Abstract

Stochastic gradient Markov chain Monte Carlo (SGMCMC) is considered the gold standard for Bayesian inference in large-scale models, such as Bayesian neural networks. Since practitioners face speed versus accuracy tradeoffs in these models, variational inference (VI) is often the preferable option. Unfortunately, VI makes strong assumptions on both the factorization and functional form of the posterior. In this work, we propose a new non-parametric variational approximation that makes no assumptions about the approximate posterior’s functional form and allows practitioners to specify the exact dependencies the algorithm should respect or break. The approach relies on a new Langevin-type algorithm that operates on a modified energy function, where parts of the latent variables are averaged over samples from earlier iterations of the Markov chain. This way, statistical dependencies can be broken in a controlled way, allowing the chain to mix faster. This scheme can be further modified in a “dropout” manner, leading to even more scalability. By implementing the scheme on a ResNet-20 architecture, we obtain better predictive likelihoods and larger effective sample sizes than full SGMCMC.

1 Introduction

There has been much recent interest in deep Bayesian neural networks (BNN) due to their reliable confidence estimates and generalization properties (Wilson and Izmailov, 2020; Jospin et al., 2020; Cardelli et al., 2019). BNNs rely on ensemble averages over model parameters typically obtained from Markov chain Monte Carlo (MCMC) algorithms, which is in contrast to regular neural networks that depend on a single set of parameters. The sheer size of these models requires scalable MCMC approaches based on inexpensive stochastic gradients, of which stochastic gradient Markov chain Monte Carlo (SGMCMC) algorithms are the gold standard (Li et al., 2016; Welling and Teh, 2011; Patterson and Teh, 2013). These algorithms owe their scalability to approximating gradients via mini-batching.

The main downside of using SGMCMC algorithms in high dimensions is their slow mixing rates since they explore the parameter space in a random walk fashion. An oftentimes faster alternative are variational inference (VI) algorithms which approximate the posterior with a simpler (typically factorized) distribution. This formulation results in an optimization problem that can be solved more efficiently using stochastic optimization (Blei et al., 2017; Zhang et al., 2018).

One downside of VI approximations is their strong distributional assumptions. A typical choice is to approximate the Bayesian posterior by a product of univariate Gaussian distributions. These distributional assumptions are frequently over-simplistic in high-dimensional models, where the posterior can be highly multi-modal and possibly heavy-tailed. Another downside is that the variational approximation typically underestimates the posterior variance, leading to poorly calibrated uncertainties and overfitting (Ormerod and Wand, 2010; Giordano et al., 2015; Zhang et al., 2018).

In this work, we derive a fundamentally new approach towards hybridizing variational inference and SGMCMC, resulting in the best of both worlds. While our approach remains a sampling algorithm resembling SGMCMC, we speed up the mixing time by systematically breaking posterior correlations. The resulting algorithm furthermore allows users to specify which posterior correlations to keep and which ones to break. It makes no assumptions on the functional
form of the approximate posterior. We call our approach structured SGMCMC since it relies on a structured (i.e., only partially factorized) variational approximation of the posterior (Wainwright and Jordan, 2008).

In more detail, assuming a functional view on variational inference, we derive the optimal variational distribution for a given posterior subject to factorization constraints. We show how to sample from this optimal distribution by running SGMCMC on a modified energy function. This energy function is obtained by marginalizing the model’s joint distribution over previously generated samples from the Markov chain, leading to an approximate factorization over user-specified parameter groups. Further, we provide a more robust and computational efficient approximation to the procedure that allows for interpolation between regular SGMCMC and our structured SGMCMC by taking inspiration from dropout techniques. Both methods are compatible with any Markovian SGMCMC algorithm, including Langevin dynamics and stochastic gradient Hamiltonian Monte Carlo.

In sum, our contributions are as follows:

- We propose a new non-parametric variational inference scheme by running SGMCMC on a modified energy function. The new approximation trades accuracy for speed and allows users to explore which posterior correlations are important to preserve. This setup effectively allows sampling from a fully joint posterior, a completely factorized posterior, and any in between.
- We prove mathematically that the resulting scheme asymptotically generates samples from the best possible posterior approximation subject to user-specified factorization constraints between groups of parameters.
- We extend this scheme further by making it more scalable with a dropout inspired approximation. This new scheme allows for smoothly interpolating between SGMCMC methods and the properly defined non-parametric mean-field VI.
- We show in both small and large scale experiments that our method well-approximates posterior marginals and gives improved results over SGMCMC on Resnet-20 architectures on CIFAR-10, Fashion MNIST, and SVHN in terms of both runtime and final accuracy.

