Deterministic Langevin Monte Carlo with Normalizing Flows for Bayesian Inference

Anonymous Author(s)
Affiliation
Address
email

Abstract

We propose a general purpose Bayesian inference algorithm for expensive likelihoods, replacing the stochastic term in the Langevin equation with a deterministic density gradient term. The particle density is evaluated from the current particle positions using a Normalizing Flow (NF), which is differentiable and has good generalization properties in high dimensions. We take advantage of NF preconditioning and NF based Metropolis-Hastings updates for a faster and unbiased convergence. We show on various examples that the method is competitive against state of the art sampling methods.

1 Introduction

The task of Bayesian inference is to determine the posterior $p(\boldsymbol{x}|\boldsymbol{y})$ of d parameters $\boldsymbol{x}$ given the likelihood $p(\boldsymbol{y}|\boldsymbol{x})$ of some data $\boldsymbol{y}$ and given the prior $p(\boldsymbol{x})$, such that the posterior is given by Bayes theorem as $p(\boldsymbol{x}|\boldsymbol{y}) = p(\boldsymbol{y}|\boldsymbol{x})p(\boldsymbol{x})/p(\boldsymbol{y})$. While we have access to the joint $p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{y}|\boldsymbol{x})p(\boldsymbol{x})$, the normalization $p(\boldsymbol{y})$ is generally unknown. Bayesian posterior inference can be related to the general task of finding a stationary distribution in an external potential by defining $U(\boldsymbol{x}) = -\ln p(\boldsymbol{y}|\boldsymbol{x}) - \ln p(\boldsymbol{x}) = \mathcal{L}(\boldsymbol{x}) + \mathcal{P}(\boldsymbol{x})$, where $\mathcal{L}(\boldsymbol{x})$ is the negative log likelihood and $\mathcal{P}(\boldsymbol{x})$ the negative log prior. A common statistical physics approach to this task is to use either the deterministic Fokker-Planck equation, which solves the partial differential equation (PDE) governing the density evolution of a system of particles, or a particle based Langevin equation, which solves a stochastic differential equation (SDE) of particle evolution (Langevin Monte Carlo, LMC). In both cases the long time equilibrium solution is that of the target stationary distribution, the posterior $p(\boldsymbol{x}|\boldsymbol{y})$. A related gradient based method is Hamiltonian Monte Carlo (HMC) (1), which uses particle positions and velocities to evolve the particles. LMC and HMC are two of the most popular gradient based implementations of Markov Chain Monte Carlo (MCMC), but for finite step size require Metropolis-Hastings (MH) adjustment to become unbiased. In this case they have theoretical convergence guarantees to the stationary distribution (under mild ergodicity assumptions), but suffer from chain element correlations, which may render the convergence to be very slow.

In this paper we propose a Deterministic Langevin Monte Carlo (DLMC) with Normalizing Flows (NF). It uses a random initialization from the prior, but the subsequent evolution is deterministic, replacing the stochastic velocity term in the Langevin equation with a deterministic density gradient term. To avoid the need to solve the Fokker-Planck equation directly we evaluate the density defined by the current particle positions via an NF, and then use its gradient to update the first order particle Langevin dynamics. NFs are differentiable and have good generalization properties in high dimensions. A prominent deterministic method is Stein Variational Gradient Descent (SVGD) (2). After the initial submission we also became aware of interacting particle solutions of (3), which proposes particle based scores for the gradient of the log-density. However, these particle based methods scale poorly to high dimensions. The main novelty of our contribution is the introduction

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of NFs to the class of deterministic methods for evaluating stationary distributions: we use NF for density estimation and its gradient evaluation, as well as for MH adjustment that makes our method asymptotically unbiased.

Our primary target application is to expensive likelihoods (wall clock time of seconds or more). An example are inverse problems in scientific applications, where often one must solve an expensive Ordinary or Partial Differential Equation (ODE or PDE) forward model, where the computational cost can be as long as days or months. In such applications the computational cost of NF (which is of order seconds in our experiments) is not dominant. For fast model evaluations standard MCMC methods suffice and our target are problems where the cost of standard methods is prohibitive. The computational cost of a forward model is unrelated to the complexity of posterior distribution: often the posteriors are simple Gaussian distributions even when the computational cost is high. In such settings the main goal of posterior analysis is to minimize the number of likelihood calls to reach some prescribed precision on the posterior.

DLMC has the following advantages in comparison to several other MCMC samplers:

- DLMC takes advantage of the gradient information of the target distribution, but without the stochastic noise, which slows down the particle evolution towards the target in LMC and HMC. As a result, DLMC gradient based optimization can rapidly move the particles into the region of high posterior mass for a fast convergence.
- DLMC is not a sequential Markov Chain, and DLMC particles can be updated in parallel at each time step, which can take advantage of trivial machine parallelization of likelihood evaluations, reducing the wall-clock time compared to standard MCMC.
- DLMC particles are initialized as a random draw from the prior, which covers the posterior. Each particle produces an independent sample in the large number of particles N limit.
- DLMC uses NF for density estimation, and takes advantage of NF preconditioning and NF based MH updates, for a faster and asymptotically unbiased convergence.
- DLMC can handle multimodal posteriors, in contrast to standard MCMC samplers.

2 Langevin and Fokker-Planck equations

The overdamped Langevin equation is a stochastic differential equation describing particle motion in an external potential and subject to random force with zero mean,

$$\dot{\boldsymbol{x}} = \boldsymbol{v} = -\boldsymbol{\nabla} U(\boldsymbol{x}) + \boldsymbol{\eta}, \tag{1}$$

where $\langle \boldsymbol{\eta(t)} \rangle = 0$ and $\langle \eta_i(t)\eta_j(t') \rangle = 2\delta_{ij}\delta(t-t')$. For simplicity we set the diffusion coefficient, temperature and mobility to unity. The Langevin equation is a first order velocity equation which has a deterministic velocity $-\boldsymbol{\nabla} U(\boldsymbol{x})$ and a stochastic velocity $\boldsymbol{\eta}$. Here the gradient operator is with respect to the parameters of $U(\boldsymbol{x})$, $\boldsymbol{\nabla} U(\boldsymbol{x}) = dU(\boldsymbol{x})/d\boldsymbol{x}$.

