mathbf{x})$ in the first place. Despite this challenge, minimizing (1) has drawn the attention of researchers because it can overcome some known limitations of the exclusive KL (Minka, 2005; MacKay, 2001).

For performing inclusive VI, Naesseth et al. (2020); Ou & Song (2020) recently proposed *Markovian score climbing* (MSC), which is a blend of Markov-chain Monte Carlo (MCMC) and variational inference. In MSC, stochastic gradients of the inclusive KL are obtained by operating a Markov-chain in parallel with the VI optimizer. In this paper, we find an interesting property of MSC when it is combined with specific types of MCMC kernels. Specifically, we show that *independent Metropolis-Hastings* (IMH, Robert & Casella 2004) type kernels can automatically trade off bias and variance when used for MSC. This family of kernels includes the *condition importance sampling* (CIS, Naesseth et al. 2020) kernel, which was originally proposed for MSC. Surprisingly, this automatic tradeoff property is unique to IMH type kernels and does not occur in MCMC kernels with state-dependent proposals such as Hamiltonian Monte Carlo (HMC, Duane et al. 1987; Neal 2011a; Betancourt 2017).

Following our analysis of the CIS kernel, we also show that its performance can degrade with the number of proposals (which is equivalent to the *per-transition computational budget*) used in each Markov-chain transition. As a simple solution to this, we propose to use parallel IMH (MSC-PIMH) chains, which reduce variance given the same amount of computation. We evaluate the performance of MSC with PIMH against other inclusive VI (Bornschein & Bengio, 2015; Naesseth et al., 2020) and exclusive VI (Ranganath et al., 2014; Kucukelbir et al., 2017) methods.

Contribution Summary **(i)** We propose the parallel state estimator for using MCMC to estimate the score function in inclusive VI (**Section 3.2**). **(ii)** We theoretically compare the bias and variance of the previously proposed MCMC estimation schemes against the parallel state estimator (**Section 3.3**). **(iii)** We experimentally compare the VI performance of the considered MCMC estimation schemes on general Bayesian inference benchmark problems (**Section 4**).

2 Background

2.1 Inclusive Variational Inference Until Now

Different inclusive variational A typical way to perform VI is to use stochastic gradient descent (SGD, Robbins & Monro 1951; Bottou 1999), which requires unbiased gradient estimates of the optimization target. In the case of inclusive variational inference, this corresponds to estimating

$$\nabla_{\lambda} D_{\mathrm{KL}}(p \parallel q_{\lambda}) = \mathbb{E}_{p(\mathbf{z}|\mathbf{x})}\left[-\nabla_{\lambda} \log q_{\lambda}(\mathbf{z}) \right] = -\mathbb{E}_{p(\mathbf{z}|\mathbf{x})}\left[s(\mathbf{z}; \boldsymbol{\lambda}) \right] \approx g(\boldsymbol{\lambda}) \tag{2}$$

with some estimator $g(\boldsymbol{\lambda})$ where $s(\mathbf{z}; \boldsymbol{\lambda}) = \nabla_{\lambda} \log q_{\lambda}(\mathbf{z})$ is known as the *score function*. Evidently, estimating $\nabla_{\lambda} D_{\mathrm{KL}}(p \parallel q_{\lambda})$ requires integrating the score function over $p(\mathbf{z} \mid \mathbf{x})$, which is prohibitive. Different inclusive variational inference methods form a different estimator g.

Importance Sampling When it is easy to sample from the variational approximation $q_{\lambda}(\mathbf{z})$, one can use importance sampling (IS, Robert & Casella 2004; Owen 2013) for estimating g since

$$\mathbb{E}_{p(\mathbf{z}|\mathbf{x})}\left[s(\mathbf{z}; \boldsymbol{\lambda}) \right] \propto \mathbb{E}_{q_{\lambda}}\left[w(\mathbf{z})\, s(\mathbf{z}; \boldsymbol{\lambda}) \right] \approx \frac{1}{N} \sum_{i=1}^{N} w(\mathbf{z}^{(i)})\, s(\mathbf{z}^{(i)}; \boldsymbol{\lambda}) = g_{IS}(\boldsymbol{\lambda}) \tag{3}$$

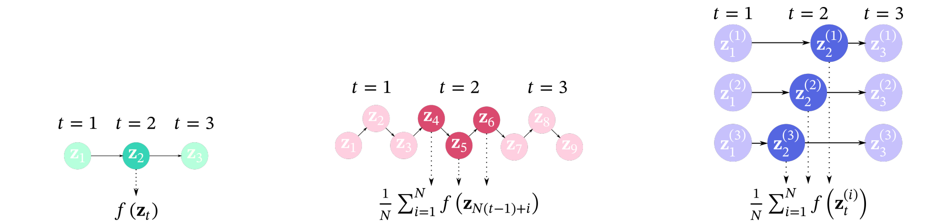
where $w(\mathbf{z}) = p(\mathbf{z}, \mathbf{x}) / q_{\lambda}(\mathbf{z})$ is known as the *importance weight*, and $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(N)}$ are N independent samples from $q_{\lambda}(\mathbf{z})$. This scheme is equivalent to adaptive IS methods (Cappé et al., 2008; Bugallo et al., 2017) since the IS proposal $q_{\lambda}(\mathbf{z})$ is iteratively optimized based on the current samples. Though IS is unbiased, it is highly unstable in practice. A more stable alternative is to use the *normalized weight* $\widetilde{w}^{(i)} = w(\mathbf{z}^{(i)}) / \sum_{i=1}^{N} w(\mathbf{z}^{(i)})$, which is known as the self-normalized IS (SNIS) approximation. Unfortunately, SNIS still fails to converge even on moderate dimensional objectives and unlike IS, it is no longer unbiased (Robert & Casella, 2004; Owen, 2013).

3 Chain Wielding Strategies for Markov-chain Monte Carlo Estimators in Inclusive Variational Inference

3.1 Overview of Previous Estimation Strategies

Overview Recently, Naesseth et al. and Ou & Song proposed two similar but independent methods for performing inclusive variational inference. Both methods estimate the score gradient by operating a Markov-chain in parallel with the VI optimization sequence. Also, they both use MCMC kernels that can effectively used the variational approximation $q_{\lambda_t}(\mathbf{z})$. Because of this, compared to previous VI approaches (Ruiz & Titsias, 2019; Hoffman, 2017) that use expensive MCMC kernels such as Hamiltonian Monte Carlo, both methods are computationally efficient.

Markovian Score Climbing and the Single State Estimator In Markovian score climbing (MSC), (Naesseth et al., 2020) estimate the score gradient by performing an MCMC iteration and update the parameters such that



(a) Single state estimator (b) Sequential state estimator (c) Parallel state estimator

Figure 1: Visualization of different ways of combining MCMC with stochastic approximation variational inference. The index t denotes the stochastic approximation iteration. The dark circles denote the MCMC samples used for estimating the score gradient at $t = 2$.

$$\mathbf{z}_t \sim K(\mathbf{z}_{t-1}, \cdot) \qquad\qquad g_{\text{single-CIS}}(\boldsymbol{\lambda}) = s(\mathbf{z}_t; \boldsymbol{\lambda}) \tag{4}$$

where $K(\mathbf{z}_{t-1}, \cdot)$ is a MCMC kernel leaving $p(\mathbf{z} \mid \mathbf{x})$ invariant and $g_{\text{single}}(\boldsymbol{\lambda})$ denotes the score estimator. For $K(\mathbf{z}_{t-1}, \cdot)$, they propose a new type of kernel inspired by particle MCMC Andrieu et al. (2010), the conditional importance sampling (CIS) kernel. Since the estimator uses *a single state* created by the CIS kernel, we call it the single state estimator with the CIS kernel (single-CIS). The CIS kernel internally uses N samples from the $q_{\boldsymbol{\lambda}}(\mathbf{z})$. Thus, when compared to MCMC kernels that only use a single sample from $q_{\boldsymbol{\lambda}}(\mathbf{z})$, it is N times more expensive, but hopefully, statistically superior. Unfortunately, we will show that this is not the case.