Our paper is structured as follows: Section 2 presents the related work to our proposal, Section 3 introduces preliminaries regarding the energy function and the stochastic gradient updates, Sections 4 and 5 derive our proposed methodology along with its variants, and Sections 6 and 7 provide our experiments, the conclusions of our proposal and its broader impact.

## 2 Related Work

Our work connects both to (stochastic) variational inference (Bishop, 2006; Hoffman et al., 2013; Ranganath et al., 2014; Blei et al., 2017; Zhang et al., 2018) and scalable MCMC (Welling and Teh, 2011; Chen et al., 2014; Ma et al., 2017; Zhang et al., 2020; Leimkuhler et al., 2019; Wenzel et al., 2020; Ilzmailov et al., 2021). For space limitations, we focus on the most related work at the intersection of both topics.

Among the earliest works to hybridize both approaches was (de Freitas et al., 2001) who constructed a variational proposal distribution in the Metropolos-Hastings step of MCMC. An improved approach to that was introduced in (Habib and Barber, 2018), where by introducing low-dimensional auxiliary variables they fit a more accurate approximating distribution.

Most recent work focuses on connections between VI and stochastic gradient-based MCMC, or between VI and stochastic gradient descent (SGD). For example, Mandt et al. (2016), Stephan et al. (2017) and Duvenaud et al. (2016) consider SGD as a type of variational inference, but their approaches did not attempt to close the gap to exact MCMC. Other works aim at explicitly interpolating between both methods. Domke (2017) proposes a divergence bound for hybridizing VI and MCMC, essentially by running Langevin dynamics on a tempered evidence lower bound (ELBO). Saltmans et al. (2015) embody MCMC steps into the variational inference approximation. Ahn et al. (2012) improve stochastic gradient Langevin dynamics by leveraging the central limit theorem and using the estimated inverse Fisher information matrix to sample from the approximate posterior distribution.

Rezende and Mohamed (2015) interpreted the path of an MCMC algorithm as a variational distribution, and then fitting parameters to tighten a variational bound. Recently, Hoffman and Ma (2020) interpreted (parametric) VI as approximate Langevin dynamics and showed that both algorithms have similar transient dynamics.

Our approach is different from all these papers in that it is a non-parametric, structured mean-field VI scheme inspired by coordinate VI updates (Bishop, 2006). At the same time, it is also an approximate SGMCMC scheme in that the variational distribution is a Markov chain and the ELBO is implicit.
3 Preliminaries

Given data \( D = \{ (x_i, y_i) \}_{i=1,...,N} \), parameters \( \theta \), a proper prior distribution \( p(\theta) \), and a likelihood \( p(D|\theta) = \prod_{i=1}^{N} p(y_i|x_i, \theta) \), suppose we are interested in the corresponding posterior distribution \( p(\theta|D) \propto p(D|\theta)p(\theta) \). A convenient representation of the posterior is as a Boltzmann distribution:

\[
p(\theta|D) \propto \exp\{-U(\theta)\} \quad \text{where} \quad U(\theta) = - \sum_{(x,y) \in D} \log p(y|x, \theta) - \log p(\theta).
\]  

\( U \) is typically referred to as the posterior energy function. Note that the posterior distribution is typically intractable due to the normalizing constant.

Should the maximum a posteriori (MAP) of \( \theta \) (i.e., \( \arg \max_{\theta} p(\theta|D) \)) be desired, it can be found directly with \( \hat{\theta}_{\text{MAP}} = \arg \min_{\theta} U(\theta) \) via various optimization methods, such as SGD. While the MAP is typically quick to optimize for, it does not afford uncertainty estimates of \( \theta \) or any downstream usages of \( \theta \) (e.g., such as predictive uncertainty).

The gold standard for approximating the entire posterior distribution is by deploying Markov chain Monte Carlo (MCMC) algorithms. These methods work by producing an empirical distribution of samples through a random walk in parameter space. While being very accurate and having asymptotic guarantees, these methods are known to not scale well with respect to both data and parameters (Brooks et al., 2011; Geyer, 1992).