In practice we need to discretize the Langevin equation, and for any finite step size Δt the result is a biased distribution. An example is Ornstein-Uhlenbeck process, where $U(\boldsymbol{x})$ is a harmonic potential, $\exp(-U(\boldsymbol{x})) = N(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$. Standard Langevin algorithm updates lead to the solution $q(\boldsymbol{x}) = N(\boldsymbol{\mu}, \boldsymbol{\Sigma}(I - \Delta t \boldsymbol{\Sigma}^{-1}/2)^{-1})$ (4). We can see that for a finite fixed stepsize Δt the solution converges to a biased answer regardless of the number of time integration steps taken, or the number of samples used. A solution to this is to supplement the Langevin updates with Metropolis-Hastings (MH) Adjustment Langevin Algorithm (MALA), where MH acceptance guarantees detailed balance (5). A similar MH adjustment is also required for HMC (1).

The Langevin equation can be viewed as a particle implementation of the evolution of particle probability density $q(\boldsymbol{x}(t))$, which is governed by the deterministic Fokker-Planck equation, a continuity equation for the density,

$$\dot{q}(\boldsymbol{x}(t)) + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0, \quad \boldsymbol{J} = -q(\boldsymbol{x}(t))[\nabla U(\boldsymbol{x}) - \nabla V(\boldsymbol{x}(t))] \equiv q(\boldsymbol{x}(t))\boldsymbol{v}. \tag{2}$$

We defined $V(\boldsymbol{x}(t)) = -\ln q(\boldsymbol{x}(t))$ and expressed current as density times velocity, where the two terms in the probability current $\boldsymbol{J}$ correspond to the two velocity terms in the Langevin equation. One can see from equation 2 that the stationary distribution $\dot{q}(\boldsymbol{x}, t) = 0$ is given by $p(\boldsymbol{x}|\boldsymbol{y}) = \exp(-U(\boldsymbol{x}))/p(\boldsymbol{y})$. The Fokker-Planck equation is a PDE, while the Langevin equation is stochastic

(SDE). Langevin diffusion provides a particle description of the density $q(\boldsymbol{x}, t)$ and in the large time limit both equations lead to a stationary distribution equal to the posterior $p(\boldsymbol{x}|\boldsymbol{y})$.

If we replace the stochastic velocity in the Langevin equation 1 with the deterministic velocity in equation 2, we obtain the deterministic Langevin equation (3; 6),

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{v} = -\boldsymbol{\nabla}[U(\boldsymbol{x}) - V(\boldsymbol{x}(t))]. \tag{3}$$

Equation 3 gives the dynamics of a particle representation of density $q(\boldsymbol{x}(t))$, which in the large time limit $t \to \infty$ converges to the same distribution as the solution of the stochastic Langevin equation 1. This follows from the fact that the stationary solution of equation 3, $\dot{\boldsymbol{x}}(t) = 0$ is given by $V(\boldsymbol{x}(t)) = U(\boldsymbol{x}) + \mathrm{c}$, with c being a constant independent of $\boldsymbol{x}$, which must thus be equal to $\log p(\boldsymbol{y})$, since $q(\boldsymbol{x}(t))$ is normalized. There is no stochastic noise in Equation 3, so it can be interpreted as a deterministic analog of the Langevin equation, which is a first order equation for velocity.

The main difficulty in solving equation 3 is the instantaneous density term $q(\boldsymbol{x}(t))$ needed to obtain $V(\boldsymbol{x})$. Here we solve this by evolving N particles together, using NF to evaluate their particle density. While this makes the particles interacting, in the limit of large N the particle evolution is independent, and each particle becomes an independent sample. Furthermore, we can use NF to do MH adjustment and make the method unbiased (section 3.2). Upon time discretization of Equation 3 we obtain Algorithm 1. We initialize at $t = 0$ by providing initial samples drawn at random from the known prior distribution $p(\boldsymbol{x})$, similar to Sequential Monte Carlo (7). This has several positive features: since the posterior is proportional to prior times likelihood, the prior always covers the posterior. Moreover, when the likelihood is weakly informative the convergence of DLMC is fast. We then apply DLMC gradient update to obtain the particle positions update. When initializing from the prior the initial density distribution cancels out the prior in the target, and the initial gradient update is the log likelihood term $\boldsymbol{\nabla}\mathcal{L}(\boldsymbol{x})$.

Equation 3 can be interpreted as a gradient based minimization of time dependent objective $U(\boldsymbol{x}) - V(\boldsymbol{x}(t))$. In this view we can optimize the objective using any optimization method. Initially, if we start the particles from the prior $p(\boldsymbol{x})$, DLMC is simply performing optimization of the target likelihood $p(\boldsymbol{y}|\boldsymbol{x})$. Later, as $q(\boldsymbol{x}(t)) \sim p(\boldsymbol{x}|\boldsymbol{y})$, the gradient of the optimization objective becomes zero, and the particles stop moving. One can use any optimization method to move the particles, so if gradient of $U(\boldsymbol{x})$ is not available we can use gradient free optimization methods to do so. For gradient based optimization we can use many of the standard optimization methods (8), such as first order (stochastic or deterministic) gradient descent, momentum based methods, or (quasi) second order methods (e.g. L-BFGS, Newton, conjugate gradient etc.). The algorithm can be stopped when the particle distribution becomes stationary. For example, we can stop when the first and second moment of posterior distribution for the relevant parameters stop changing.