Joint Stochastic Approximation and the Sequential State Estimator On the other hand, at each SGD iteration t, (Ou & Song, 2020) perform N sequential Markov-chain transitions and use the average of the intermediate states for estimation. That is, for the index $i \in \{1, \ldots, N\}$,

$$\mathbf{z}_{T+i} \sim K^i(\mathbf{z}_T, \cdot) \qquad\qquad g_{\text{seq.-IMH}}(\boldsymbol{\lambda}) = \frac{1}{N}\sum_{i=1}^{N} s(\mathbf{z}_{T+i}; \boldsymbol{\lambda}) \tag{5}$$

where $\mathbf{z}_T$ is the last Markov-chain state of the previous SGD iteration. For the MCMC kernel, they use the classic independent Metropolis-Hastings (IMH, Robert & Casella 2004, Algorithm 25 Hastings 1970) algorithm, which uses only a single sample from $q_{\boldsymbol{\lambda}}(\mathbf{z})$. Therefore, the cost of N state transitions with IMH is similar to the cost of a single transition with CIS. Since the estimator uses sequential states, we call it the sequential state esimator with the IMH kernel (seq.-IMH)

Additional Notes on JSA Before preoceeding, we acknowledge that the setup of Ou & Song (2020) is slightly different than what we described. Their MCMC kernel leave $p\left(\mathbf{z}_j \mid \mathbf{x}_j\right)$ invariant for a single datapoint $\mathbf{x}_j$, which is only possible when the datapoints are independently, identically distributed (*iid*) under the probabilistic model. We interpret their method more generally and assume that we only have a kernel that can leave $p(\mathbf{z} \mid \mathbf{x})$ invariant.

3.2 Overview of Markov-Chain Monte Carlo Score Estimation Strategies

Single State and Sequential State Estimators The two different MCMC estimators used in MSC and JSA represent two different ways of using a fixed computational budget. The former uses a computationally expensive, but hopefully statistically superior, MCMC kernel with less samples, while the latter uses a cheaper MCMC kernel with more samples. Illustrations of the two schemes are shown in Figures 1a and 1b. Detailed pseudocodes of the considered schemes are provided in the *supplementary material*.

Parallel State Estimator In this work, we will add a new scheme into the mix: the parallel state estimator. Similarly with the sequential state estimator, we use the cheaper IMH kernel, but instead of applying the MCMC kernel N times to a single chain, we apply the MCMC kernel a single time to N *parallel Markov-chains*. That is, for each Markov-chain $i \in \{1, \ldots, N\}$,

$$\mathbf{z}_t^{(i)} \sim K\big(\mathbf{z}_{t-1}^{(i)}, \cdot\big) \qquad\qquad g_{\text{par.-IMH}}(\boldsymbol{\lambda}) = \frac{1}{N}\sum_{i=1}^{N} s(\mathbf{z}_t^{(i)}; \boldsymbol{\lambda}) \tag{6}$$

where $\mathbf{z}_{t-1}^{(i)}$ is the state of the ith chain at the previous SGD step. Computationally speaking, we are still applying $K\big(\mathbf{z}_{t-1}^{(i)}\big)$ N times in total, so the cost is similar to the sequential state estimator.

Table 1: Computational Cost of Markov-chain Schemes

	Estimation			Stochastic gradient	
	$p(\mathbf{z}, \mathbf{x})$ # Eval.	$q_{\boldsymbol{\lambda}}(\mathbf{z})$ # Eval.	$q_{\boldsymbol{\lambda}}(\mathbf{z})$ # Samples	$p(\mathbf{z}, \mathbf{x})$ # Grad.	$q_{\boldsymbol{\lambda}}(\mathbf{z})$ # Grad.
ADVI	0	0	N	N	0
Single state estimator with CIS	$N-1$	N	$N-1$	0	1^1 or N^2
Sequential state estimator with IMH	N	N	N	0	N
Parallel state estimator with IMH	N	N	N	0	N

[*] N is the number of samples used in each method.
[1] Vanilla CIS kernel.
[2] Rao-Blackwellized CIS kernel.

However, the Markov-chain are N times shorter, which, in a traditional MCMC view, might seem to result in worse statistical performance. An illustration of the parallel state estimator is shown in Figure 1c

Computational Cost The three scheme using the CIS kernel and the IMH kernel can have different computational cost depending on the parameter N. The computational costs of each scemes are organized in Table 1. In the CIS kernel, N controls the number of internal proposals sampled from $q_{\boldsymbol{\lambda}}(\mathbf{z})$. In the sequential and parallel state estimators, the IMH kernel only uses a single sample from $q_{\boldsymbol{\lambda}}(\mathbf{z})$, but applies the kernel N times. When estimating the score, the single state estimator computes $\nabla_{\boldsymbol{\lambda}} \log q_{\boldsymbol{\lambda}}(\mathbf{z})$ only once, while for the sequential and parallel state estimators compute it N times. However, Naesseth et al. (2020) also discuss a Rao-Blackwellized version of the CIS kernel, which also computes the gradient N times.

3.3 Theoretical Analysis of Bias

Adaptive MCMC and Ergodicity For bounded functions, a bound on the bias of MCMC estimators can be easily derived from the convergence rates of MCMC kernels as shown by Jiang et al. (2021, Theorem 4). In the context of MSC, the convergence rate of an MCMC kernel is a subtle subject since the kernel is now *adaptive* as it depends on $\boldsymbol{\lambda}_t$, which is in turn dependent on all of the past MCMC samples. This is clearly the type of problem adaptive MCMC algorithms have been concerned with (Andrieu & Moulines, 2006). However, our setting crucially differs with adaptive MCMC in that our goal is not to obtain asymptotically unbiased samples. Instead, we use the MCMC samples acquired during each SGD step, in which $\boldsymbol{\lambda}_t$ is fixed. That is, our MCMC kernel is instantaneously not adaptive, and we are thus we are free to use the ergodicity results of these kernels. However, we note that, as far as Deoblin's condition holds such that $w^* = \sup_{\mathbf{z}, \boldsymbol{\lambda}} p(\mathbf{z}|\mathbf{x})/q_{\boldsymbol{\lambda}}(\mathbf{z}) < \infty$ and the SGD stepsize sequence satisfies the diminishing adaptation condition (Roberts & Rosenthal, 2007), the MCMC kernel will indeed result in asymptotically unbised samples.

Boundedness Assumption Since convergence rates are defined with the total-variation distance, our bias results assume that the score function is bounded. That is, $\| \nabla_{\boldsymbol{\lambda}} \log q_{\boldsymbol{\lambda}}(\mathbf{z}) \| < L$ for any $\boldsymbol{\lambda}$. This boundedness assumption is reasonable since theoretical guarentees of SGD often assume Lipschitz-continuity of the gradients, from which boundedness follows as a consequence.

Assuming $w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\boldsymbol{\lambda}_t}(\mathbf{z}) < \infty$ for $\forall \boldsymbol{\lambda}$ and the score function is bounded such that $| s(\mathbf{z}; \boldsymbol{\lambda}) | \leq \frac{L}{2}$, the bias of the sequential state estimator with an IMH kernel at iteration t is bounded as

$$\mathrm{Bias}\left[g_{\mathrm{seq.,t}}\right] \leq \frac{L}{N}\left(w^* - 1\right)$$

Proof. The proof is in the *supplementary material.*

Theorem 1. *Assuming* $w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\boldsymbol{\lambda}_\tau}(\mathbf{z}) < \infty$ *for* $\forall \boldsymbol{\lambda}$ *and that the score function is bounded as* $| s(\mathbf{z}; \boldsymbol{\lambda}) | \leq \frac{L}{2}$, *the bias of the parallel state estimator with an IMH kernel at iteration t is bounded as*

$$\mathrm{Bias}\left[g_{\mathrm{par.,t}}\right] \leq L\left(1 - \frac{1}{w^*}\right).$$

Proof. The proof is in the *supplementary material.*

Finally, we analyze the bias of the single-CIS estimator. Our proof is based on the fact that the CIS kernel is identical to the iterated sampling importance resampling (i-SIR) algorithm by Andrieu et al. (2018). Especially, we utilize the the convergence rate of the i-SIR kernel. In addition, we note that the CIS kernel can be reformulated as an accept-reject type kernel that uses Barker's acceptance function (Barker, 1965). With this perspective, it is identical to the ensemble MCMC sampler independently proposed by Austad (2007); Neal (2011b). It can also be found in the review on multiple-try MCMC methods by Martino (2018, Table 12).

Theorem 2. *For a CIS kernel with N internal proposals, assuming $w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\lambda}(\mathbf{z}) < \infty$ for $\forall \lambda$, $N > 2$, and that the score function is bounded such that $|s(\mathbf{z};\boldsymbol{\lambda})| \leq \frac{L}{2}$, the bias of the single state estimator at iteration t is bounded as*

$$\text{Bias}\left[g_{\text{cis.},t}\right] \leq L\,C \quad \textit{where} \quad C = \left(1 - \frac{N}{w^*}\right) < 1.$$

Proof. The proof is in the *supplementary material*.

Reducing Bias by Increasing N Our results suggest that, for the seq.-IMH estimator and single-CIS estimator, increasing N improves the bias decrease rate. However, it is important to note that all bias bounds depend on w^*. By the following proposition, in the initial stages of VI where the KL divergence is large, w^* is bounded below exponentially.

