Preferential data subsampling in stochastic gradient MCMC

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Background and Notation

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The **posterior density** for $\theta \in \mathbb{R}^d$ given data $\mathbf{y} = \{y_1, y_2, \ldots, y_N\}$, up to a constant of proportionality, is

$$\pi(\theta) := p(\theta \,|\, \mathbf{y}) \propto p(\theta) \prod_{i=1}^{N} p(y_i \,|\, \theta),$$

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where $p(\theta)$ is a **prior** for the parameters θ.

For notational convenience we define $f_i(\theta) = -\log p(y_i \,|\, \theta)$ for $i = 1, \ldots, N$, where $f_0(\theta) = -\log p(\theta)$ and $f(\theta) = \sum_{i=0}^{N} f_i(\theta)$ is the **potential function**.

In this setting, the posterior density can be rewritten as,

$$\pi(\theta) \propto \exp(-f(\theta))$$

Langevin diffusion

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The Langevin diffusion, $\theta(t)$, is defined by the **stochastic differential equation** (SDE),

$$d\theta(t) = -\frac{1}{2}\nabla f(\theta(t))dt + dB_t,$$

where $\nabla f(\theta(t))dt$ is a **drift term** and B_t denotes a d-dimensional Wiener process.

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For a small step-size $\epsilon > 0$, the Langevin diffusion can be approximated by the **unadjusted Langevin algorithm** (ULA),

$$\theta^{(t+1)} = \theta^{(t)} - \frac{\epsilon}{2}\nabla f\left(\theta^{(t)}\right) + \sqrt{\epsilon}\,\eta^{(t)},$$

where the noise $\eta^{(t)} \sim \mathcal{N}_d(\mathbf{0}, I_{d\times d})$ is drawn independently at each update.

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The stochastic gradient Langevin dynamics (SGLD) algorithm improves the per-iteration computational burden of MCMC by replacing the full-data gradient $\nabla f(\theta)$ with an unbiased estimate $\nabla \hat{f}(\theta)$.

If the full-data gradient is

$$\nabla f(\theta) = \nabla f_0(\theta) + \sum_{i=1}^{N} \nabla f_i(\theta)$$

then an unbiased estimate is given by

$$\nabla \hat{f}(\theta) = \nabla f_0(\theta) + \frac{N}{n} \sum_{i \in \mathcal{S}} \nabla f_i(\theta),$$

where $\mathcal{S}$ is a subset of $\{1, \ldots, N\}$ with $|\mathcal{S}| = n$, $(n \ll N)$.

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A single update of the vanilla SGLD algorithm is thus given by,

$$\theta^{(t+1)} = \theta^{(t)} - \frac{\epsilon^{(t)}}{2} \cdot \nabla \hat{f}(\theta^{(t)}) + \xi^{(t)}, \qquad \xi^{(t)} \sim \mathcal{N}_d(0, \epsilon^{(t)} I_{d \times d}),$$

where $\{\epsilon^{(t)}\}$ corresponds to a schedule of step-sizes which may be fixed or decreasing.

Controlling the variance of the gradients

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Dalalyan & Karagulyan (2019) Thm.3

Let $\tilde{\pi}_t$ be the posterior distribution after t iterations of the SGLD algorithm and be its distribution. If π satisfies the strongly log-concave assumption then

$$W_2(\tilde{\pi}_t, \pi) \leq (1 - C_0\epsilon)^t W_2(\tilde{\pi}_0, \pi) + C_1(\epsilon d)^{1/2} + C_2(\epsilon d)^{1/2}\sigma,$$

where C_0, C_1 and C_2 are constants and σ^2 is the variance of $\nabla \hat{f}(\theta)$ and $W_2(\cdot, \cdot)$ is the 2-Wasserstein distance.

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Under SGLD, the variance σ^2 is of order N^2/n. Therefore the bound on $W_2(\tilde{\pi}_k, \pi)$ is dominated by a term of order $N(\epsilon d/n)^{1/2}$.

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The quality of the posterior approximation is directly tied to the variance in the gradient estimate. A similar story follows for **minibatching the Metropolis-Hastings ratio** (Quiroz et al. 2018) and **piecewise deterministic Markov process** (PDMP) algorithms, such as the zig-zag sampler (Bierkens et al. 2019).

SGLD with control variates

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Let $\hat{\theta}$ be a fixed value of the parameter, typically chosen to be close to the *maximum a posteriori* value of the target posterior density. The **control variate gradient estimator** takes the form (Baker et al. 2019),

$$\nabla \hat{f}_{cv}(\theta^{(t)}) = \left[\nabla f(\hat{\theta}) + \nabla f_0\left(\theta^{(t)}\right) - \nabla f_0(\hat{\theta})\right] + \frac{N}{n} \sum_{i \in \mathcal{S}} \left[\nabla f_i\left(\theta^{(t)}\right) - \nabla f_i(\hat{\theta})\right].$$

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Implementing the SGLD-CV estimator involves a **one-off pre-processing step** to find $\hat{\theta}$, which is typically done using stochastic gradient descent (SGD). The gradient terms $\nabla f_i\left(\hat{\theta}\right)$ are calculated and stored. While these steps are both $O(N)$ in computational cost, the optimisation step to find the mode can replace the typical burn-in phase of the SGLD chain.