3 Normalizing Flows density estimation

Normalizing Flows provide a powerful framework for density estimation and sampling (9; 10; 11; 12). These models map the d-dimensional data $\boldsymbol{x}$ to d-dimensional latent variables $\boldsymbol{z}$ through a sequence of invertible transformations $f = f_1 \circ f_2 \circ ... \circ f_L$, such that $\boldsymbol{z} = f(\boldsymbol{x})$ and $\boldsymbol{z}$ is mapped to a base distribution $\pi(\boldsymbol{z})$, which is chosen to be a standard Normal distribution $N(0, \boldsymbol{I})$. The probability density of data $\boldsymbol{x}$ can be evaluated using the change of variables formula:

$$q(\boldsymbol{x}) \equiv e^{-V(\boldsymbol{x})} = \pi(f(\boldsymbol{x}))\left|\det\left(\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}}\right)\right| = \pi(f(\boldsymbol{x}))\prod_{l=1}^{L}\left|\det\left(\frac{\partial f_l(\boldsymbol{x})}{\partial \boldsymbol{x}}\right)\right|. \tag{4}$$

The Jacobian determinant of each transform $J_l = |\det(\frac{\partial f_l(\boldsymbol{x})}{\partial \boldsymbol{x}})|$ must be easy to compute for evaluating the density, and the transformation f_l should be easy to invert for efficient sampling. In this paper we use Sliced Iterative Normalizing Flow (SINF) (12), which has been shown to achieve better performance for small training data (below a few thousand particles), and is considerably faster, than alternatives.

3.1 Normalizing Flow as a preconditioner

While the core of DLMC is NF based density gradient, the same NF can be used for additional convergence acceleration towards the target. The proposed algorithm is gradient based, and can be

Algorithm 1 Deterministic Langevin Monte Carlo with Normalizing Flows

Input: initial samples $\boldsymbol{x}^i(t=0)$ drawn at random from prior $p(\boldsymbol{x})$, size N, access to $\mathcal{L}(\boldsymbol{x}) + \mathcal{P}(\boldsymbol{x}) = U(\boldsymbol{x})$ and its gradient.
Initial update:
for $i = 1, N$ **do**
  $\boldsymbol{x}^i(\Delta t) = \boldsymbol{x}^i(t=0) - \boldsymbol{\nabla}\mathcal{L}(\boldsymbol{x}^i(t))\Delta t$
end for
while not converged **do**
  $t \to t + \Delta t$
  run Normalizing Flow on current particle positions to obtain $q(\boldsymbol{x}(t)) = \exp(-V(\boldsymbol{x}(t)))$
  for $i = 1, N$ **do**
    DL update: $\boldsymbol{x}^i(t+\Delta t) = \boldsymbol{x}^i(t) - \boldsymbol{\nabla}[U(\boldsymbol{x}^i(t)) - V(\boldsymbol{x}^i(t))]\Delta t$
    MH update: draw a sample $\tilde{\boldsymbol{x}}^i \sim q(\boldsymbol{x}(t))$, replace $\boldsymbol{x}^i$ with $\tilde{\boldsymbol{x}}^i$ with probability $r(\boldsymbol{x}^i, \tilde{\boldsymbol{x}}^i)$
  end for
end while
Output: a set of particles $\boldsymbol{x}^i(t)$ distributed as a target distribution $p(\boldsymbol{x}|\boldsymbol{y})$.

slow when the condition number of the problem is high. A typical solution is to precondition with a covariance matrix, which mimics the global curvature of the problem. This becomes more difficult if the curvature is position dependent. NF can address this problem by warping the space in which we perform the optimization: this warping or transport map maps spatially varying curvature to the latent space where the curvature is constant and isotropic (13; 14). We can implement DLMC in the NF latent space $\boldsymbol{z}$, where the target density distribution $p(\boldsymbol{x}|\boldsymbol{y})$ is transformed into

$$p(\boldsymbol{z}|\boldsymbol{y}) = p(\boldsymbol{f}^{-1}(\boldsymbol{z})|\boldsymbol{y})J(\boldsymbol{z}), \tag{5}$$

where $J(\boldsymbol{z}) = \left|\det\left(\frac{\partial \boldsymbol{f}^{-1}(\boldsymbol{z})}{\partial \boldsymbol{z}}\right)\right|$ is the absolute value of the Jacobian determinant. We can define the potential in latent space as

$$U(\boldsymbol{z}) = U(\boldsymbol{f}^{-1}(\boldsymbol{z})) - \ln J(\boldsymbol{z}). \tag{6}$$

If we can evaluate $\boldsymbol{\nabla}\boldsymbol{U}(\boldsymbol{x})$ using methods such as auto-differentiation and if the NF Jacobian is also differentiable we can also evaluate the gradient in latent space $\boldsymbol{z}$ as

$$\boldsymbol{\nabla}U(\boldsymbol{z}) = \boldsymbol{\nabla}U(\boldsymbol{x})\frac{d\boldsymbol{x}}{d\boldsymbol{z}} - \boldsymbol{\nabla}\ln J(\boldsymbol{z}) \tag{7}$$

In latent space the latent variables are distributed as $\pi(\boldsymbol{z}) = \exp(-V(\boldsymbol{z})) = N(0, \boldsymbol{I})$, so $V(\boldsymbol{z}) = \boldsymbol{z}^T\boldsymbol{z}/2 + (d/2)\ln(2\pi)$ and $\boldsymbol{\nabla}V(\boldsymbol{z}) = \boldsymbol{z}$. This gives the deterministic Langevin gradient descent updates as

$$\boldsymbol{z}(t+\Delta t) = \boldsymbol{z}(t) - \boldsymbol{\nabla}U(\boldsymbol{z}(t))\Delta t + \boldsymbol{z}(t)\Delta t. \tag{8}$$