Proposition 1. *$w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\lambda}(\mathbf{z})$ is bounded below expoentially by the KL divergence such that* $\exp\left(D_{\text{KL}}(p(\cdot \mid \mathbf{x}) \,\|\, q_{\boldsymbol{\lambda}}(\cdot))\right) \leq w^*$.

Proof. $D_{\text{KL}}(p(\cdot \mid \mathbf{x}) \,\|\, q_{\boldsymbol{\lambda}}(\cdot)) = \int p(\mathbf{z} \mid \mathbf{x}) \log \frac{p(\mathbf{z}|\mathbf{x})}{q_{\boldsymbol{\lambda}}(\mathbf{z})}\, d\mathbf{z} \leq \int p(\mathbf{z} \mid \mathbf{x}) \log M \, d\mathbf{z} = \log w^*$ □

Thus, in the initial steps of VI, the bias decrease rate C will be close to 1, making the effect of N minimal. On the other hand, in the later steps of VI, the KL divergence is small. However, in this case t will be larege, therefore making the bias small regardless.

3.4 Theoretical Analysis of Variance

Geometric ergodicity of the CIS and IMH kernels guarentee that the bias will be small regardless of the kernel and parameter N. In contrast, variance often dominate the mean-square error of MCMC estimators. Therefore, analyzing the variance will be more relevant in practice.

Theorem 3. *The variance of the sequential state estimator is*

Proof. The proof is in the *supplementary material*.

Theorem 4. *The variance of the single mode estimator with a CIS kernel $\mathbb{V}_{q_\lambda}\left[\, g_{\text{single}} \,\right]$ is approximately bounded below such that*

$$\mathbb{V}_{q_\lambda}\left[\, g_{\text{single}} \,\right] \geq \frac{N^4 Z^4}{(w(\mathbf{z}_{t-1}) + NZ)^4} \mathbb{V}_{q_\lambda}\left[\, f_{IS} \,|\, \mathbf{z}_{t-1} \,\right], \tag{7}$$

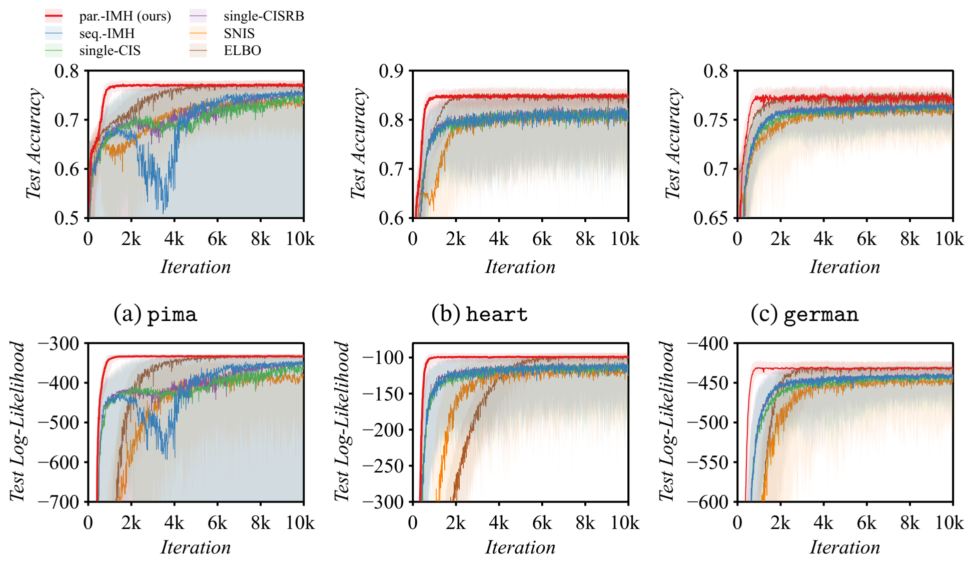
where $Z = \mathbb{E}_{q_\lambda}[p(\mathbf{z},\mathbf{x})/q_\lambda(\mathbf{z})] = \int p(\mathbf{z},\mathbf{x}) d\mathbf{z}$ is the normalizing constant.

Proof. The proof is in the *supplementary material*.

4 Evaluations

4.1 Experimental Setup

Implementation We implemented MSC with PIMH on top of the Turing (Ge et al., 2018) probabilistic programming framework. Our implementation works with any model described in Turing, which automatically handles distributions with constrained support (Kucukelbir et al., 2017). We use the ADAM optimizer by Kingma & Ba (2015) with a learning rate of 0.01 in all of the experiments. We set the computational budget $N = 10$ and $T = 10^4$ for all experiments unless specified.



(a) pima (b) heart (c) german

(d) pima (e) heart (f) german

Figure 2: Test accuracy and log-likelihood of logistic regression problems. The solid lines and colored regions are the medians and 80% percentiles computed from 100 repetitions.

Considered Baselines We compare MSC-PIMH with **(i)** MSC using the CIS kernel (**MSC-CIS**, Naesseth et al. 2020), **(ii)** MSC using the CIS kernel with Rao-Blackwellization (**MSC-CISRB**, Naesseth et al. 2020), **(iii)** the adaptive IS method using SNIS as introduced in Section 2.1 (**SNIS**), **(iv)** the reweighted wake-sleep algorithm (**RWS**, Bornschein & Bengio 2015), and **(v)** evidence lower-bound maximization (**ELBO**, Ranganath et al. 2014). Specifically, we use automatic differentiation VI (ADVI, Kucukelbir et al. 2017) implemented by Turing.

Reinterpreting RWS The original RWS algorithm assumes that independent samples from $p(\mathbf{z} \mid \mathbf{x})$ are available, possibly with an additional cost. Since this is not the case in our setting, we reinterpret RWS as alternating between cheap (*sleep update*) and expensive (*wake update*) estimates. We respectively use SNIS and HMC for the sleep and wake updates, and perform the wake update every $K = 5$ steps as originally recommended by Bornschein & Bengio (2015).

4.2 Hierarchical Logistic Regression

Experimental Setup We evaluate MSC-PIMH on logistic regression with the Pima Indians diabetes (`pima`, $\mathbf{z} \in \mathbb{R}^{11}$, Smith et al. 1988), German credit (`german`, $\mathbf{z} \in \mathbb{R}^{27}$), and heart disease (`heart`, $\mathbf{z} \in \mathbb{R}^{16}$, Detrano et al. 1989) datasets obtained from the UCI repository (Dua & Graff, 2017). 10% of the data points were randomly selected in each of the 100 repetitions as test data.

Probabilistic Model Instead of the usual single-level probit/logistic regression models used in VI, we choose a more complex hierarchical logistic regression model

$$y_i \sim \text{Bernoulli-Logit}\,(p),\;\; p \sim \mathcal{N}(\mathbf{x}_i^\top \boldsymbol{\beta} + \alpha,\, \sigma_\alpha^2),\;\; \boldsymbol{\beta} \sim \mathcal{N}(\mathbf{0},\, \sigma_\beta^2 \mathbf{I}),\;\; \sigma_\beta,\, \sigma_\alpha \sim \mathcal{N}^+(0, 1.0) \tag{8}$$

where $\mathcal{N}^+(\mu, \sigma)$ is a positive constrained normal distribution with mean μ and standard deviation σ, $\mathbf{x}_i$ and y_i are the feature vector and target variable of the ith datapoint. The extra degrees of freedom σ_β and σ_α make this model relatively more challenging.

Results The test accuracy and test log-likelihood results are shown in Figure 2. Our proposed MSC-PIMH is the fastest to converge on all the datasets. Despite having access to high-quality HMC samples, RWS fails to achieve a similar level of performance to MSC-PIMH. However, RWS converges faster than MSC-CIS and MSC-CISRB. Among the two, MSC-CISRB performs only marginally better than MSC-CIS. Meanwhile, SNIS converges the most slowly among inclu-

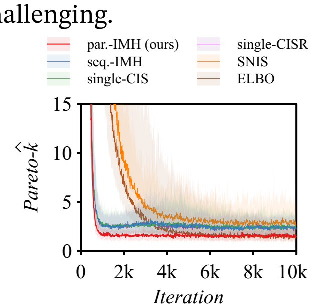
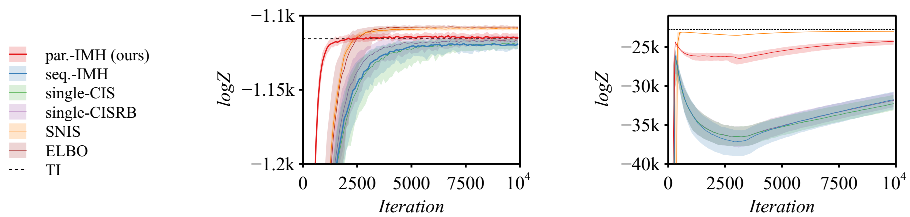


Figure 3: Pareto-$\hat{k}$ statistics result on `german`. The solid lines and colored regions are the medians and 80% percentiles computed from 100 repetitions.

sive VI methods. Although much slower to converge, ELBO achieves competitive results.