Simple Gaussian model

Simulated $N = 10{,}000$ data point from,

$$y_i \sim \mathcal{N}(\theta, 1)$$

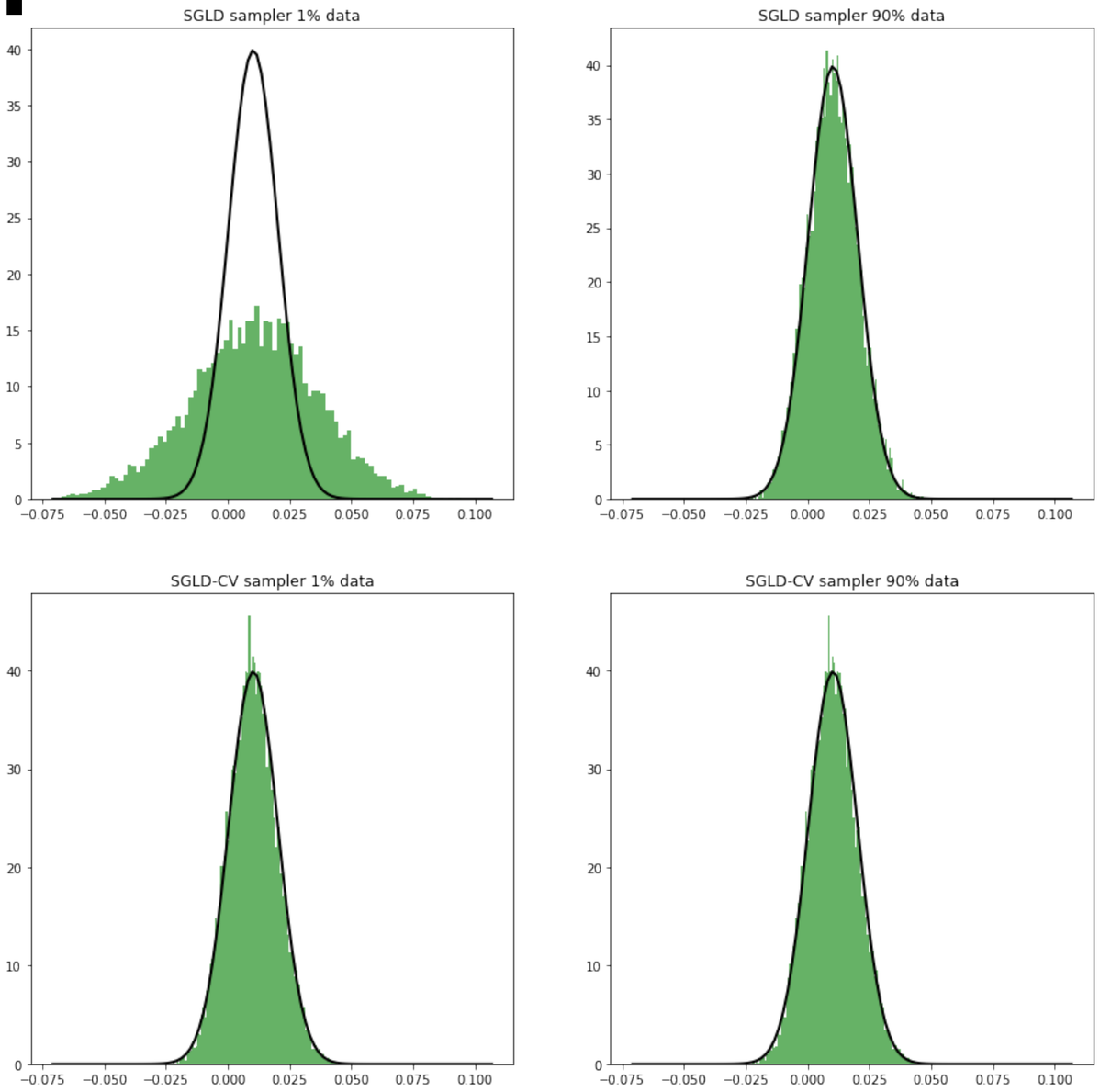
with $\theta = 0$.