It is interesting to compare this deterministic update to the standard stochastic Langevin equation update, which in latent space is

$$\boldsymbol{z}(t+\Delta t) = \boldsymbol{z}(t) - \boldsymbol{\nabla}U(\boldsymbol{z}(t))\Delta t + \boldsymbol{\eta}', \tag{9}$$

where $\boldsymbol{\eta}' \sim N(0, 2\boldsymbol{I}\Delta t)$. Both updates have the potential gradient term, which is the deterministic drift velocity. The difference between the two is that DLMC also uses the current position of the sample $\boldsymbol{z}$ for a deterministic update of density gradient $\boldsymbol{z}(t)\Delta t$, which moves the particles radially outwards from the center of the latent space, while the stochastic Langevin algorithm adds a Gaussian random variable $\boldsymbol{\eta}'$ to the update. We will show in examples that NF latent space accelerates the convergence of DLMC.

3.2 Normalizing Flow for Metrolopolis-Hastings adjustment

The main requirement of DLMC is that $q(\boldsymbol{x}(t))$ properly describes the density of samples $\boldsymbol{x}(t)$ at time t. This can only be ensured in the large N limit. Moreover, for non-convex optimization problems it

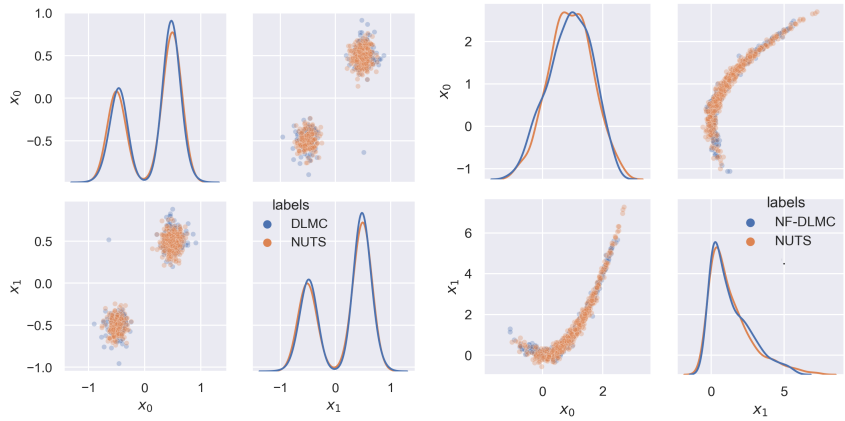
is possible that the samples get stuck at local minima far from the global minimum. One can add a Metropolis-Hastings (MH) adjustment to make DLMC unbiased, and to eliminate the samples that get stuck far from the global minimum. This step is particularly necessary for disconnected multi-modal peaks of $p(\boldsymbol{x})$ to be properly equilibrated. It plays the same role as the MH adjustment in LMC (i.e. MALA) and in HMC, making DLMC aymptotically unbiased (note however that LMC/HMC cannot properly equilibrate between separate posterior peaks without the use of specialized methods like annealing/tempering).

Specifically, at a given t we can draw independent particles $\tilde{\boldsymbol{x}}^i \sim q(\boldsymbol{x}(t))$, one for each existing particle $\boldsymbol{x}^i$. We compare the new particle against an existing particle to decide whether we accept or reject it. Since these new samples are independent, the transition kernel is particularly simple, and to achieve detailed balance the MH acceptance rate is (e.g. (15))

$$r(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \min\left\{1, \frac{p(\tilde{\boldsymbol{x}}, \boldsymbol{y})q(\boldsymbol{x})}{p(\boldsymbol{x}, \boldsymbol{y})q(\tilde{\boldsymbol{x}})}\right\}. \tag{10}$$

Note that the normalization constant cancels out in this ratio, so we can evaluate this with knowledge of $U(\boldsymbol{x})$ only. The corresponding expression in NF latent space is $r(\boldsymbol{z}, \tilde{\boldsymbol{z}}) = \min\left\{1, \frac{p(\tilde{\boldsymbol{z}}, \boldsymbol{y})\pi(\boldsymbol{z})}{p(\boldsymbol{z}, \boldsymbol{y})\pi(\tilde{\boldsymbol{z}})}\right\}$.

Initially, when $q(\boldsymbol{x}(t))$ is very broad compared to $p(\boldsymbol{x}|\boldsymbol{y})$, the acceptance rate of MH will be low, since most of the samples drawn will have low $p(\boldsymbol{x}|\boldsymbol{y})$, so this process may only eliminate the worst performers, and replace them with samples in the higher density region of $p(\boldsymbol{x}|\boldsymbol{y})$. As DLMC progresses $q(\boldsymbol{x}(t))$ becomes closer to $p(\boldsymbol{x}|\boldsymbol{y})$, and the acceptance increases and reaches $r(\boldsymbol{z}, \tilde{\boldsymbol{z}}) = 1$ if NF learns the target perfectly. In high dimensions MH acceptance can remain low, however MH update is still necessary, as it ensures proper equilibration of multi-modal peaks.