Inclusive VI v.s. Exclusive VI The results of Figure 2 might be misleading to conclude that inclusive and exclusive VI deliver similar results. However, in the parameter space, they choose different optimization paths. This is shown in Figure 3 through the Pareto-$\hat{k}$ diagnostic (Dhaka et al., 2020; Vehtari et al., 2021), which determines how reliable the importance weights are when computed using $q_{\lambda}(\mathbf{z})$. While the test accuracy suggests that ELBO converges around $t = 2000$, in terms of Pareto-$\hat{k}$, it takes much longer to converge (about $t = 5000$). This shows that, even if their predictive performance is similar, the inclusive VI chooses paths that have better density coverage as expected.

4.3 Marginal Likelihood Estimation



(a) `radon` (b) `stock`

Figure 4: Marginal log-likelihood ($\log Z$) estimates of considered methods. ELBO is omitted in Figure 4b as it failed to deliver reasonable estimates. The solid lines and colored regions are the medians and 80% percentiles computed from 100 repetitions.

Experimental Setup We now estimate the marginal log-likelihood $\log Z$ of a stochastic volatility model (`stock`, $\mathbf{z} \in \mathbb{R}^{2613}$, Kim et al. 1998) and a hierarchical regression model with partial pooling (`radon`, $\mathbf{z} \in \mathbb{R}^{175}$, Gelman & Hill 2007) for modeling radon levels in U.S homes. For `stock`, we use 10 years of the S&P index daily closing price (May 3, 2007, to May 3, 2017). `stock` is highly challenging as it is both high dimensional and strongly correlated. We estimated the reference marginal likelihood using *thermodynamic integration* (TI, Gelman & Meng 1998; Neal 2001; Lartillot & Philippe 2006) with HMC implemented by Stan (Carpenter et al., 2017; Betancourt, 2017).

Results The results are shown in Figure 4. On `radon`, MSC-PIMH converges quickly and provides the most accurate estimate. By contrast, MSC-CIS and MSC-CISRB converge much slowly. SNIS and ELBO, on the other hand, overestimate $\log Z$, which can be attributed to the mode-seeking behavior of ELBO and the small sample bias of SNIS. On `stock`, SNIS is unexpectedly the most accurate. Unfortunately, MSC-PIMH, MSC-CIS, MSC-CISRB all underestimate $\log Z$. Nevertheless, MSC-PIMH provides much better estimates than the latter two. Lastly, we observe that only ELBO fails to converge given the same amount of SGD steps.

5 Related Works

Inclusive VI with SGD Our method directly builds on top of MSC (Naesseth et al., 2020), which is a method for minizing the inclusive KL divergence. While many works minimizing the inclusive KL have emerged (Bornschein & Bengio, 2015; Li et al., 2017; Minka, 2001; Ou & Song, 2020; Kim et al., 2021), only a few have been proposed for general VI based on SGD. Notably, Bornschein & Bengio (2015) use SNIS for estimating the stochastic gradients, while Li et al. (2017) use an MCMC kernel to refine samples from $q_{\lambda}(\mathbf{z})$ to better resemble samples from $p(\mathbf{z} \mid \mathbf{x})$. Meanwhile, a synonymous method to MSC, *general stochastic approximation* (GSA) by Ou & Song (2020, Algorithm 1) has been proposed concurrently in the context of discrete latent variables. Kim et al. (2021) recently proposed a method that essentially blends GSA/MSC with RWS.

Adaptive MCMC As pointed out by Ou & Song (2020), MSC is structurally equivalent to adaptive MCMC methods. Strong resemblence can be found in methods using stochastic approximation for adapting the proposal distribution used inside the MCMC kernel. In particular, Andrieu & Thoms (2008); Garthwaite et al. (2016) discuss the use of stochastic approximation in adaptive MCMC.

Adaptive IMH Among adaptive MCMC methods, those that use independent proposals (Andrieu & Moulines, 2006; Keith et al., 2008; Holden et al., 2009; Giordani & Kohn, 2010) are the most related to our work. Keith et al. (2008) propose to use *cross-entroy minimization* (Barbakh et al., 2009), which is mathematically identical to inclusive VI, for adaptation. Our work, on the other hand, contrasts with previous adaptive IMH algorithms in that we use SGD for adapting $q_{\lambda}(\mathbf{z})$. This enables VI methods such as ADVI to consider proposals that are much more complex (Kucukelbir et al., 2017).

Ergodicity and Inclusive VI Meanwhile, in the context of MCMC, Mengersen & Tweedie (1996) showed that it is necessary to ensure $\sup_{\mathbf{z}} w(\mathbf{z}) = M < \infty$ (finite weight condition) for an IMH kernel to be geometrically ergodic. While this might seem less relevant for inclusive VI, the bound

$$D_{\mathrm{KL}}(p \parallel q_{\lambda}) = \int p(\mathbf{z} \mid \mathbf{x}) \log w(\mathbf{z})\, d\mathbf{z} \leq \int p(\mathbf{z} \mid \mathbf{x}) \log M \, d\mathbf{z} = \log M. \tag{9}$$

suggests that it is in fact a sufficient condition for the KL divergence to be finite. This condition can easily be violated as shown by Andrieu & Thoms (2008). To ensure this does not happen, Giordani & Kohn (2010); Holden et al. (2009) use proposal distributions of the form of $w\, q_0(\mathbf{z}) + (1 - w)\, q_{\lambda}(\mathbf{z})$ for some $0 < w < 1$ for their adaptive IMH sampler. Here, q_0 is supposed to be a heavy tailed distribution in the spirit of defensive mixtures (Hesterberg, 1995). A research direction in the interest of both adaptive MCMC and inclusive VI would be to investigate whether such precaution is actually necessary for convergence. If that is the case, it would be beneficial to consider variational families of heavy-tailed distributions as proposed by Domke & Sheldon (2018) for exclusive VI.

6 Conclusions

In this paper, we investigated the properties of Markovian score climbing (MSC) with independent Metropolis-Hastings (IMH) type Markov-chain Monte Carlo (MCMC) kernels. We proved that IMH type kernels are able to automatically perform bias-variance tradeoff using their accept-reject mechanism. We also analyzed the limitation of the conditional importance sampling (CIS) kernel originally used in MSC. We then proposed parallel IMH (PIMH) as an alternative that enjoys the benefits of CIS without its limitations. Our experiments verify that MSC combined with PIMH performs well on the considered Bayesian inference problems, even compared to exclusive variational inference methods.

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A Relationship Between Sampling Methods

We organize the sampling methods described in this work in Table 2.

Table 2: Comparison of Sampling Method Designs

Algorithm	Origin	Proposal	M-H Test	Acceptance Ratio	Multiple Proposals	Reference
RWMH[1]	MCMC	Dependent	✓	M-H	✗	
HMC	MCMC	Dependent	✓	M-H	✗	Duane et al. (1987)
SNIS	IS	Independent	✗		✓	
IMH	MCMC	Independent	✓	M-H	✗	
CIS	PMCMC[4]	Independent	✓	Barker	✓	Naesseth et al. 2020
En. MCMC[2]	MCMC	Both	✓	Barker	✓	Neal 2011b
PMP MCMC[3]	MCMC	Dependent	✓	Barker	✓	Austad 2007

[1] Random-walk Metropolis-Hastings
[2] Ensemble MCMC
[3] Parallel multiple proposals MCMC
[4] Particle MCMC

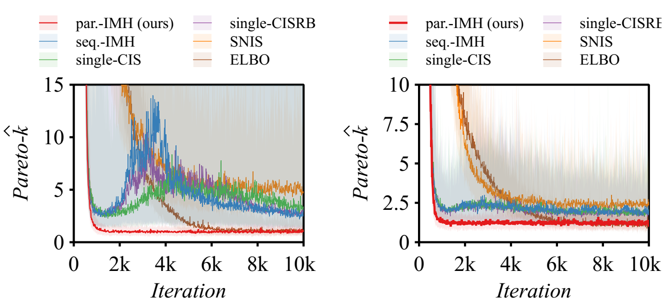
In this paper, we designated kernels that use independent proposals and perform a Metropolis-Hastings (M-H) test as "IMH type" kernels. While the original paper of CIS does not mention it as an IMH type, we have shown in **??** that it is indeed an IMH type kernel that uses Barker's acceptance ratio and multiple proposals per transition. This, in turn, reveals close connections with ensemble MCMC by Neal (2011b). While parallel multiple proposals MCMC by Austad (2007) also uses Barker's acceptance ratio and multiple proposals, it only considers dependent proposals, unlike ensemble MCMC. Although in principle, it should work with independent proposals without modification.