Stochastic gradient MCMC (SGMCMC) is a class of scalable MCMC algorithms that is able to produce posterior approximations of continuous-time diffusion processes. Examples of these algorithms include stochastic gradient Langevin dynamics (SGLD) (Welling and Teh, 2011), preconditioned SGLD (pSGLD) (Li et al., 2016), and stochastic gradient Hamiltonian Monte Carlo (SGHMC) (Chen et al., 2014).

As alluded to, the basis of SGMCMC algorithms is using a sampled minibatch of data \( \tilde{D} \) from \( D \) to produce an unbiased estimate of the gradient of the posterior energy function:

\[
\nabla_{\theta} U(\theta) \approx \tilde{\nabla}_{\theta} U(\theta) =: N \nabla_{\theta} G(\theta; \tilde{D})
\]

where \( G(\theta; \tilde{D}) = -\frac{1}{|\tilde{D}|} \sum_{(x,y) \in \tilde{D}} \log p(y|x, \theta) - \frac{1}{N} \log p(\theta). \)

\( G(\cdot) \) can be seen as representing a normalized minibatch loss (with regularization from the prior). Different algorithms use this gradient approximation in different ways to propose new samples of \( \theta \) in their random walks. The update rules for SGLD, pSGLD, and SGHMC are defined as follows:

\[
\text{SGLD} \quad \theta^{(t+1)} = \theta^{(t)} - \frac{\epsilon_t}{2} \tilde{\nabla}_{\theta} U(\theta^{(t)}) + N(0, \epsilon_t I)
\]

\[
\text{pSGLD} \quad \theta^{(t+1)} = \theta^{(t)} - \frac{\epsilon_t}{2} \left[ R(\theta^{(t)}) \tilde{\nabla}_{\theta} U(\theta^{(t)}) + \sum_{\delta} \nabla_{\theta} R(\theta^{(t)}) \right] + N(0, \epsilon_t R(\theta^{(t)}))
\]

\[
\text{SGHMC} \quad \theta^{(t+1)} = \theta^{(t)} + \epsilon_t M^{-1} m^{(t+1)}
\]

\[
m^{(t+1)} = (1 - \gamma \epsilon_t M^{-1}) m^{(t)} - \epsilon_t \tilde{\nabla}_{\theta} U(\theta^{(t)}) + N(0, 2\gamma - \epsilon_t \hat{V}(\theta^{(t)}))
\]

where \( \epsilon_t \) is the step size at time step \( t \), \( R(\cdot) \) and \( M \) are preconditioners, \( \gamma \geq 0 \) is a friction term, and \( \hat{V}(\cdot) \) is an estimate of the covariance induced by the stochastic gradient. All of these methods produce a chain of samples up to time step \( t \) that ultimately form an empirical distribution \( \hat{p}^{(t)}(\theta|D) \). Should the algorithms converge, then \( \lim_{t \to \infty} \hat{p}^{(t)}(\theta|D) = p(\theta|D) \).

4 Structured SGMCMC

By design, SGMCMC methods produce a completely joint posterior distribution over parameters \( \theta \). For models with a large amount of parameters, this can lead to various complications due to the curse of dimensionality. This is typically seen with slow convergence times and potentially unexplored parameter spaces. A viable solution is to break

\footnote{Note that we abuse notation in Eqs.\cite{4}, where the addition of \( N(\mu, \Sigma) \) denotes the addition of a normally distributed random variable with mean \( \mu \) and covariance \( \Sigma \).}
dependencies in the posterior distribution by leveraging variational inference (VI). This would reduce the number of various potential posterior correlations that the model would need to capture while sampling.

To do so, we first start by partitioning the parameters into $M > 1$ distinct groups: $\theta_1, \ldots, \theta_M$. The structured, approximate posterior distribution will be denoted as $q(\theta) = \prod_{i=1}^{M} q_i(\theta_i)$; however, it should be noted that unlike traditional VI, we are not assuming a parametric form of $q$ — only structural. $q(\theta)$ is encouraged to best approximate the posterior $p(\theta|D)$ by seeking to minimize the KL-divergence between the two:

$$J(q(\theta)) = D_{\text{KL}}(q(\theta)||p(\theta|D))$$

$$= \mathbb{E}_{\theta \sim q} \left[ \log \frac{q(\theta)}{p(\theta|D)} \right]$$

(8)

(9)

**Theorem 1.** The unique solution to the KL minimization problem given in Eq. (9) is given by the Boltzmann distribution $Z^{-1} \exp\{- \sum_{i=1}^{M} U_i^{(S)}(\theta_i)\}$ where $U_i^{(S)}(\theta_i) = \mathbb{E}_{\theta_i \sim q_i} \left[ \log p(\theta_i; \hat{\theta}_{\setminus i}, D) \right]$ for $i = 1, \ldots, M$ and $Z$ is a normalizing constant.