(a) Double Gaussian

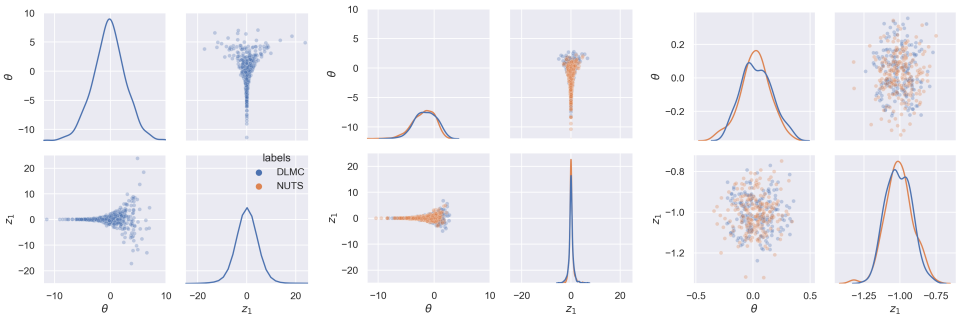
(b) Rosenbrock

Figure 1: Left: results on $d = 100$ Gaussian mixture after 90 DLMC iterations (blue), compared to the true distribution (orange). We show 1d density projections and 2d particle distributions along the first two parameters. Right: same for Rosenbrock function in $d = 32$ after 50 DLMC iterations. The Gaussian mixture uses 500 particles, whilst the Rosenbrock uses 1000.

4 Related work

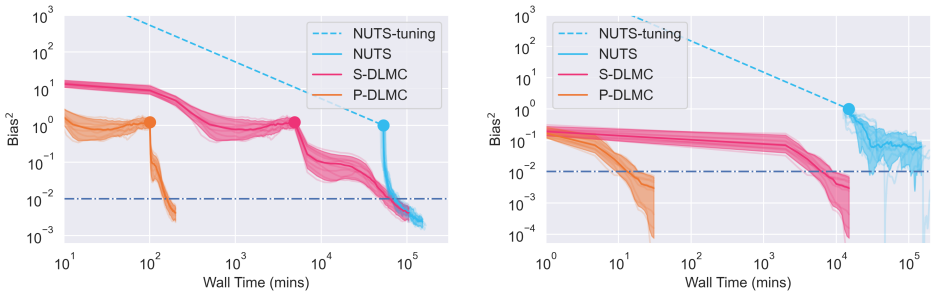
NFs and transport maps for Bayesian posterior analysis have been explored in (13; 14; 16). These approaches use NF as a latent space preconditioner, using standard MCMC methods such as HMC, LMC or MH deployed in latent space, where geometry may be more favorable for a fast mixing of the chains. In (15) NF is used as a MH transition proposal, giving independent samples. DLMC goes beyond these NF applications in that it also uses NF for the density gradient in the deterministic Langevin equation.

DLMC is an ensemble method, in that all of the particles inform the NF density evaluation, which is in turn used to update each particle position. There have been many other ensemble methods proposed in the literature, such as the Affine Invariant Ensemble Sampler (17) or the Differential

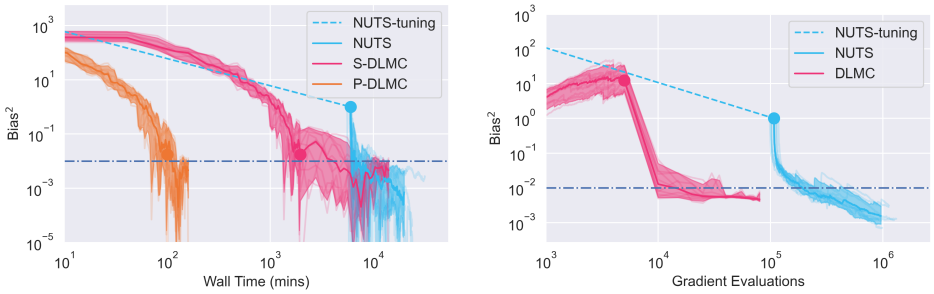


(a) Neal's funnel ($\sigma = \infty$) (b) $\sigma = 5$ (c) $\sigma = 0.1$

Figure 2: DLMC results on $d = 100$ hierarchical variance problem (funnel problem), compared to a very long NUTS run. We show posteriors of θ and z_1. Left panel shows Neal's funnel: it corresponds to noise $\sigma \to \infty$, so no updates are needed since likelihood update is zero. Middle panel shows $\sigma = 5$: despite the large noise, $d = 100$ latent variables are informative of σ and the posterior is narrower than the prior. Right panel shows $\sigma = 0.1$: here the posterior is narrowed further, and is close to a Gaussian.



(a) Rosenbrock (b) funnel $\sigma = 5$



(c) funnel $\sigma = 0.1$ (d) sparse logistic regression

Figure 3: Bias-squared on the second moment for the $d = 32$ Rosenbrock function (panel (a)), $d = 100$ dimensional hierarchical funnel vs wall clock time (panels (b) and (c)) and for $d = 51$ sparse logistic regression versus number of likelihood gradient evaluations (panel (d)). In panels (a)-(c) we show sequential (S-DLMC) and parallel (P-DLMC) versions. Solid circles denote the end of any burnin phases.

Evolution MCMC (18). DLMC differs from these methods in that it evaluates the particle density explicitly, and uses the density and target gradient to update the particle evolution.

Two deterministic algorithms related to DLMC that have recently been proposed are the Stein Variational Gradient Descent (SVGD) (2), which uses direct pair summation over all particles, and score based interacting particles (3), inspired by generative score based models (6), which use the particles to estimate directly the density gradient term. DLMC differs from these in using NF instead

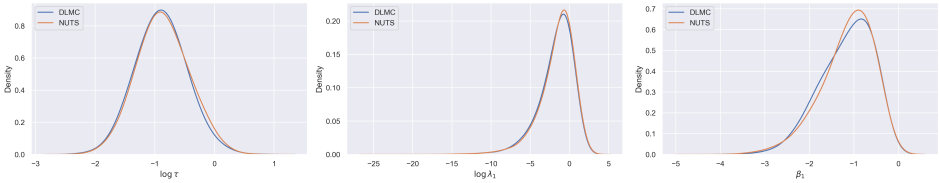


Figure 4: Results on $d = 51$ sparse logistic regression after 100 iterations (blue), compared to a very long run NUTS HMC distribution (orange). We show three representative variables, showing good agreement. The corresponding bias squared is 0.01 (figure 4).

of direct pair interactions, which as we show below leads to better performance in terms of number of particles needed to represent the density.