Set the prior to be $\mathcal{N}(0, 10)$ then the posterior is given in closed-form

$$\theta \,|\, y \sim \mathcal{N}(\mu, \sigma^2).$$

Run SGLD and SGLD-CV with data subsample sizes of 1% and 90%.

https://tinyurl.com/2tdh97z4



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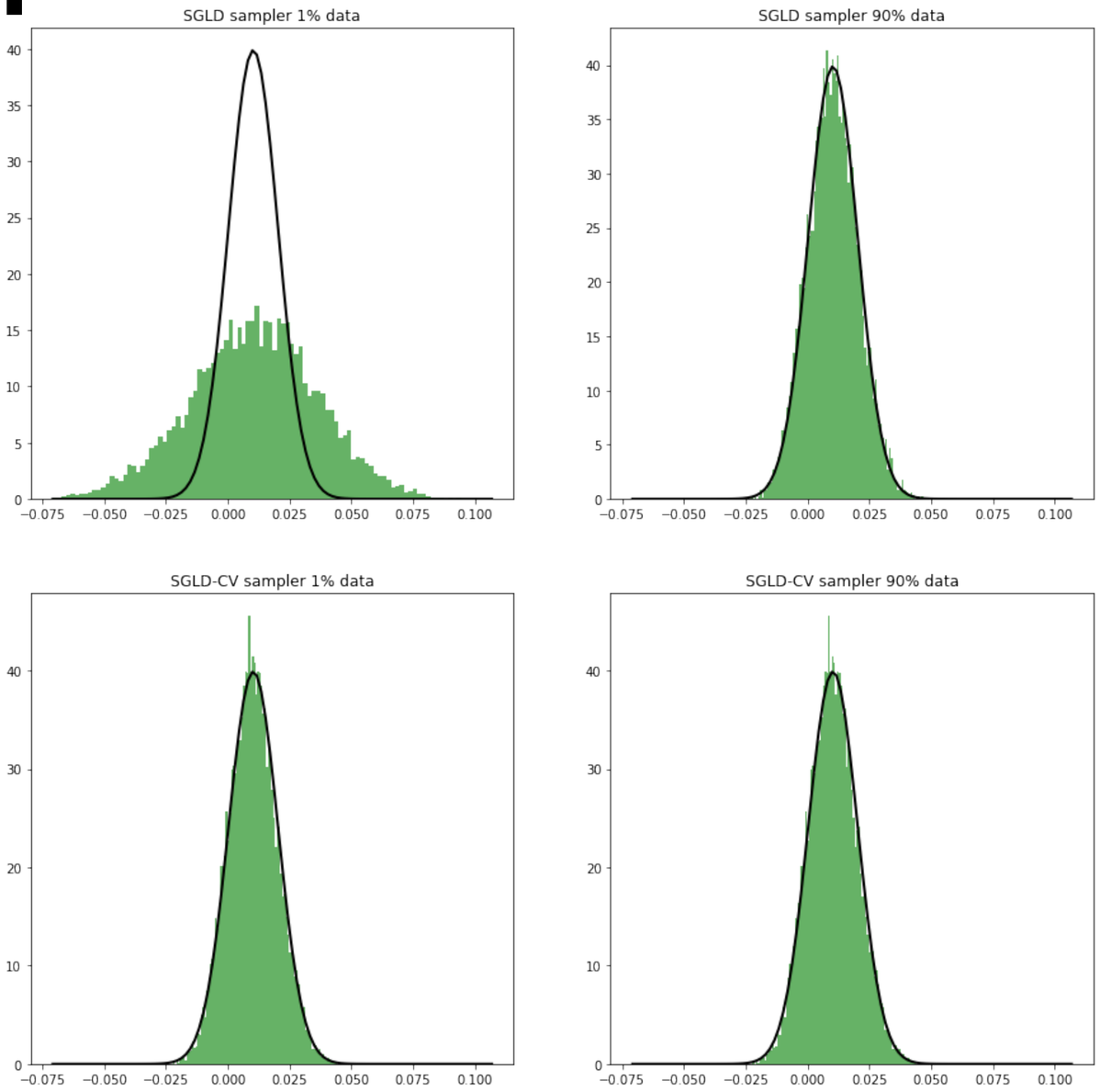

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Preferential data subsampling

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An alternative gradient estimator for SGLD can be given by reweighting the simple estimator

$$\nabla \hat{f}_{ps}(\theta^{(t)}) = \nabla f_0\left(\theta^{(t)}\right) + \frac{1}{n} \sum_{i \in \mathcal{S}} \frac{1}{p_i^t} \nabla f_i\left(\theta^{(t)}\right),$$

where $\mathcal{S} \subset \{1, \ldots, N\}$ is selected according to $\mathbf{p}^{(t)} = (p_1^t, \ldots, p_N^t)^T$ and $|\mathcal{S}| = n \quad (n \ll N)$.

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Our goal is to find a **preferential subsampling distribution $\mathbf{p}$**, which minimises the gradient variance:

$$\min_{\mathbf{p}^{(t)}, p_i^t \in [0,1], \sum_i p_i^t = 1} \mathrm{Var}\Big[\nabla \hat{f}_{ps}(\theta^{(t)})\Big] .$$

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Note that $p_i = 1/N$ gives us the original gradient estimator.