**Proof.** We begin by rewriting Eq. (9) as follows:

$$J(q(\theta)) = \mathbb{E}_{\theta \sim q} \left[ \log q(\theta) \right] - \mathbb{E}_{\theta \sim q} \left[ \log p(\theta, D) \right] + C$$

$$= \mathbb{E}_{\theta_i \sim q_i} \left[ \log q_i(\theta_i) \right] + \sum_{i \neq j} \mathbb{E}_{\theta_j \sim q_j} \left[ \log q_j(\theta_j) \right] - \int \log p(\theta, D) q_i(\theta_i) d\theta_i \prod_{i \neq j} q_j(\theta_j) d\theta_j + C$$

(10)

(11)

for some $i \in \{1, \ldots, M\}$, where $\setminus i := \{1, \ldots, M\} \setminus \{i\}$ and $C = \log p(D)$. In order to find the optimal distribution that respects the factorization constraints imposed between parameter groups, we need to minimize this functional over $q$ — or rather every $q_i$. This is done by taking the functional derivative of $J$ with respect to $q_i$, setting it equal to zero, and solving for $q_i$:

$$\frac{\delta J(q(\theta))}{\delta q_i(\theta_i)} = \int \log p(\theta, D) \prod_{i \neq j} q_j(\theta_j) d\theta_j - 1 - \log q_i(\theta_i) := 0$$

$$\implies \log q_i(\theta_i) = \mathbb{E}_{\theta_i \sim q_i} \left[ \log p(\theta_i, \hat{\theta}_{\setminus i}, D) \right] - 1$$

$$\implies q_i(\theta_i) \propto \exp \left\{ \mathbb{E}_{\theta_i \sim q_i} \left[ \log p(\theta_i, \hat{\theta}_{\setminus i}, D) \right] \right\}.$$ 

(12)

(13)

(14)

By defining the energy $U_i^{(V)}(\theta_i) = -\mathbb{E}_{\theta_i \sim q_i} \left[ \log p(\theta_i, \hat{\theta}_{\setminus i}, D) \right]$, we realize that by minimizing the KL-divergence in Eq. (9), the approximate posterior distribution $q = \prod_{i=1}^{M} q_i$ takes the form of a Boltzmann distribution as in Eq. (1) with $U^{(V)}(\theta) = \sum_{i=1}^{M} U_i^{(V)}(\theta_i)$.

It remains to be shown that the solution is unique. To this end, we refer to the convexity of the KL divergence in function space [Cover and Thomas 2001]. This implies that the stationary point of the KL is indeed a global optimum and unique.

We will now show how to leverage the results of Theorem 1 to construct an algorithm that can produce samples from the approximate posterior $q(\theta)$. Since $U^{(S)}$ is properly defined, samples that approximate $q(\theta)$ can be generated using SGMCMC algorithms. Similar to $\hat{q}^{(t)}(\theta|D)$, we will denote the empirical distribution of samples up to time step $t$ from $q(\theta)$ as $\tilde{q}^{(t)}(\theta)$. The only requirement is to use these algorithms to define the stochastic estimate of the energy function’s gradient $\nabla_\theta U^{(S)}(\theta)$:

$$\nabla_\theta U^{(S)}(\theta) \approx \nabla_\theta U^{(S)}(\theta) := N \nabla_\theta G^{(S)}(\theta; \hat{D})$$

$$G^{(S)}(\theta; \hat{D}) = \sum_{i=1}^{M} \mathbb{E}_{\theta_i \sim q_i} G(\{\theta_i, \hat{\theta}_{\setminus i}\}; \hat{D})$$

(15)

(16)

In practice, $\mathbb{E}_{\theta_i \sim q_i} G(\{\theta_i, \hat{\theta}_{\setminus i}\}; \hat{D})$ is approximated using a single-sample, Monte Carlo estimate:

$$\mathbb{E}_{\theta_i \sim q_i} G(\{\theta_i^{(t)}, \hat{\theta}_{\setminus i}\}; \hat{D}) \approx G(\{\theta_i^{(t)}, \hat{\theta}_{\setminus i}^{(t)}\}; \hat{D})$$

(17)

where $\theta_i^{(t)}$ is sampled from the chain $q_i^{(t)}$. Putting Eq. (17) into words, the minibatch loss specific to $\theta_i^{(t)}$ is approximated by substituting $\theta_i^{(t)}$ in the model with a sample from the empirical approximate posterior $q_i^{(t)}$. 