DLMC is related to Variational Inference (e.g. (19)) in that both approximate the posterior with a parametrized normalized function $q(\boldsymbol{x})$. However, DLMC does not use standard variational optimization such as KL minimization to optimize $q(\boldsymbol{x})$, and does not use $q(\boldsymbol{x})$ for the posterior, which is reported by the particles instead. In our experiments we observe that the posterior distribution of DLMC particles agrees better with the exact posteriors than the samples from the NF density. This is expected, since we use the MH step to correct NF. DLMC thus contains components of both sampling and optimization: sampling as optimization in the space of distributions has been pursued in many directions since (20)), and in recent years the line between optimization and sampling has been significantly blurred.

5 Examples

The main DLMC application is for expensive likelihoods such as ODE or PDE. We can simulate this by synthetically creating expensive model evaluations, but in most examples we will compare the performance in terms of the number of likelihood evaluations. The implementation of DLMC requires NF and particle evolution. For NF we use SINF, which has very few hyper-parameters (12), is fast, and is iterative, so the number of layers L can be chosen based on cross-validation, where we set aside 20% of the samples, and iterate until validation data start to diverge from the training data. Typical SINF training time is of order seconds on a CPU.

The implementation of particle evolution requires us to specify the learning rate for the particle updates. At each iteration, we take Adagrad updates in the $\nabla(U(\boldsymbol{x}) - V(\boldsymbol{x}(t)))$ direction. We use learning rates between 0.001 and 0.1, with smaller learning rates being more robust for targets with complicated geometries such as funnel distributions.

In our plots we focus on the quality of marginal posteriors, because that is typically the primary goal of Bayesian inference. To quantify the quality of the posteriors numerically we follow (14) and show the squared bias of the relative variance versus wall clock time or number of gradient evaluations. The precision of this number is limited by the effective number of samples (ESS). Here we choose bias squared of 0.01 as sufficient in terms of posteriors, and corresponds for a Gaussian distribution to ESS of 200. The number of particles N is a hyperparameter that must exceed this ESS. We choose to start with $N = 200$, and we verify the results by doubling it. In some examples this requires to increase the number of particles up to 5000. Overall we find there is a tradeoff between number of particles and number of iterations, such that starting with a larger number of particles does not always imply a higher overall computational cost.

The main baseline we compare against is NUTS HMC (21), implemented in the NumPyro library (22). It requires tuning and burn-in, which need to be included in the computational budget. NUTS HMC is a standard baseline since it typically outperforms other samplers such as LMC, SVGD and SMC. Where we include NUTS as a baseline, we use 500 tuning steps. NUTS has the number of leapfrog steps as a tunable parameter, and when it is one HMC becomes LMC/MALA (23).

In some of our experiments we compare default DLMC (denoted sequential, S-DLMC) to parallel DLMC (P-DLMC), where for the latter we show the wall clock time based on the assumption that we can evaluate the likelihood gradient in parallel on N CPU cores. We assume the likelihood gradient cost of 1 minute, and the cost of NF itself (seconds) is negligible.

5.1 Gaussian mixture

Multimodal distributions are a failure mode for many standard MCMC samplers, such as LMC, HMC and MHMC, as they cannot move from one peak to another when the potential barrier between them is too high. They need to be augmented with an annealing procedure, where one is slowly morphing the target distribution from the prior to the posterior. Annealed Importance Sampling (24) and Sequential MC (SMC) (7) are examples of annealing methods that can handle multi-modality. They require equilibrating the distribution at every temperature level using standard MCMC (e.g. MH or HMC), and as a result are significantly slower than standard MCMC. DLMC uses a different strategy from annealing, but can also handle multi-modal distributions, as long as NF can approximate it. As an example we take a Gaussian mixture with 1/3 of the posterior mass in the first peak and 2/3 in the second peak, in $d = 100$.

We choose $N = 500$, drawn from a broad initial prior $(-2, 2)^d$. The log of prior to posterior volume ratio is 415, which is a challenge for non-gradient based MCMCs, as they become very slow in such settings. We apply logit transforms to all the variables such that we sample in an unconstrained space. DLMC is gradient based and makes rapid progress towards the region of posterior mass. The resulting DLMC posterior after 90 iterations for the first two variables is shown in figure 1, and is in a near perfect agreement with the true distribution.

5.2 Rosenbrock function

The 32-d example comes from a popular variant of multidimensional Rosenbrock function (25), which is composed of 16 uncorrelated 2-d bananas. The model likelihood is $\ln \mathcal{L} = -\sum_{i=1}^{n/2} \left[(g(x_{2i-1})^2 - x_{2i})^2/Q + (x_{2i-1} - 1)^2 \right], Q = 0.1$, with Gaussian prior $N(0, 6)$ on all the parameters. We assume $g(x) = x$ and use an initial burnin phase with $N = 10$ for 50 iterations, before upsampling to $N = 1000$. The posterior for first two variables is shown in figure 1. We see that DLMC perfectly matches NUTS. The quality of the posterior versus wall clock time is shown in figure 3, where we are idealizing a data assimilation process by assigning a high computational cost of 1 minute to the evaluation of $g(x)$. This allows us to compare sequential and parallel DLMC. S-DLMC achieves results that are competitive with NUTS HMC. P-DLMC can improve the wall clock time by $N = 1000$.