Optimal preferential data subsampling

Proposition

For the SGLD with preferential subsampling gradient estimator $\nabla \hat{f}_{ps}(\theta)$, the variance is given by

$$\min_{\mathbf{p}^{(t)},\, p_i^t \in [0,1],\, \sum_i p_i^t = 1} \frac{1}{n} \sum_{i=1}^{N} \frac{1}{p_i^t} \left\| \nabla f_i\left(\theta^{(t)}\right) \right\|^2,$$

and the optimal weights which minimise the gradient variance are,

$$p_i^t = \frac{\| \nabla f_i\left(\theta^{(t)}\right) \|}{\sum_{k=1}^{N} \| \nabla f_k\left(\theta^{(t)}\right) \|} \quad \text{for } i = 1, \ldots, N.$$

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Proposition

For the SGLD-CV with preferential subsampling gradient estimator $\nabla \hat{f}_{ps}(\theta)$, the variance is given by

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The optimal weights, $p_i^t = \|\nabla f_i\left(\theta^{(t)}\right)\| / \sum_{k=1}^{N} \|\nabla f_k\left(\theta^{(t)}\right)\|$, depend on the current state of the Markov chain $\theta^{(t)}$ and require N gradient calculations at each iteration t.

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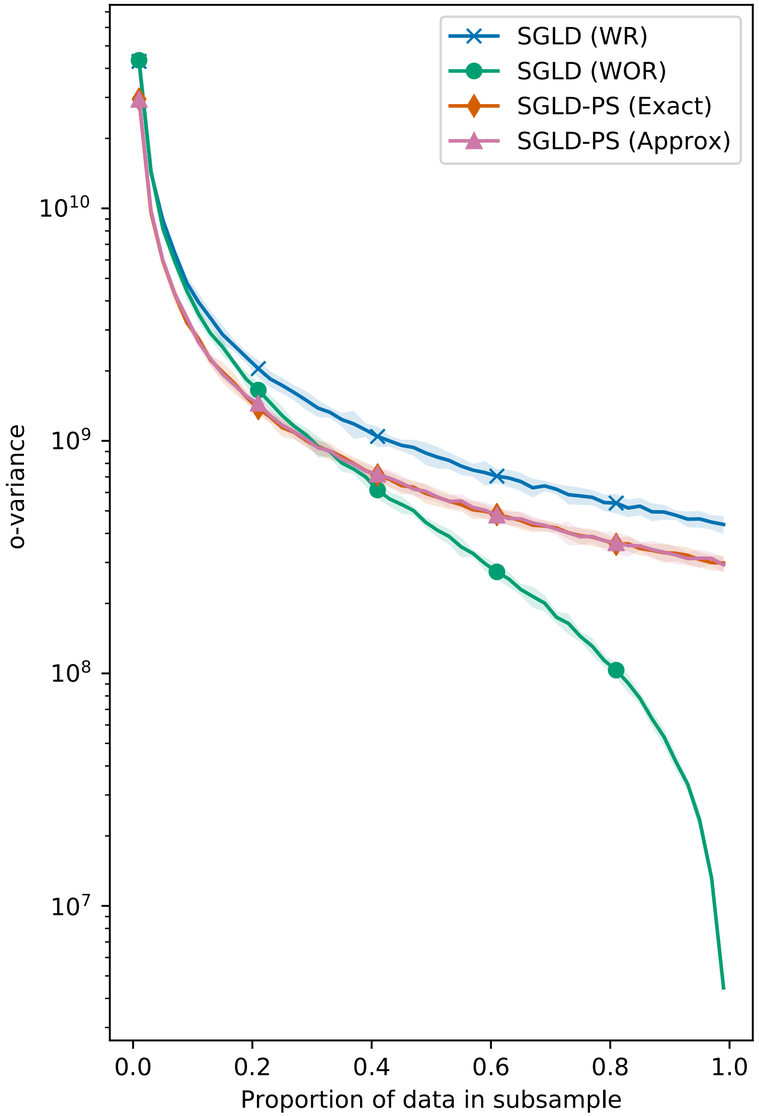
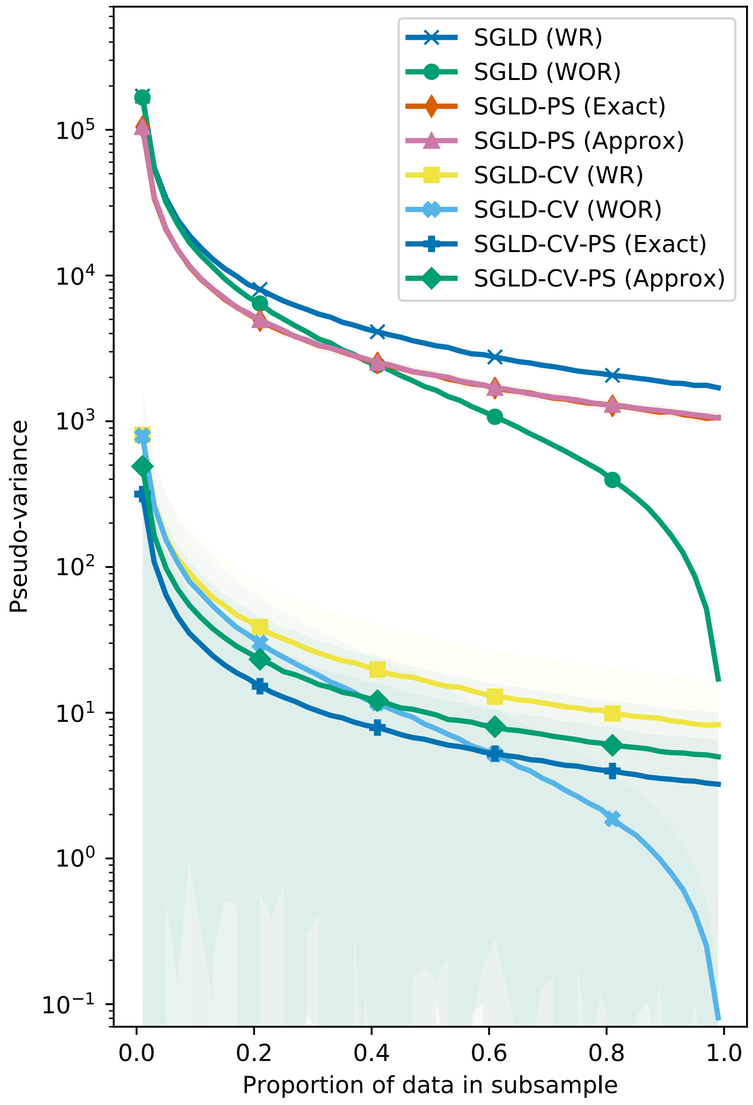
In this case, the approximate subsampling scheme would be given by,