B Additional Experimental Results

B.1 Experimental Environment

All of our experiments presented in this paper were executed on a server with 20 Intel Xeon E5–2640 CPUs and 64GB RAM. Each of the CPUs has 20 logical threads with 32k L1 cache, 256k L2 cache, and 25MB L3 cache. All of our experiments can be executed within a few days on a system with similar computational capabilities.

B.2 Additional Results of Logistic Regression Experiments



(a) Pima (b) Heart

Figure 5: Pareto-$\hat{k}$ results of logistic regression problems. The solid lines are the median of 100 repetitions while the colored regions are the 80% empirical percentiles.

C PSEUDOCODES OF THE CONSIDERED SCHEMES

Algorithm 1: Single State Estimator

Input: MCMC kernel $K(\mathbf{z}, \cdot)$, initial sample $\mathbf{z}_0$, initial parameter $\boldsymbol{\lambda}_0$, number of iterations T, stepsize schedule γ_t

for $t = 1, 2, \dots, T$ **do**
- $\mathbf{z}_t \sim K(\mathbf{z}_{t-1}, \cdot)$
- $s(\mathbf{z}; \boldsymbol{\lambda}) = \nabla_{\boldsymbol{\lambda}} \log q_{\boldsymbol{\lambda}}(\mathbf{z})$
- $g_{\text{single}} = s(\mathbf{z}_t; \boldsymbol{\lambda}_{t-1})$
- $\boldsymbol{\lambda}_t = \boldsymbol{\lambda}_{t-1} + \gamma_t \, g_{\text{single}}$

end

Algorithm 2: Sequential State Estimator

Input: initial sample $\mathbf{z}_0$, initial parameter $\boldsymbol{\lambda}_0$, number of iterations T, stepsize schedule γ_t

for $t = 1, 2, \dots, T$ **do**
- $T = N(t-1)$
- **for** $i = 1, 2, \dots, N$ **do**
  - $\mathbf{z}_t \sim K(\mathbf{z}_{T+i}, \cdot)$
- **end**
- $s(\mathbf{z}; \boldsymbol{\lambda}) = \nabla_{\boldsymbol{\lambda}} \log q_{\boldsymbol{\lambda}}(\mathbf{z})$
- $g_{\text{seq.}} = \frac{1}{N} \sum_{i=1}^{N} s(\mathbf{z}_{T+i}; \boldsymbol{\lambda}_{t-1})$
- $\boldsymbol{\lambda}_t = \boldsymbol{\lambda}_{t-1} + \gamma_t \, g_{\text{seq.}}$

end

Algorithm 3: Parallel State Estimator

Input: initial samples $\mathbf{z}_0^{(1)}, \dots, \mathbf{z}_0^{(N)}$, initial parameter $\boldsymbol{\lambda}_0$, number of iterations T, stepsize schedule γ_t

for $t = 1, 2, \dots, T$ **do**
- **for** $i = 1, 2, \dots, N$ **do**
  - $\mathbf{z}_t^{(i)} \sim K(\mathbf{z}_{t-1}^{(i)}, \cdot)$
- **end**
- $s(\mathbf{z}; \boldsymbol{\lambda}) = \nabla_{\boldsymbol{\lambda}} \log q_{\boldsymbol{\lambda}}(\mathbf{z})$
- $g_{\text{par.}} = \frac{1}{N} \sum_{i=1}^{N} s(\mathbf{z}_t^{(i)}; \boldsymbol{\lambda}_{t-1})$
- $\boldsymbol{\lambda}_t = \boldsymbol{\lambda}_{t-1} + \gamma_t \, g_{\text{par.}}$

end

Algorithm 4: Conditional Importance Sampling Kernel

Input: previous sample $\mathbf{z}_{t-1}$, previous parameter $\boldsymbol{\lambda}_{t-1}$, number of proposals N

$\mathbf{z}^{(0)} = \mathbf{z}_{t-1}$

$\mathbf{z}^{(i)} \sim q_{\boldsymbol{\lambda}_{t-1}}(\mathbf{z})$ for $i = 1, 2, \dots, N$

$w(\mathbf{z}^{(i)}) = p(\mathbf{z}^{(i)}, \mathbf{x}) \,/\, q_{\boldsymbol{\lambda}_{t-1}}(\mathbf{z}^{(i)})$ for $i = 0, 1, \dots, N$

$\widetilde{w}^{(i)} = w(\mathbf{z}^{(i)}) / \sum_{i=0}^{N} w(\mathbf{z}^{(i)})$ for $i = 0, 1, \dots, N$

$\mathbf{z}_t \sim \text{Multinomial}(\widetilde{w}^{(0)}, \widetilde{w}^{(1)}, \dots, \widetilde{w}^{(N)})$

Algorithm 5: Independent Metropolis-Hastings Kernel

Input: previous sample $\mathbf{z}_{t-1}$, previous parameter $\boldsymbol{\lambda}_{t-1}$,

$\mathbf{z}^* \sim q_{\boldsymbol{\lambda}_{t-1}}(\mathbf{z})$

$w(\mathbf{z}) = p(\mathbf{z}, \mathbf{x}) / q_{\boldsymbol{\lambda}_{t-1}}(\mathbf{z})$

$\alpha = \min\left(w\left(\mathbf{z}^*\right) / w\left(\mathbf{z}_{t-1}\right), 1\right)$

$u \sim \text{Uniform}(0, 1)$

if $u < \alpha$ **then**

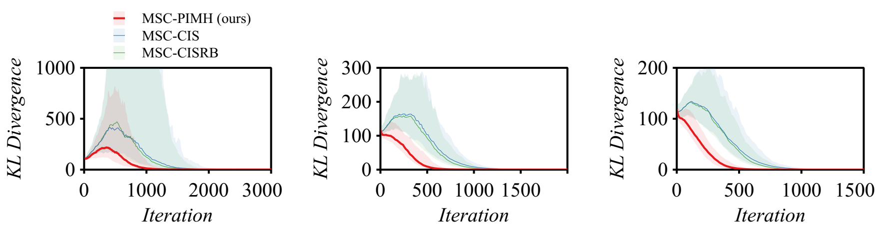
  $\mathbf{z}_t = \mathbf{z}^*$

else

  $\mathbf{z}_t = \mathbf{z}_{t-1}$

end

C.1 Isotropic Gaussian Experiments



(a) $N = 2^2$ (b) $N = 2^4$ (c) $N = 2^6$

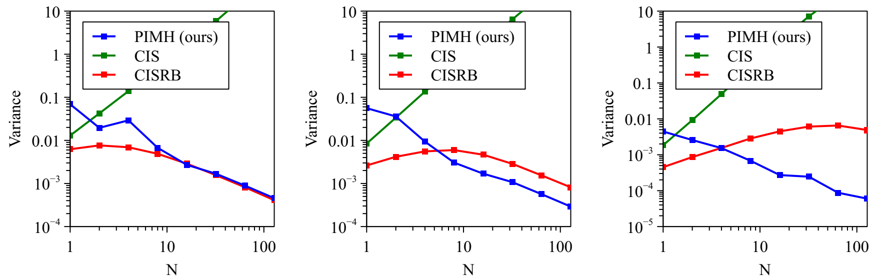
Figure 6: 100-D isotropic Gaussian example with a varying computational budget N. MSC-PIMH converges faster than MSC-CIS and MSC-CISRB regardless of N. Also, the convergence of MSC-PIMH becomes more stable/monotonic as N increases. The solid lines and colored regions are the medians and 80% percentiles computed from 100 repetitions.

We perform experiments with a 100-D isotropic multivariate Gaussian distribution. With Gaussian distributions, convergence can be evaluated exactly since their KL divergence is available in a closed form. We compare the performance of MSC-PIMH, MSC-CIS, and MSC-CISRB with respect to the N (number of proposals for MSC-CIS, MSC-CISRB; number of parallel chains for MSC-PIMH). The results are shown in Figure 6. While MSC-PIMH shows some level of overshoot wih $N = 4$, it shows monotonic convergence with larger N. On the other hand, both MSC-CIS and MSC-CISRB overshoots even with $N = 64$. This clearly shows that PIMH enjoys better gradient estimates compared to the CIS kernel.

D Numerical Simulation

We present numerical simulations of our analyses in **??** and **??**. In particular, we visualize the fact that the variance of the CIS kernel can increase with the number of proposals N when the KL divergence is large, as described in (**??**).