5.3 Hierarchical Bayesian analysis

Hierarchical Bayesian analyses are very common in many applications. They often lead to funnel type posteriors, which are challenging for standard samplers. Moreover, forward models relating the variance of latent space to some parameters of interest can be expensive. As an example, in cosmology data analysis applications we measure Fourier modes and want to determine their power spectrum, which in turn informs of cosmological parameters. The evaluation of the power spectrum as a function of cosmological parameters requires an expensive PDE evolution of structure in the universe as a function of time (26). Here we choose a simplified version where the power variance $P = g(\theta)$ is determined by cosmological parameter θ and controls the variance of parameters z_i. Parameters z_i are not directly observable, and instead we observe their noisy version with a likelihood of the data $\boldsymbol{y}$, so a combined prior and likelihood are

$$p(\theta) = N(0, 3), P = g(\theta), \quad p(z_i|\theta) = N(0, P), \quad p(y_i|z_i, \theta) = N(z_i, \sigma^2), i = 1..d-1, \quad (11)$$

where σ^2 is the measurement noise and $g(\theta)$ is an expensive function that evaluates the power spectrum P as a function of θ. To connect to Neal's funnel we assume the result of the PDE is that the power spectrum depends exponentially on θ, with an approximate relation $P = g(\theta) = \exp(\theta/2)$, with a 1 minute computational cost of performing $g(\theta)$. The goal is the posterior of parameter θ marginalized over z_i. We use $N = 500$.

In the limit $\sigma^2 \to \infty$ the setup corresponds to Neal's funnel problem, which is deemed problematic for many samplers such as HMC (27), which require millions of likelihood calls. Note however that DLMC solution in the $\sigma^2 \to \infty$ is trivial: the data likelihood is non-informative, and after drawing samples from the prior of equation 11 the likelihood updates of equation 11 are zero, so DLMC stopping criterion (stationary posterior) is satisfied immediately. This shows that drawing the initial samples from the prior has a significant advantage over other initializations of DLMC.

To make the problem closer to actual applications in cosmology we analyze it with a finite noise σ^2, such that the data are informative of the parameter θ. We create a simulated data set with the true value $\theta_{\text{true}} = 0$ and use $d = 100$. The resulting posterior for $\sigma = 5$ and $\sigma = 0.1$ is compared to NUTS HMC in figure 2. We also show the prior (i.e. Neal's funnel) to highlight that the posterior is narrow compared to the prior. For $\sigma = 5$ we used 15,000 likelihood calls, which is orders of magnitude fewer likelihood evaluations than HMC NUTS baseline, which struggles to converge at all (figure 3) without the help of a reparametrization or a preconditioner (14).

To highlight the advantage of DLMC with parallelization we further show the performance of (embarrassingly) parellel DLMC, where we evaluate the likelihood update for all 500 particles in parallel, so each iteration is 1 minute. This converges to the required precision $b^2 = 10^{-2}$ in 30 minutes. Sequential MCMC methods such as NUTS cannot be efficiently parallelized, and cannot take advantage of parallelization because they require hyperparameter tuning and burn-in phase (each of order 10^4 likelihood calls). This leads to 3-4 orders of magnitude larger wall clock time. SMC can take advantage of parallelization, but needs a lot of temperature levels and a lot of steps to equilibriate at each temperature level (7; 28), such that the overall wall clock time is still orders of magnitude larger than parallel DLMC.

5.4 Sparse logistic regression

Hierarchical logistic regression with a sparse prior applied to the German credit dataset is a popular benchmark for sampling methods (29). We use the example from (14) with $d = 51$, applying a log-transform to bounded variables such that we sample in an unconstrained space. This is a challenging example for HMC, with samples requiring on average 125 leapfrog steps.

We run an extended burnin phase with 10 particles to shrink from the prior to posterior volume, using 500 iterations. We then upsample to 5000 samples, with DLMC converging to the correct solution within 10 iterations. Upsampling to lower sample sizes, such as 1000 particles, would also converge to the correct solution, but requires more DLMC iterations such that the computational cost is not reduced. The resulting posteriors are shown in figure 4 for three representative variables showing good agreement.

5.5 Ablation studies and comparison to particle deterministic methods

In the supplementary material we present results of ablation studies. We show DLMC without MH, DLMC without NF preconditioning, DLMC with particle based density instead of NF, and pure NF MH without DLMC. In all cases the results are inferior to DLMC with preconditioning and with MH adjustment. We also show NF with MH without DL is inferior to DLMC. We compare to kernel density estimation based DLMC and SVGD, both of which give inferior results, confirming that NF is the key ingredient for success of deterministic methods.

6 Conclusions

We present a new general purpose Bayesian inference algorithm we call Deterministic Langevin Monte Carlo with Normalizing Flows. The method uses deterministic Langevin equation, which requires density gradient, which we propose to be evaluated using a Normalizing Flow determined by the positions of all the particles at a given time. Particle positions are then updated in the direction of log target density minus log current density gradient. To make it asymptotically unbiased we add MH step, which is also based on NF. The process is repeated until the particle distribution becomes stationary, which happens when the particle density equals the target density.

In our experiments we find that DLMC significantly outperforms baselines such as LMC, HMC and SVGD, and even more in terms of wall-clock time when likelihoods can be evaluated in parallel on a multi-core computer. A possible limitation is that NF training may not learn the true target distribution for small N. While DLMC with MH is asymptotically unbiased, it can fail in situations where MH acceptance rate is very low, so that it cannot reach the stationary distribution in a finite number of steps. In this case a possible alternative is a short MCMC with local transitions at the end of DLMC. This was however not necessary in our examples. It would be interesting to explore what NF architectures, regularization, and training procedures safeguard against low MH acceptance rates.

References

[1] S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, *Hybrid monte carlo*, *Physics letters B* **195** (1987) 216.