While a formal proof of convergence needs to be shown, one can see that the approximate posterior is a fixed point of the sampling scheme. Namely, if $q_{\theta}(\theta \rightarrow \theta)$ is stationary, then the Monte-Carlo gradient of Eq. (17) with respect to $\theta$, will be an unbiased gradient estimator of the energy function’s true gradient Eq. (16) and the Langevin chain will converge to the correct marginal, and in particular remain stationary. In practice, we find that the scheme converges to a stationary distribution (Section 6).

This formulation of $\nabla_{\theta} U(\theta)$ can be plugged in anywhere $\nabla_{\theta} U(\theta)$ appears in the original SGMCMC algorithms. The resulting class algorithms will be referred to as structured SGMCMC (S-SGMCMC). We will denote specific structured variants of SGMCMC algorithms with a ‘$S$’ prefix (e.g., S-SGLD, S-pSGLD, and S-SGHMC). The full algorithm can be seen in Algorithm 1.

5 Structured Dropout SGMCMC

With just a slight shift in perspective, it is actually possible to further generalize $U(S)$ and consequently S-SGMCMC to produce a broader class of approximate sampling algorithms. This is done by first noting that $U(S)$ can be represented with a scaled double-expectation:

$$U(S)(\theta) = -\frac{E_{r \sim p(S)} \left[ \sum_{i=1}^{M} r_i \right]}{E_{r \sim q(S)} \left[ \log p(r \theta + (1 - r) \tilde{\theta}, D) \right]}$$

where $p(S)(r) = \text{Cat}(r; M^{-1}, \ldots, M^{-1})$ and $(r \theta + (1 - r) \tilde{\theta})$, is equal to $\theta$ if $r = 1$ and $\tilde{\theta}$ otherwise for $i = 1, \ldots, M$.

Note that this is constructed in this manner specifically so that $U(S)$ remains differentiable with respect to $\theta$. Also note that though the denominator appears superfluous as $E_{r \sim p(S)} \left[ \sum_{i=1}^{M} r_i \right] = 1$, it is necessary for certain theoretic properties, as seen in Theorem 2.

By replacing $p(S)$ with a more flexible distribution, we can further generalize and encapsulate different energy functions to sample from. One such choice is $p^{(S_d)}(r; \rho) = \prod_{i=1}^{M} \text{Bern}(r_i; \rho) \mathbb{1}(\sum_{i=1}^{M} r_i > 0)$ with $\rho \in (0, 1)$. Substituting $p(S)$ for $p^{(S_d)}$ in Eq. (18) yields a new energy function that we will refer to as $U(S_d)$. We note that this choice in distribution leads to a dropout-like behavior of Nalisnick et al. [2019], Srivastava et al. [2014], where the composition of model parameters as $r \theta + (1 - r) \tilde{\theta}$ leads to each parameter group $\theta_i$ having a probability of approximately $\rho$ to be used in a prediction and a $(1 - \rho)$ probability of being replaced by $\tilde{\theta}_i$ from the approximate posterior (traditional dropout, $\theta_i$ would instead be replaced with 0). Likewise, we will denote methods that use this energy function for sampling as structured dropout SGMCMC ($S_d$-SGMCMC) with different variants all sharing the same $S_d$ prefix (e.g. S_d-SGHMC).

**Theorem 2.** For a given set of parameters $\theta$ partitioned into $M$ groups, the following holds true: (i) $U(S_d) \to U$ as $\rho \to 1$ and (ii) $U(S_d) \to U(S)$ as $\rho \to 0$. Thus, distributions approximated by $S_d$-SGMCMC lie on a continuum with those generated by S-SGMCMC at one extreme and with those from SGMCMC at the other.

Please refer to the Supplement for the full, formal proof. Informally, a dropout rate of $\rho = 1$ implies that $r \theta + (1 - r) \tilde{\theta}$ is equivalent to just $\theta$. This, in effect, recovers the original energy function $U$ as every parameter group is updated together. Likewise, when $\rho \to 0$ it can be shown that $p^{(S_d)} (r_i = 1, r_{-i} = 0; \rho) \to M^{-1}$ for $i = 1, \ldots, M$. As such, this implies that $p^{(S_d)} \to \text{Cat}(M^{-1}, \ldots, M^{-1})$ which in turn recovers $U(S)$ from $U(S_d)$ by design.