$$\hat{p}_i^t = \frac{\|\nabla f_i\left(\hat{\theta}\right)\|}{\sum_{k=1}^{N} \|\nabla f_k\left(\hat{\theta}\right)\|} \quad \text{for } i = 1, \ldots, N.$$

Variance of the gradients



Gaussian model



Logistic regression model

Bivariate Gaussian example

We want to simulate independent data from:

$$Y_i \,|\, \theta \sim \mathcal{N}_2(\theta, \Sigma_x) \;\; \text{for } i = 1, \ldots, N\,.$$

The conjugate prior for θ is set to be

$$\theta \sim \mathcal{N}_2(\mu_0, \Lambda_0)\,.$$

The conjugate posterior that we are ultimately trying to simulate from using SGLD is known to be:

$$\pi(\theta \,|\, \mathbf{y}) \propto \exp\left(-\frac{1}{2}(\theta - \mu_1)^T \Lambda_1^{-1} (\theta - \mu_1) \right) \stackrel{D}{=} \mathcal{N}_2(\mu_1, \Lambda_1),$$

where $\mu_1 = (\Lambda_0^{-1} + N\Sigma_x^{-1})^{-1}(\Lambda_0^{-1}\mu_0 + N\Sigma_x^{-1}\bar{y})$,

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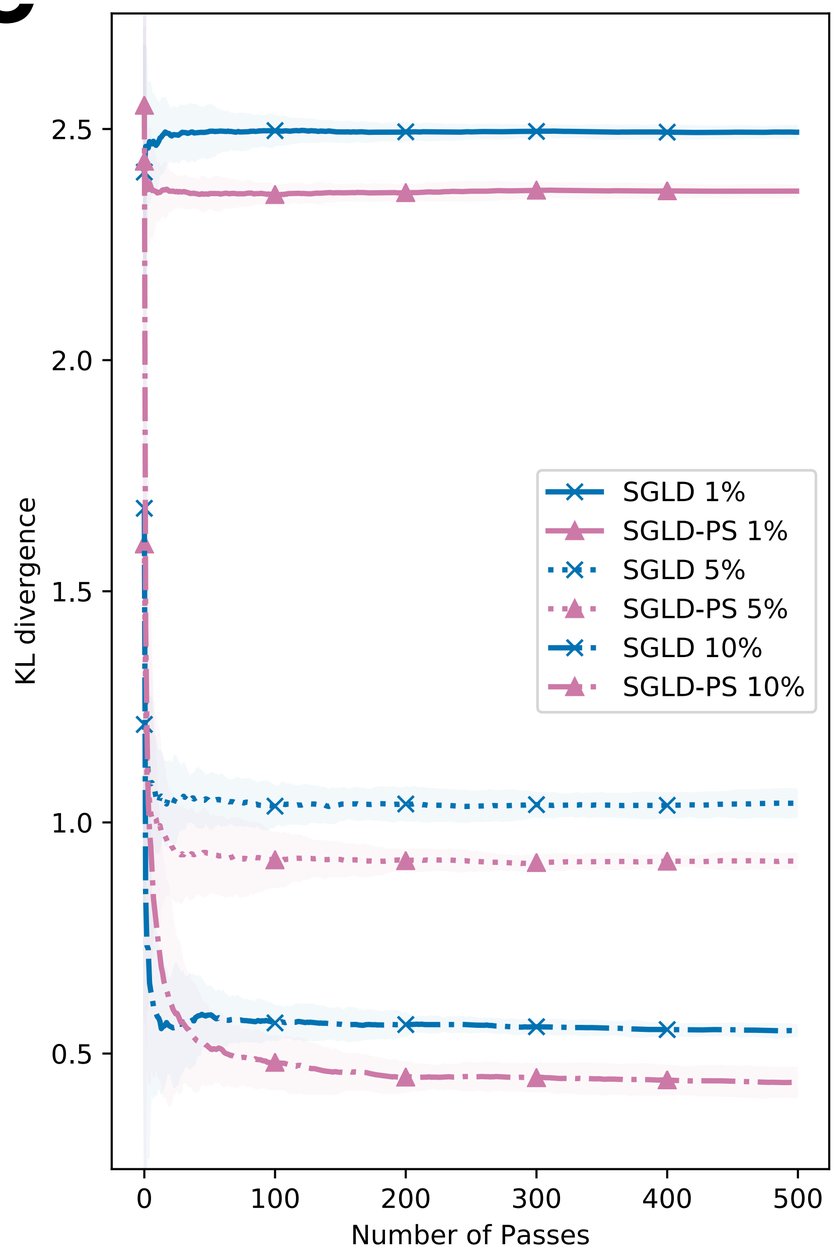