Experimental Setup We first set the target distribution as $p(z \mid x) = \mathcal{N}(0, 1)$ and the proposal distribution as $q(z; \mu) = \mathcal{N}(\mu, 2)$ with varying mean. We measure the variance of estimating the score function $s(z, \mu) = \frac{\partial q(z;\mu)}{\partial \mu}$ using the CIS, CISRB, and PIMH kernels, given the previous Markov-chain denoted bystate z_{t-1} and computational budget N. For CIS and CISRB, we set a fixed z_{t-1}, while for PIMH, we randomly sample N samples from $\mathbf{z}_{t-1} \sim p(z \mid z)$ (we obtained similar trends regardless of the distribution of z_{t-1}). The variance is estimated using 2^{14} samples from $K(\mathbf{z}_{t-1}, \cdot)$. We report the variance across varying N and varying KL divergence between $q_{\lambda}(z)$ and $p(\mathbf{z} \mid \mathbf{x})$. The latter is performed by varying the difference between the mean of the proposal and the target distributions denoted by $\Delta\mu = \mathbb{E}_{p(\mathbf{z}|\mathbf{x})}[\, z\,] - \mathbb{E}_{q_{\lambda}}[\, z\,]$.



(a) $\Delta\mu = 0$ (b) $\Delta\mu = 2$ (c) $\Delta\mu = 4$

Figure 7: Conditional variance of different MCMC kernels with varying N and varying difference between the mean of the target and proposal distributions.

Results Summary The results are presented in Figure 7. We can see that, when the difference of the mean of the p and q is large, the variance of CISRB *increases* with N. This increasing trend becomes stronger as the KL divergence between p and q increases. While this simulation suggests that CISRB has much smaller variance compared to CIS, our realistic experiments in Section 4 did not reveal such levels of performance gains. Is also visible that PIMH has a slightly larger variance compared to CIS in the small N regime. This is due to the higher acceptance rate of the Metropolis-Hastings acceptance ratio used by PIMH compared to Barker's acceptance ratio used by CIS (Peskun, 1973; Minh & Minh, 2015).

E Probabilistic Models Considered in Section 4

E.1 Hierarchical Logistic Regression

The hierarchical logistic regression used in Section 4.2 is

$$\begin{aligned}
\sigma_\beta &\sim \mathcal{N}^+(0, 1.0) \\
\sigma_\alpha &\sim \mathcal{N}^+(0, 1.0) \\
\boldsymbol{\beta} &\sim \mathcal{N}\left(\mathbf{0}, \sigma_\beta^2 \mathbf{I}\right) \\
\alpha &\sim \mathcal{N}\left(0, \sigma_\alpha^2\right) \\
p &\sim \mathcal{N}\left(\mathbf{x}_i^\top \boldsymbol{\beta} + \alpha,\, \sigma_\alpha^2\right) \\
y_i &\sim \text{Bernoulli-Logit}\,(p)
\end{aligned}$$

where $\mathbf{x}_i$ and y_i are the predictors and binary target variable of the ith datapoints.

E.2 Stochastic Volatility

The stochastic volatility model used in Section 4.3 is

$$\begin{aligned}
\mu &\sim \text{Cauchy}(0, 10) \\
\phi &\sim \text{Uniform}\,(-1, 1) \\
\sigma &\sim \text{Cauchy}^+(0, 5) \\
h_1 &\sim \mathcal{N}\left(0, \frac{\sigma^2}{1-\phi^2}\right) \\
h_{t+1} &\sim \mathcal{N}\left(\mu + \phi\,(h_t - \mu), \sigma^2\right) \\
y_t &\sim \mathcal{N}\left(0, \exp\left(h_t\right)\right)
\end{aligned}$$

where y_t is the stock price at the tth point in time. We used the reparameterized version where h_t is sampled from a white multivariate Gaussian described by the Stan Development Team (2020).

E.3 Radon Hierarchical Regression

The partially pooled linear regression model used in Section 4.3 is

$$
\begin{aligned}
\sigma_{a_1} &\sim \text{Gamma}\,(\alpha = 1, \beta = 0.02) \\
\sigma_{a_2} &\sim \text{Gamma}\,(\alpha = 1, \beta = 0.02) \\
\sigma_{y} &\sim \text{Gamma}\,(\alpha = 1, \beta = 0.02) \\
\mu_{a_1} &\sim \mathcal{N}\,(0, 1) \\
\mu_{a_2} &\sim \mathcal{N}\,(0, 1) \\
a_{1,c} &\sim \mathcal{N}\left(\mu_{a_1}, \sigma_{a_1}^2\right) \\
a_{2,c} &\sim \mathcal{N}\left(\mu_{a_2}, \sigma_{a_2}^2\right) \\
y_i &\sim \mathcal{N}\left(a_{1,c_i} + a_{2,c_i}\, x_i,\, \sigma_y^2\right)
\end{aligned}
$$

where $a_{1,c}$ is the intercept at the county c, $a_{2,c}$ is the slope at the county c, c_i is the county of the ith datapoint, x_i and y_i are the floor predictor of the measurement and the measured radon level of the $i$the datapoint, respectively. The model pools the datapoints into their respective counties, which complicates the posterior geometry (Betancourt, 2020).

F Proofs

Assuming $w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\lambda_t}(\mathbf{z}) < \infty$ for $\forall \boldsymbol{\lambda}$ and the score function is bounded such that $|\, s(\mathbf{z}; \boldsymbol{\lambda})\,| \leq \frac{L}{2}$, the bias of the sequential state estimator with an IMH kernel at iteration t is bounded as

$$
\text{Bias}\left[g_{\text{seq.,t}}\right] \leq \frac{L}{N}\,(w^* - 1)
$$

Proof of section 3.3. We employ a similar proof strategy with the works of Jiang et al. (2021, Theorem 4).

Let us first denote the empirical distribution of the Markov-chain states at iteration t as

$$
\eta_{\text{seq.},\,t}(\mathbf{z}) = \frac{1}{N} \sum_{i=1}^{N} K^i(\mathbf{z}_T, \mathbf{z}), \tag{10}
$$

where $\mathbf{z}_T$ is the last state of the Markov-chain at the previous SGD iteration. Consequently, the estimator can be described as

$$
g_{\text{seq},t}(\boldsymbol{\lambda}) = \int s\,(\mathbf{z}; \boldsymbol{\lambda})\; \eta_{\text{seq.},\,t}(\mathbf{z})\, d\mathbf{z}. \tag{11}
$$

Now,

$$
\begin{aligned}
\left\| \eta_{seq.,\,t}(\cdot) - p\,(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} &= \left\| \frac{1}{N} \sum_{i=1}^{N} K^i(\mathbf{z}_T, \cdot) - p\,(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} &\quad (12) \\
&\leq \frac{1}{N} \sum_{i=1}^{N} \left\| K^i(\mathbf{z}_T, \cdot) - p\,(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} \qquad \text{(Triangle inequality)} &\quad (13)
\end{aligned}
$$

For an IMH kernel with $w^* < \infty$, the geometric ergodicity of the IMH kernel (Mengersen & Tweedie, 1996, Theorem 2.1) gives the bound

$$
\left\| K^t(\mathbf{z}_0, \cdot) - p(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} \leq \left(1 - \frac{1}{w^*}\right)^t. \tag{14}
$$

For the SGD step t, $\boldsymbol{\lambda}_t$ is fixed, temporarily enabling ergodicity to hold. Therefore,

$$\begin{aligned}
\left\| \eta_{\text{seq.},\,t}(\cdot) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} &\leq \frac{1}{N} \sum_{i=1}^{N} \left(1 - \frac{1}{w^*}\right)^{i} && (15)\\
&= \frac{1}{N} \sum_{i=1}^{N} C^{i} && (16)\\
&= \frac{1}{N} \left(\frac{C\left(1 - C^{N}\right)}{1 - C} \right) && (17)\\
&= \frac{C}{N} \frac{\left(1 - C^{N}\right)}{1 - C} && (18)\\
&\leq \frac{1}{N} \frac{C}{1 - C} && (19)\\
&= \frac{1}{N} \frac{1 - {}^{1}/_{w^*}}{{}^{1}/_{w^*}} && (20)\\
&= \frac{1}{N} \left(w^* - 1\right) && (21)
\end{aligned}$$

Finally, by the definition of the total-variation distance,

$$\begin{aligned}
\text{bias}\left[g_{\text{seq.,t}}\right] &\leq \left\| \eta_{seq.,\,t}(\cdot) - p(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} && (22)\\
&\leq \sup_{h:\mathcal{Z}\rightarrow[-L/2,L/2]} \left| \mathbb{E}_{\eta_{\text{seq.},\,t}(\cdot)}\left[\,h\,\right] - \mathbb{E}_{p(\cdot\mid\mathbf{x})}\left[\,h\,\right] \right| && (23)\\
&= L \left\| \eta_{\text{seq.},\,t}(\cdot) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} && (24)\\
&\leq \frac{L}{N} \left(w^* - 1\right). && (25)
\end{aligned}$$

□

Theorem 1. *Assuming* $w^* = \sup_{\mathbf{z}} {}^{p(\mathbf{z}\mid\mathbf{x})}/_{q_{\lambda_T}(\mathbf{z})} < \infty$ *for* $\forall \boldsymbol{\lambda}$ *and that the score function is bounded as* $\left| s\left(\mathbf{z}; \boldsymbol{\lambda}\right) \right| \leq \frac{L}{2}$, *the bias of the parallel state estimator with an IMH kernel at iteration t is bounded as*

$$\text{Bias}\left[g_{\text{par.},\,\text{t}}\right] \leq L \left(1 - \frac{1}{w^*}\right).$$

*Proof of **Theorem** 1.* We denote the empirical distribution of the Markov-chain states at iteration t as

$$\eta_{\text{par.},\,t}(\mathbf{z}) = \frac{1}{N} \sum_{i=1}^{N} K\left(\mathbf{z}_{t-1}^{(i)}, \mathbf{z}\right). \tag{26}$$

and consequently,

$$g_{\text{par.},t}(\boldsymbol{\lambda}) = \int s\left(\mathbf{z}; \boldsymbol{\lambda}\right) \eta_{\text{par.},\,t}(\mathbf{z})\, d\mathbf{z}. \tag{27}$$

Similarly with Section 3.3,

$$\begin{aligned}
\left\| \eta_{\text{par.},\,t}(\mathbf{z}) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} &= \left\| \frac{1}{N} \sum_{i=1}^{N} K\left(\mathbf{z}_{t-1}^{(i)}, \mathbf{z}\right) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} && (28)\\
&\leq \frac{1}{N} \sum_{i=1}^{N} \left\| K\left(\mathbf{z}_{t-1}^{(i)}, \cdot\right) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} && \text{(Triangle inequality)} \quad (29)\\
&= \left\| K(\mathbf{z}_t, \cdot) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} && \text{(Uniform ergodicity)} \quad (30)\\
&\leq 1 - \frac{1}{w^*}. && (31)
\end{aligned}$$

And, finally the bias is given as

$$\text{bias}\left[g_{\text{par.,t}}\right] \leq L \left\| \eta_{\text{par.},t}(\cdot) - p(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} \tag{32}$$

$$\leq L \sup_{h : \mathcal{Z} \to [-L/2, L/2]} \left| \mathbb{E}_{\eta_{\text{par.},t}(\cdot)}\left[h \right] - \mathbb{E}_{p(\cdot \mid \mathbf{x})}\left[h \right] \right| \tag{33}$$

$$= L \left\| \eta_{\text{par.},t}(\cdot) - p(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} \tag{34}$$

$$\leq L \left(1 - \frac{1}{w^*} \right) \tag{35}$$

□

Theorem 2. *For a CIS kernel with N internal proposals, assuming $w^* = \sup_{\mathbf{z}} p(\mathbf{z}|\mathbf{x})/q_{\boldsymbol{\lambda}}(\mathbf{z}) < \infty$ for $\forall \boldsymbol{\lambda}$, $N > 2$, and that the score function is bounded such that $|s(\mathbf{z};\boldsymbol{\lambda})| \leq \frac{L}{2}$, the bias of the single state estimator at iteration t is bounded as*

$$\text{Bias}\left[g_{\text{cis.,t}}\right] \leq L\,C \quad \textit{where} \quad C = \left(1 - \frac{N}{w^*}\right) < 1.$$

*Proof of **Theorem** 2.* Let us first denote the empirical distribution of the Markov-chain states at iteration t as

$$\eta_{\text{cis.},t}(\mathbf{z}) = K\left(\mathbf{z}_{t-1}, \mathbf{z}\right), \tag{36}$$

and consequently,

$$g_{\text{cis},t}(\boldsymbol{\lambda}) = \int s\left(\mathbf{z};\boldsymbol{\lambda}\right)\, \eta_{\text{cis.},t}(\mathbf{z})\, d\mathbf{z}. \tag{37}$$

The CIS sampler is identical to the iterated sampling importance resampling (i-SIR) algorithm described by Andrieu et al. (2018). They showed that the i-SIR kernel achieves a geometric convergence rate such that

$$\left\| K^t\left(\mathbf{z}_{t-1}, \cdot\right) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} \leq \left(1 - \frac{N-1}{2\,w^* + N - 2}\right)^t. \tag{38}$$

From this, the bound can be shown as

$$\text{bias}\left[g_{\text{cis.,t}}\right] \leq \left\| \eta_{cis.,t}(\cdot) - p(\cdot \mid \mathbf{x}) \right\|_{\text{TV}} \tag{39}$$

$$\leq \sup_{h : \mathcal{Z} \to [-L/2, L/2]} \left| \mathbb{E}_{\eta_{\text{cis.},t}(\cdot)}\left[h \right] - \mathbb{E}_{p(\cdot \mid \mathbf{x})}\left[h \right] \right| \tag{40}$$

$$= L \left\| \eta_{\text{cis.},t}(\cdot) - p\left(\cdot \mid \mathbf{x}\right) \right\|_{\text{TV}} \tag{41}$$

$$\leq L \left(1 - \frac{N-1}{2\,w^* + N - 2}\right) \tag{42}$$

$$\leq L \left(1 - \frac{N}{w^*}\right) \qquad \text{(Monotonicity)} \tag{43}$$

given that $N > 2$. □

Theorem 3. *The variance of the sequential state estimator is*

*Proof of **Theorem** 3.* For notational convenience, let us define $g\left(\mathbf{z}\right) = s\left(\mathbf{z};\boldsymbol{\lambda}\right)$.

$$\mathbb{V}\left[\, g_{\text{seq.,t}} \,\right] = \mathbb{E}\left[\, \mathbb{V}\left[\, g \mid \mathbf{z}_T \,\right] \right] + \mathbb{V}\left[\, \mathbb{E}\left[\, g \mid \mathbf{z}_T \,\right] \right] \tag{44}$$

$$
\begin{aligned}
&\mathbb{E}\left[\,\mathbb{V}\left[\,g \mid \mathbf{z}_T\,\right]\,\right] && (45)\\
&= \mathbb{E}\left[\,\frac{1}{N^2}\sum_{i=1}^{N}\mathbb{V}\left[\,g\left(\mathbf{z}_{T+i}\right) \mid \mathbf{z}_T\,\right] + \frac{2}{N^2}\sum_{i<j}\mathrm{Cov}\left(\,g\left(\mathbf{z}_{T+1}\right), g\left(\mathbf{z}_{T+i}\right) \mid \mathbf{z}_T\,\right)\,\right] && (46)\\
&= \frac{1}{N^2}\sum_{i=1}^{N}\mathbb{E}\left[\,\mathbb{V}\left[\,g\left(\mathbf{z}_{T+i}\right) \mid \mathbf{z}_T\,\right]\,\right] && (47)\\
&\qquad + \frac{2}{N^2}\sum_{i<j}\mathbb{E}\left[\,\mathrm{Cov}\left(\,g\left(\mathbf{z}_{T+1}\right), g\left(\mathbf{z}_{T+i}\right) \mid \mathbf{z}_T\,\right)\,\right] && (48)\\
&= \frac{1}{N}\sigma^2 + \frac{2}{N^2}\sum_{i<j}\mathbb{E}_{p(\mathbf{z}_T\mid\mathbf{x})}\left[\,\mathrm{Cov}\left(\,g\left(\mathbf{z}_{T+i}\right), g\left(\mathbf{z}_{T+j}\right) \mid \mathbf{z}_T\,\right)\,\right] && \text{(Stationarity)} \quad (49)\\
&= \frac{1}{N}\sigma^2 + \frac{2}{N^2}\sum_{i<j}\mathbb{E}_{p(\mathbf{z}_T\mid\mathbf{x})}\left[\,\mathrm{Cov}\left(\,g\left(\mathbf{z}_{T+i}\right), g\left(\mathbf{z}_{T+j}\right) \mid \mathbf{z}_T\,\right)\,\right] && (50)
\end{aligned}
$$

□

Theorem 4. *The variance of the single mode estimator with a CIS kernel $\mathbb{V}_{q_\lambda}\left[\,g_{\text{single}}\,\right]$ is approximately bounded below such that*

$$
\mathbb{V}_{q_\lambda}\left[\,g_{\text{single}}\,\right] \geq \frac{N^4 Z^4}{(w(\mathbf{z}_{t-1}) + NZ)^4}\mathbb{V}_{q_\lambda}\left[\,f_{IS} \,|\, \mathbf{z}_{t-1}\,\right], \tag{7}
$$

where $Z = \mathbb{E}_{q_\lambda}[p(\mathbf{z},\mathbf{x})/q_\lambda(\mathbf{z})] = \int p(\mathbf{z},\mathbf{x})d\mathbf{z}$ is the normalizing constant.