In practice, the double-expectation in $U(S_d)$ is jointly approximated using a Monte Carlo estimate with $K$ samples. This leads to the following approximated gradients to use with SGMCMC algorithms:

$$\nabla_{\theta} U^{(S_d)}(\theta^{(t)}) \approx \nabla_{\theta} U^{(S_d)}(\theta^{(t)}) =: N \nabla_{\theta} G^{(S_d)}(\theta^{(t)}; \tilde{D}) \quad \text{(19)}$$

$$G^{(S_d)}(\theta^{(t)}; \tilde{D}) \approx \frac{1}{Kp} \sum_{k=1}^{K} G(r^{(t,k)} \theta^{(t,k)} + (1 - r^{(t,k)}) \tilde{\theta}^{(t,k)}; \tilde{D}) \quad \text{(20)}$$

where $r^{(t,k)} \sim p^{(S_d)}$ and $\tilde{\theta}^{(t,k)} \sim \tilde{q}^{(t)}$ for $k = 1, \ldots, K$. We note that by approximating $U^{(S_d)}$ in this way, computing a gradient no longer scales on the order of $O(M)$, but rather $O(K)$. This means that the choice of structure imposed on the posterior distribution remains independent of computing resources. As such, configurations with large amounts of parameter groups are typically only feasible when using $S_d$-SGMCMC as S-SGMCMC would use too much memory and/or compute per sample.

2Other choices of distribution that are well justified include any with support over $[0, 1]^M$ and with measure 0 over $\{0\}^M$. Exploring the effects these distributions have are an interesting line of future inquiry.
Algorithm 1: S-SGMCMC

Input: Initial sample $\theta^{(0)}$; parameter partitions $\theta_1, \ldots, \theta_M$; step sizes $\{\epsilon_t\}_{t=1}^{T-1}$.

Output: $\hat{q}^{(T)}(\theta) := \{\hat{\theta}^{(t)}\}_{t=1}^{T}$.

1. for $t = 0$ to $T - 1$
2. Sample minibatch $\tilde{D}^{(t)} \subset \mathcal{D}$
3. for $i = 1$ to $M$
4. Sample $\tilde{\theta}^{(t)} \sim \hat{q}^{(t)}$
5. $G_{i}^{(S,t)} = G(\{\tilde{\theta}^{(t)}, \theta^{(t)}\}; \tilde{D}^{(t)})$
6. end
7. $\hat{\nabla}_{\theta} U^{(S,t)} = N \sum_{i=1}^{M} \nabla_{\theta} G_{i}^{(S,t)}$
8. $\tilde{\theta}^{(t+1)} = \hat{\text{SGMCMC\_step}}(\tilde{\theta}^{(t)}, \hat{\nabla}_{\theta} U^{(S,t)}, \epsilon_t)$
9. end
10. return $\hat{q}^{(T)}(\theta)$

6 Experiments

Overview In this section we evaluate our proposed approach on various models and datasets. To directly visualize and compare the posterior approximations of our different proposed methods, Section 6.1 analyzes a low-dimensional regression data set. Section 6.2 investigates the impact of the variational approximation on the algorithms’ mixing and autocorrelation times using a fully-connected network architecture on MNIST (LeCun et al., 2010). Section 6.3 studies our methods with ResNet-20 (He et al., 2016) on CIFAR-10 (Krizhevsky et al., 2009), SVHN (Netzer et al., 2011), and Fashion MNIST (Xiao et al., 2017) and compares them for their accuracy and speed of convergence. Our experiments reveal that our methods converge faster than SGMCMC and sometimes even achieve higher accuracies.

Metrics For the evaluation of our proposal we examine the resulting modeling capabilities in classification accuracy. We take the average of an ensemble of 100 models whose weights are sampled from the past samples of the parameters chains in order to calculate the accuracy. Identifying convergence for these kind of methods is challenging due to there being an “official” metric (Gelman et al., 1992). For the convergence of our methods, we decided to use two convergence criteria: integrated autocorrelation time (IAC) (Sokal, 1997; Goodman and Weare, 2010) and effective sample size (ESS) (Geyer, 1992).