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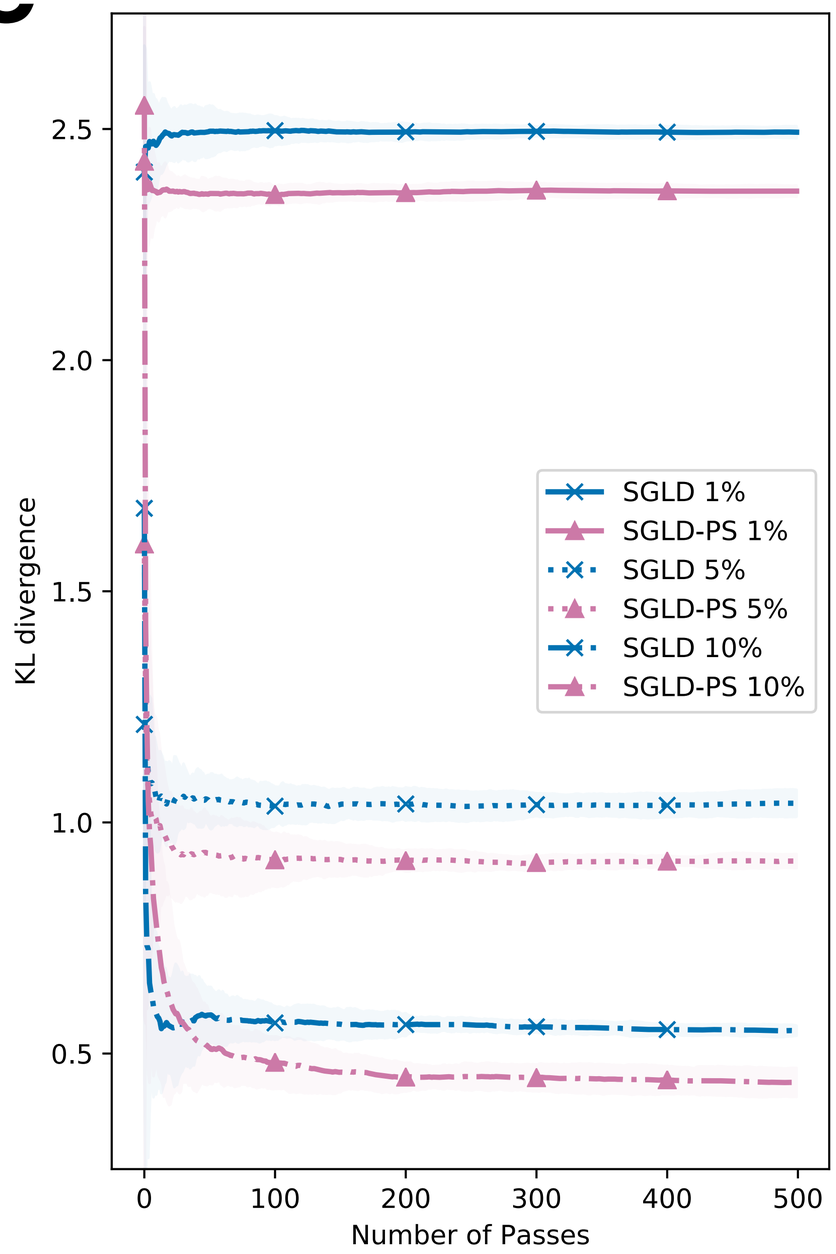