*Proof of **Theorem** 4.* By the law of total variance,

$$
\begin{aligned}
\mathbb{V}_{q_\lambda}\left[\,g_{\text{single}}\,\right] &= \mathbb{V}\left[\,\mathbb{E}_{q_\lambda}\left[\,g \mid \mathbf{z}_{t-1}\,\right]\,\right] + \mathbb{E}\left[\,\mathbb{V}_{q_\lambda}\left[\,g \mid \mathbf{z}_{t-1}\,\right]\,\right] && (51)\\
&= \mathbb{V}\left[\,\mathbb{E}_{q_\lambda}\left[\,\mathbb{E}\left[\,g \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\,\right]\,\right]\\
&\quad + \mathbb{E}\left[\,\mathbb{V}_{q_\lambda}\left[\,\mathbb{E}\left[\,g \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\,\right] + \mathbb{E}_{q_\lambda}\left[\,\mathbb{V}\left[\,g \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\,\right]\,\right] && (52)\\
&= \mathbb{V}\left[\,\mathbb{E}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right] + \mathbb{E}\left[\,\mathbb{V}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right]\\
&\quad + \mathbb{E}\left[\,\mathbb{E}_{q_\lambda}\left[\,\mathbb{V}\left[\,g \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\,\right]\,\right] && (53)\\
&= \mathbb{V}\left[\,\mathbb{E}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right] + \mathbb{E}\left[\,\mathbb{V}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right]\\
&\quad + \mathbb{E}\left[\,\mathbb{E}_{q_\lambda}\left[\,\mathbb{E}\left[\,g_{\text{IS}}^2 \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\,\right] + \left(\mathbb{E}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)}\,\right]\right)^2\,\right] && (54)
\end{aligned}
$$

where g_{IS} denotes the importance sampling estimator given $\mathbf{z}^{(1:N)}$ and $\mathbf{z}^{(0)} = \mathbf{z}_{t-1}$ defined as $g_{\text{IS}} = \sum_{i=0}^{N}\frac{w\left(\mathbf{z}^{(i)}\right)}{\sum_{i=0}^{N}w\left(\mathbf{z}^{(i)}\right)}s\left(\mathbf{z}^{(i)}\right)$.

If we use Rao-Blackwellization, the last variance term vanishes, and we are left with

$$
\mathbb{V}_{q_\lambda}\left[\,g_{\text{single}}\,\right] = \mathbb{V}\left[\,\mathbb{E}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right] + \mathbb{E}\left[\,\mathbb{V}_{q_\lambda}\left[\,g_{\text{IS}} \mid \mathbf{z}_{t-1}\,\right]\,\right]. \tag{55}
$$

Therefore, in expectation,

Now,

$$\begin{aligned}
&\mathbb{E}_{q_\lambda}\left[\, g_{\text{IS}} \mid \mathbf{z}_{t-1} \,\right] && (56)\\
&= \mathbb{E}_{q_\lambda}\left[\frac{\sum_{i=0}^{N} w\left(\mathbf{z}^{(i)}\right) s\left(\mathbf{z}^{(i)}\right)}{\sum_{i=0}^{N} w\left(\mathbf{z}^{(i)}\right)} \middle| \mathbf{z}_{t-1} \right] && (57)\\
&= \mathbb{E}_{q_\lambda}\left[\frac{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) s\left(\mathbf{z}^{(i)}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} + \frac{w\left(\mathbf{z}_{t-1}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} s\left(\mathbf{z}_{t-1}\right) \middle| \mathbf{z}_{t-1} \right] && (58)\\
&= \mathbb{E}_{q_\lambda}\left[\frac{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) s\left(\mathbf{z}^{(i)}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} \middle| \mathbf{z}_{t-1} \right] && (59)\\
&\qquad + \mathbb{E}_{q_\lambda}\left[\frac{w\left(\mathbf{z}_{t-1}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} \middle| \mathbf{z}_{t-1} \right] s\left(\mathbf{z}_{t-1}\right) && (60)\\
&= \mathbb{E}_{q_\lambda}\left[\frac{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) s\left(\mathbf{z}^{(i)}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} \middle| \mathbf{z}_{t-1} \right] + r\left(\mathbf{z}_{t-1}\right) s\left(\mathbf{z}_{t-1}\right) && (61)\\
&= \mathbb{E}_{q_\lambda}\left[\frac{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) + w\left(\mathbf{z}_{t-1}\right)} \frac{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right) s\left(\mathbf{z}^{(i)}\right)}{\sum_{i=1}^{N} w\left(\mathbf{z}^{(i)}\right)} \middle| \mathbf{z}_{t-1} \right] + r\left(\mathbf{z}_{t-1}\right) s\left(\mathbf{z}_{t-1}\right) && (62)
\end{aligned}$$

Write

$$\mathbb{V}_{q_\lambda}[f|\mathbf{z}_{t-1}] = \mathbb{V}_{q_\lambda}\left[\frac{\sum_{i=1}^{N} w(\mathbf{z}^{(i)})}{\sum_{i=0}^{N} w(\mathbf{z}^{(i)})} \frac{\sum_{i=1}^{N} w(\mathbf{z}^{(i)}) f(\mathbf{z}^{(i)})}{\sum_{i=1}^{N} w(\mathbf{z}^{(i)})} + \frac{w(\mathbf{z}_{t-1})}{\sum_{i=0}^{N} w(\mathbf{z}^{(i)})} f(\mathbf{z}_{t-1}) \middle| \mathbf{z}_{t-1} \right]. \tag{63}$$

Note that if $a > 0$, then we can approximate the function $\sum_{i=1}^{N} x_i/(a + \sum_{i=1}^{N} x_i)$ using the first-order Taylor series expansion about $(Z, \dots, Z)$ by

$$\frac{\sum_{i=1}^{N} x_i}{a + \sum_{i=1}^{N} x_i} \approx \frac{NZ}{a + NZ} + \sum_{i=1}^{N} \frac{a}{(a + NZ)^2}(x_i - Z).$$

Hence, given $\mathbf{z}_{t-1}$, we approximate $\sum_{i=1}^{N} w(\mathbf{z}^{(i)}) / \sum_{i=0}^{N} w(\mathbf{z}^{(i)})$ by

$$\begin{aligned}
\frac{\sum_{i=1}^{N} w(\mathbf{z}^{(i)})}{\sum_{i=0}^{N} w(\mathbf{z}^{(i)})} &\approx \frac{NZ}{w(\mathbf{z}_{t-1}) + NZ} + \sum_{i=1}^{N} \frac{w(\mathbf{z}_{t-1})}{(w(\mathbf{z}_{t-1}) + NZ)^2}(w(\mathbf{z}^{(i)}) - Z) && (64)\\
&= \frac{N^2 Z^2 + w(\mathbf{z}_{t-1}) \sum_{i=1}^{N} w(\mathbf{z}^{(i)})}{(w(\mathbf{z}_{t-1}) + NZ)^2} && (65)
\end{aligned}$$

so that

$$\begin{aligned}
\mathbb{V}_{q_\lambda}[f|\mathbf{z}_{t-1}] \approx \mathbb{V}_{q_\lambda}\Bigg[&\frac{N^2 Z^2}{(w(\mathbf{z}_{t-1}) + NZ)^2} f_{IS} + \frac{w(\mathbf{z}_{t-1})}{(w(\mathbf{z}_{t-1}) + NZ)^2} \sum_{i=1}^{N} w(\mathbf{z}^{(i)}) f(\mathbf{z}^{(i)}) && (66)\\
&+ \frac{w(\mathbf{z}_{t-1})}{\sum_{i=0}^{N} w(\mathbf{z}^{(i)})} f(\mathbf{z}_{t-1}) \Bigg| \mathbf{z}_{t-1} \Bigg]. && (67)
\end{aligned}$$

Observe that $\sum_{i=1}^{N} w(\mathbf{z}^{(i)}) f(\mathbf{z}^{(i)}) = O(N)$ since $\{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}\}$ are independent and identically distributed and that $w(\mathbf{z}_{t-1}) f(\mathbf{z}_{t-1}) / \sum_{i=0}^{N} w(\mathbf{z}^{(i)}) = o(N)$. Combining these, we obtain

$$\mathbb{V}_{q_\lambda}\left[\, f \mid \mathbf{z}_{t-1}, \mathbf{z}^{(1:N)} \,\right] \approx \frac{N^4 Z^4}{(w(\mathbf{z}_{t-1}) + NZ)^4} \mathbb{V}_{q_\lambda}\left[\, f_{\text{IS}} \,|\, \mathbf{z}_{t-1} \,\right], \tag{68}$$

as was to be shown. □