[2] Q. Liu and D. Wang, *Stein variational gradient descent: A general purpose bayesian inference algorithm*, in *Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain*, D. D. Lee, M. Sugiyama, U. von Luxburg, I. Guyon and R. Garnett, eds., pp. 2370–2378, 2016, https://proceedings.neurips.cc/paper/2016/hash/b3ba8f1bee1238a2f37603d90b58898d-Abstract.html.

[3] D. Maoutsa, S. Reich and M. Opper, *Interacting Particle Solutions of Fokker-Planck Equations Through Gradient-Log-Density Estimation*, *Entropy* **22** (2020) 802 [2006.00702].

[4] A. Wibisono, *Sampling as optimization in the space of measures: The langevin dynamics as a composite optimization problem*, in *Conference on Learning Theory*, pp. 2093–3027, PMLR, 2018.

[5] G. O. Roberts and R. L. Tweedie, *Exponential convergence of langevin distributions and their discrete approximations*, *Bernoulli* (1996) 341.

[6] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon and B. Poole, *Score-based generative modeling through stochastic differential equations*, *arXiv preprint arXiv:2011.13456* (2020) .

[7] P. Del Moral, A. Doucet and A. Jasra, *Sequential monte carlo samplers*, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **68** (2006) 411.

[8] J. Nocedal and S. J. Wright, *Numerical Optimization*. Springer, New York, 2nd ed., 2006.

[9] L. Dinh, J. Sohl-Dickstein and S. Bengio, *Density estimation using real NVP*, in *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*, OpenReview.net, 2017, https://openreview.net/forum?id=HkpbnH9lx.

[10] G. Papamakarios, I. Murray and T. Pavlakou, *Masked autoregressive flow for density estimation*, in *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, I. Guyon, U. von Luxburg, S. Bengio, H. M. Wallach, R. Fergus, S. V. N. Vishwanathan et al., eds., pp. 2338–2347, 2017.

[11] D. P. Kingma and P. Dhariwal, *Glow: Generative flow with invertible 1x1 convolutions*, in *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, S. Bengio, H. M. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi and R. Garnett, eds., pp. 10236–10245, 2018.

[12] B. Dai and U. Seljak, *Sliced iterative normalizing flows*, in *Proceedings of the 38th International Conference on Machine Learning, ICML 2021, 18-24 July 2021, Virtual Event*, M. Meila and T. Zhang, eds., vol. 139 of *Proceedings of Machine Learning Research*, pp. 2352–2364, PMLR, 2021, http://proceedings.mlr.press/v139/dai21a.html.

[13] M. D. Parno and Y. M. Marzouk, *Transport map accelerated markov chain monte carlo*, *SIAM/ASA Journal on Uncertainty Quantification* **6** (2018) 645.

[14] M. Hoffman, P. Sountsov, J. V. Dillon, I. Langmore, D. Tran and S. Vasudevan, *Neutra-lizing bad geometry in hamiltonian monte carlo using neural transport*, *arXiv preprint arXiv:1903.03704* (2019) .

[15] M. Albergo, G. Kanwar and P. Shanahan, *Flow-based generative models for markov chain monte carlo in lattice field theory*, *Physical Review D* **100** (2019) 034515.

[16] M. Arbel, A. G. de G. Matthews and A. Doucet, *Annealed flow transport monte carlo*, in *Proceedings of the 38th International Conference on Machine Learning, ICML 2021, 18-24 July 2021, Virtual Event*, M. Meila and T. Zhang, eds., vol. 139 of *Proceedings of Machine Learning Research*, pp. 318–330, PMLR, 2021, http://proceedings.mlr.press/v139/arbel21a.html.

[17] J. Goodman and J. Weare, *Ensemble samplers with affine invariance*, *Communications in applied mathematics and computational science* **5** (2010) 65.

[18] C. J. Ter Braak, *A markov chain monte carlo version of the genetic algorithm differential evolution: easy bayesian computing for real parameter spaces*, *Statistics and Computing* **16** (2006) 239.

[19] D. M. Blei, A. Kucukelbir and J. D. McAuliffe, *Variational inference: A review for statisticians*, *Journal of the American statistical Association* **112** (2017) 859.

[20] R. Jordan, D. Kinderlehrer and F. Otto, *The variational formulation of the fokker–planck equation*, *SIAM journal on mathematical analysis* **29** (1998) 1.

[21] M. D. Hoffman, A. Gelman et al., *The no-u-turn sampler: adaptively setting path lengths in hamiltonian monte carlo.*, *J. Mach. Learn. Res.* **15** (2014) 1593.

[22] D. Phan, N. Pradhan and M. Jankowiak, *Composable effects for flexible and accelerated probabilistic programming in numpyro*, *arXiv preprint arXiv:1912.11554* (2019) .

[23] M. Girolami and B. Calderhead, *Riemann manifold langevin and hamiltonian monte carlo methods*, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **73** (2011) 123.

[24] R. M. Neal, *Annealed importance sampling*, *Statistics and computing* **11** (2001) 125.

[25] H. Rosenbrock, *An automatic method for finding the greatest or least value of a function*, *The Computer Journal* **3** (1960) 175.

[26] A. Lewis, A. Challinor and A. Lasenby, *Efficient Computation of Cosmic Microwave Background Anisotropies in Closed Friedmann-Robertson-Walker Models*, *ApJ* **538** (2000) 473.

[27] R. M. Neal et al., *Mcmc using hamiltonian dynamics*, *Handbook of markov chain monte carlo* **2** (2011) 2.

[28] Y. Wu, Y. Burda, R. Salakhutdinov and R. Grosse, *On the quantitative analysis of decoder-based generative models*, 2017.

[29] D. Dua and C. Graff, *UCI machine learning repository*, 2017.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A]
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   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]

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