IAC quantifies the Monte Carlo error between samples and hence the inefficiency of a MCMC algorithm. IAC is computed as $\tau_f = \sum_{\tau=-\infty}^{\infty} \rho_f(\tau)$ where $\rho_f$ is the normalized autocorrelation function of the stochastic process that generated the chain for $f$ and is calculated as $\hat{\rho}_f(\tau) = \hat{c}_f(\tau)/\hat{c}_f(0)$, where $\hat{c}_f(\tau) = \frac{1}{N-\tau} \sum_{n=1}^{N-\tau} (f_n - \mu_f)(f_{n+\tau} - \mu_f)$ and $\mu_f = \frac{1}{N} \sum_{n=1}^{N} f_n$. We note that we calculated $\hat{c}_f(\tau)$ with a fast Fourier transform as it is more computationally efficient than using the direct sum. ESS measures how many independent samples would be equivalent to an chain of correlated samples and is calculated as $n_{\text{eff}} = \frac{n}{\sum_{n=1}^{N} (n - 1)^2}$, where $n$ is the number of samples and $\rho$ is the autocorrelation. We note that a model with higher ESS and lower IAC converges faster. See the Supplement for the detailed implementation details and experimental setup for the metrics and our models.

6.1 Qualitative Differences in a Simulation

First, we aim to showcase qualitative differences in the empirical posterior distributions generated by a baseline SGMCMC algorithm and our proposed variants. To do so, we consider a regression task where 100 randomly sampled three-dimensional covariates $\{\tilde{x}_i = [x_{i1}, x_{i2}, x_{i3}]^{T}\}_{i=1}^{100}$ are used to sample response values $y_i \sim \mathcal{N}(\tilde{w}^{T} \tilde{x}_i + b, \sigma^2)$ where $\tilde{w} = [w_1, w_2, w_3]^{T} = [1.5, -0.8, 1.3]^{T}$, $b = 0.5$, and $\sigma^2 = 1$. More details on the generation process for $\tilde{x}$ can be found in the Supplement.

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4We used the tensorflow implementation for ESS which uses the direct sum for the autocorrelation.
We choose to fit a linear regression model of the same form as the generation process. \( \sigma^2 \) is assumed to be known. Thus, \( \theta = [w_1, w_2, w_3, b] \). A standard normal distribution is used as the prior for each parameter. Due to conjugacy, the posterior distribution can be calculated analytically. As such, the MAP is roughly \( \hat{\theta}_{\text{MAP}} \approx [0.52, 0.31, 0.47, 0.84] \).

The approximated posterior distributions for \( \theta \) are found using SGLD, S-SGLD, and S\(_d\)-SGLD. For the latter two sampling schemes, two parameter partitions are tested: (i) two groups of parameters where \( \theta_1 = [w_1, w_2] \) and \( \theta_2 = [w_3, b] \) and (ii) four groups of parameters where \( \theta_1 = w_1, \theta_2 = w_2, \theta_3 = w_3, \) and \( \theta_4 = b \). For S\(_d\)-SGLD, \( \rho = 0.5 \) and \( K = 4 \) was used.

The resulting posterior distributions for \( (w_1, w_2) \) and \( (w_1, w_3) \) from all five scenarios, with SGLD in the leftmost column as our baseline, can be seen in Fig. 1. We observe that, as expected, correlations between \( (w_1, w_2) \) still exist when they are allocated to the same parameter group and become apparently independent when assigned to different groups. We also note that the variance of the distributions shrink as the parameter space is partitioned into smaller groups. The underestimation of posterior variance is a commonly reported finding for VI techniques and is interesting to note that our non-parametric methods appear to exhibit this behavior as well. Finally, it appears that the S\(_d\)-SGLD adequately approximates S-SGLD with just slightly higher variances and very minor correlations between parameter groups being exhibited.

### 6.2 Dropout Rate & Group Size Investigation

The aim of this set of experiments is to study the effects that the number of independent parameter groups (or alternatively, the amount of allowed posterior correlations) has on accuracy and convergence when using our proposed methods. We compare pSGLD, S-pSGLD, and S\(_d\)-pSGLD with dropout rates \( \rho \in \{0.1, 0.3, 0.5\} \) on a fully-connected neural network with 2 hidden layers, each with 50 hidden units, trained and evaluated with MNIST using the standard train and test split.

The model has 42,200 parameters in total. For S-pSGLD and S\(_d\)-pSGLD, these parameters are evenly distributed into \( M \) groups where \( M \) ranges from 4 to 42,200. Accuracy, IAC, and ESS are reported in Fig. 2 using 100,000 posterior samples after a 150,000 burn-in period. More details on the implementation of the model regarding training and evaluation can be found in the Supplement.
As shown in Fig. 2(a), for S-pSGLD we observe that as we increase the number of groups the accuracy drops dramatically whereas S_d-pSGLD’s accuracy improves slightly and then remains fairly stable. In the best case, S_d-pSGLD achieves an accuracy of 96.3% with 32 groups and dropout rate of 0.5 which outperforms pSGLD with accuracy of 94.2%. We speculate that the dropout-like behavior is beneficial for regularizing the model (much like normal dropout), hence the improved accuracy across all dropout rates. Similarly, a single sample used for the Monte Carlo estimate in S-SGMCMC may not be enough as the number of groups \( M \) increase; however, increasing the number of samples in this scenario is infeasible due to S-SGMCMC scaling as \( O(M) \).

Fig. 2(b-c) portrays the comparison between number of groups and convergence metrics IAC and ESS. As the number of groups gradually increase, we note that S-pSGLD converges faster, as does S_d-pSGLD to lesser and lesser degrees as \( \rho \) increases.

This behavior is to be expected due to Theorem 2 with S_d-pSGLD exhibiting convergence rates more similar to pSGLD when \( \rho = 0.5 \) and more similar to S-pSGLD when \( \rho = 0.1 \).

### 6.3 Systematic Comparison on Real-World Data

We test the proposed methodology on larger-scale datasets which mimic real-world data: CIFAR-10, SVHN, and FMNIST. It is worth-mentioning that for these datasets we employ ResNet-20 without any data augmentation for the assessment of our methods. We evaluate the precision of the methods on accuracy over time and the overall convergence of them on IAC and ESS with 2 base algorithms: pSGLD and SGHMC.

In Fig. 3, we observe how quickly the proposed methods and the baseline SGMCMC methods approach their optimum accuracy over the course of training. As is shown, S_d-SGMCMC appears to achieve optimal accuracy values much faster than SGMCMC on all datasets and with all base sampling schemes. S-SGMCMC appears to do the same to a lesser extent in all but one case (FMNIST with SGHMC). In some cases, the variational methods appear to even achieve better accuracy values than the baseline methods, as seen in Fig. 3(a)(i-iii).

IAC and ESS were calculated for the same methods using the latest 5,000 samples after sampling for 300 epochs; the results of which can be found in Table 1. For CIFAR-10, we see that S-pSGLD with 2 evenly split parameter groups converges the fastest against all other methods. Likewise, for SVHN and FMNIST, S_d-pSGLD with every parameter belonging to its own group converges faster than all other methods. At times it does appear that increasing the number of parameter groups causes slower convergence for S-SGMCMC. This could potentially be attributed to large variance in the gradients from using only a single sample per Monte Carlo estimate.

To ensure that our methods produce well-calibrated uncertainties, similar to the baseline SGMCMC methods, we also evaluated our proposed algorithms on expected calibration error (ECE) (Guo et al., 2017).

We find that the variational methods produce comparable ECE values to the baseline. These results can be found in more detail in the Supplement.
7 Conclusions

In an attempt to hybridize MCMC and VI, we proposed S-SGMCMC: an approach that produces samples from an structured posterior by running SGMCMC on a modified energy function. The resulting Markov chain becomes asymptotically decoupled across user-specified groups of parameters, resulting in faster convergence.

For better computational efficiency, we proposed $S_d$-SGMCMC: a further generalization of S-SGMCMC inspired by dropout. This extension allows interpolating between a SGMCMC algorithm and its corresponding S-SGMCMC method. Our experimental results demonstrate that the proposed methods impose structure over posterior distributions, increase convergence speeds, and result in similar or better posterior predictive accuracies compared to SGMCMC on a variety of (deep) models. Our experimental evaluations have provided strong empirical evidence for the efficacy of our approach.

Despite its proven capabilities, our proposed methodology does come with some limitations. Namely, for quick access our methods require keeping chains of samples on the GPU whereas the baseline SGMCMC methods can simply save samples to disk.

Additionally, S-SGMCMC scales poorly with respect to the number of parameter groups. $S_d$-SGMCMC manages to break this dependency; however, it still requires more compute than SGMCMC per sample. Possible future work could focus on more theoretical analyses of S-SGMCMC, such as formal proofs of convergence.

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