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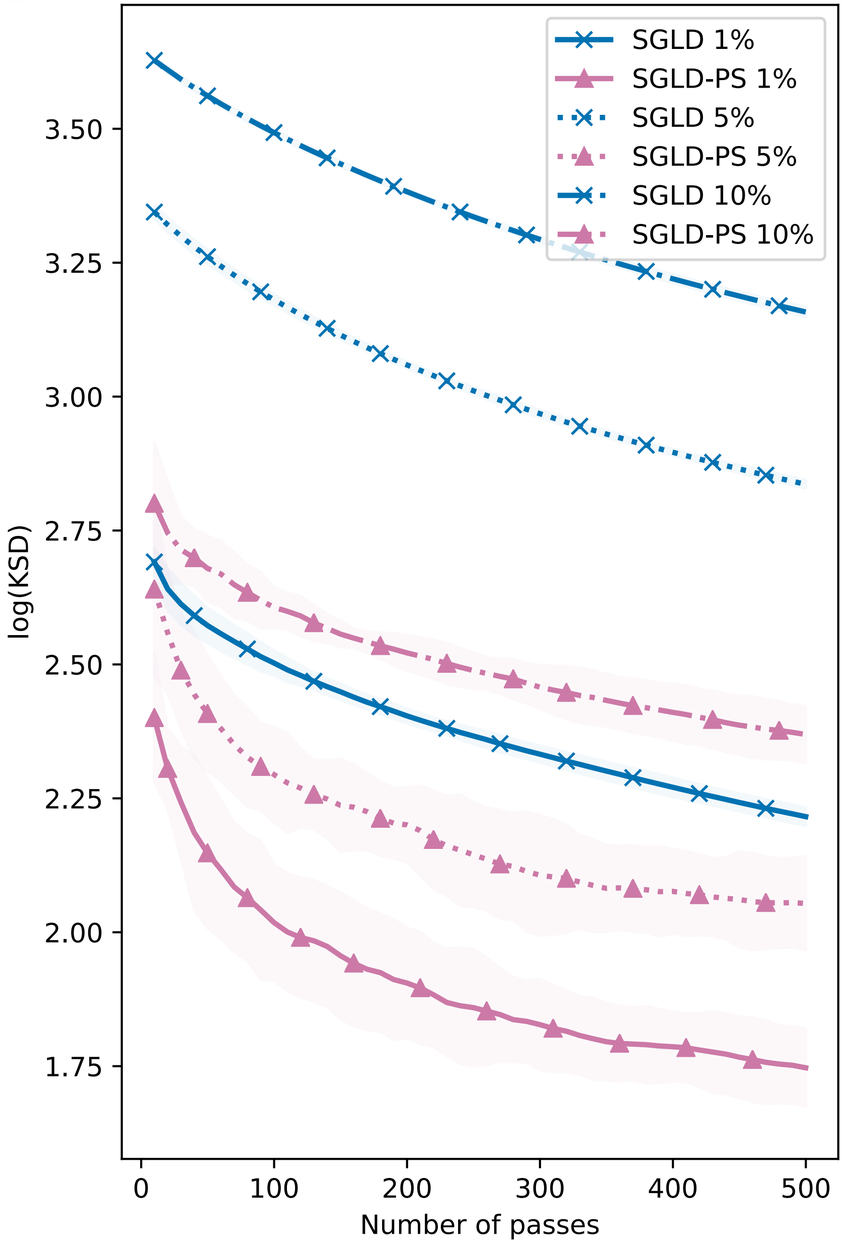
A logistic regression model with parameters $\theta = (\beta_0, \beta_1, \ldots, \beta_p)$ representing the coefficients β_j for $j = 1, \ldots, p$ and bias β_0 will have likelihood

$$p(X, y \mid \theta) = \prod_{i=1}^{N} \left[\frac{1}{1 + e^{-\theta^T x_i}} \right]^{y_i} \left[1 - \frac{1}{1 + e^{-\theta^T x_i}} \right]^{1-y_i}$$

The prior for θ is set to be $\theta \sim \text{MVN}(\mu_0, \Lambda_0)$. The hyper-parameters of the prior are $\mu_0 = (0, \ldots, 0)^T$ and $\Lambda_0 = \text{diag}(10, d)$.

We use the *covertype* dataset, where $N = 581{,}012$ and $p = 55$.



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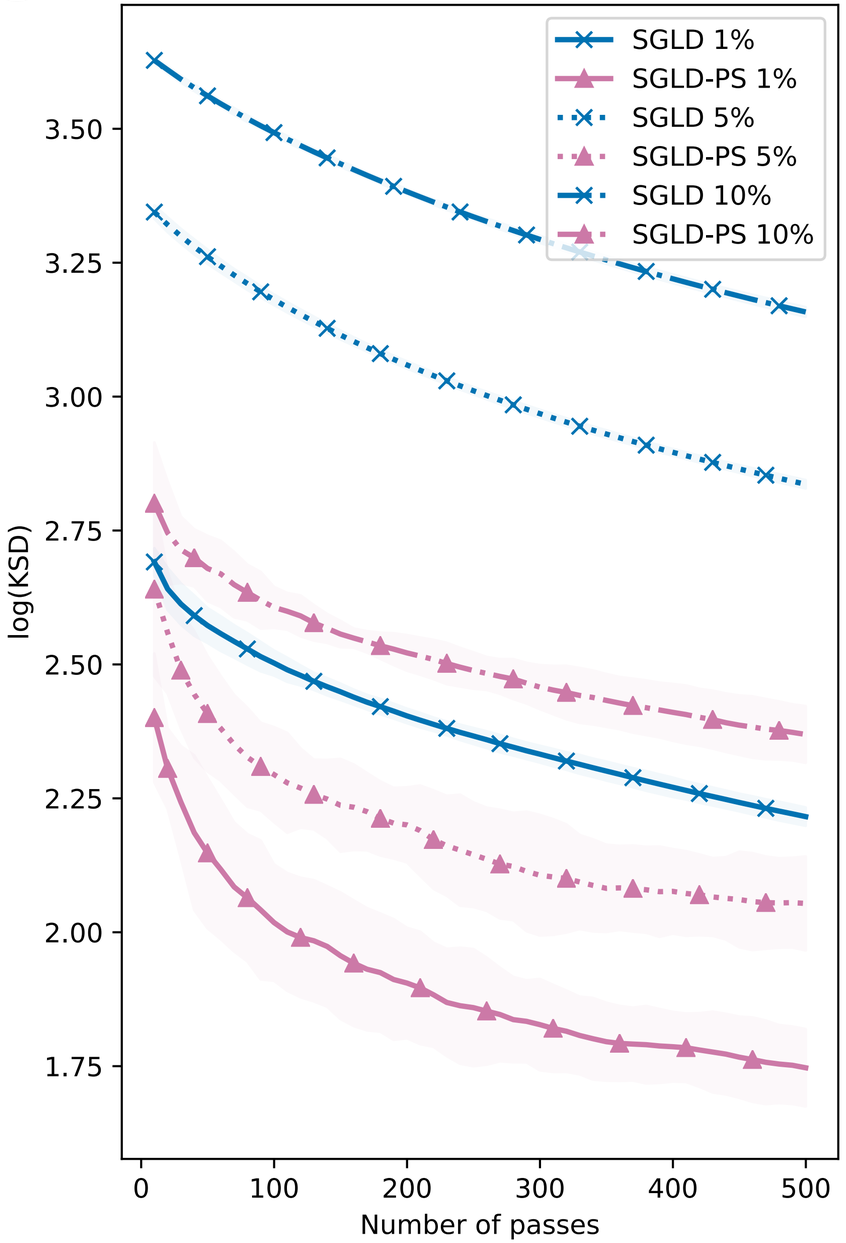

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There exists constants $L_0, \ldots, L_N$ such that

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Under the Lipschitz assumption, the variance of the stochastic gradient estimator can be bounded above by

$$\text{Var}[\nabla \hat{f}_{ps}(\theta^{(t)})] \leq \frac{1}{n} \|\theta^{(t)} - \hat{\theta}\|^2 \left(\sum_{i=1}^{N} \frac{L_i^2}{p_i^t} \right)$$

where $(p_1^t, \ldots, p_N^t)^T$ is a set of user-defined discrete weights (chosen such that $\sum_{i=1}^{N} p_i^T = 1$).

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We can set the upper threshold of the variance to be some fixed value $V_0 > 0$,

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Rearranging this inequality we obtain the following lower bound on the subsample size,

$$n > \frac{1}{V_0}\|\theta^{(t)} - \hat{\theta}\|^2 \left(\sum_{i=1}^{N} \frac{L_i^2}{p_i^t} \right).$$

Adaptive subsample size

$$\text{Var}[\nabla \hat{f}_{ps}(\theta^{(t)})] \leq \frac{1}{n}\|\theta^{(t)} - \hat{\theta}\|^2 \left(\sum_{i=1}^{N} \frac{L_i^2}{p_i^t} \right).$$

We can set the upper threshold of the variance to be some fixed value $V_0 > 0$,

$$\frac{1}{n}\|\theta^{(t)} - \hat{\theta}\|^2 \left(\sum_{i=1}^{N} \frac{L_i^2}{p_i^t} \right) < V_0 .$$

Rearranging this inequality we obtain the following lower bound on the subsample size,

$$n > \frac{1}{V_0}\|\theta^{(t)} - \hat{\theta}\|^2 \left(\sum_{i=1}^{N} \frac{L_i^2}{p_i^t} \right).$$

This result tells us that for fixed $L_i, \hat{p}_i^t$ and V_0, we should choose a subsample size of $n \propto \|\theta^{(t)} - \hat{\theta}\|^2$.

Wrap-Up

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- Paper and code will be on *arXiv* soon.

New Stochastic Gradient MCMC Package

SGMCMCJax

latest

Search docs

HOW TO USE SGMCMCJAX

Overview

Build a sampler function

Build a transition kernel

Build a diffusion solver

EXAMPLES

Gaussian posterior

Logistic Regression

Bayesian Neural Network

Flax CNN

Sample from a PyMC model using SGMCMCJax

» Welcome to SGMCMCJax's documentation!

Edit on GitHub

Welcome to SGMCMCJax's documentation!

SGMCMCJax is a lightweight library of stochastic gradient Markov chain Monte Carlo (SGMCMC) algorithms. The aim is to include both standard samplers (SGLD, SGHMC) as well as state of the art samplers (SVRG-langevin, others, ...).

The target audience for this library is researchers and practitioners: simply plug in your JAX model and easily obtain samples.

You can find the source code on Github.

"Hello World" example

Estimate the mean of a Gaussian using SGLD: