Gradient-Based Markov Chain Monte Carlo for Bayesian Inference With Non-differentiable Priors

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ABSTRACT

The use of nondifferentiable priors in Bayesian statistics has become increasingly popular, in particular in Bayesian imaging analysis. Current state-of-the-art methods are approximate in the sense that they replace the posterior with a smooth approximation via Moreau-Yosida envelopes, and apply gradient-based discretized diffusions to sample from the resulting distribution. We characterize the error of the Moreau-Yosida approximation and propose a novel implementation using underdamped Langevin dynamics. In misscritical cases, however, replacing the posterior with an approximation may not be a viable option. Instead, we show that piecewise-deterministic Markov processes (PDMP) can be used for exact posterior inference from distributions satisfying almost everywhere differentiability. Furthermore, in contrast with diffusion-based methods, the suggested PDMP-based samplers place no assumptions on the prior shape, nor require access to a computationally cheap proximal operator, and consequently have a much broader scope of application. Through detailed numerical examples, including a nondifferentiable circular distribution and a nonconvex genomics model, we elucidate the relative strengths of these sampling methods on problems of moderate to high dimensions, underlining the benefits of PDMP-based methods when accurate sampling is decisive. Supplementary materials for this article are available online.

1. Introduction

Estimating and quantifying the uncertainty of the parameters in a Bayesian statistical model often involves intractable, high-dimensional integrals. One of the most widely applied methods to estimate these integrals is Markov chain Monte Carlo (MCMC), which involves simulating a Markov chain that has the posterior distribution as its invariant, and subsequently estimating quantities of interest from the resulting trajectory. More recently, algorithms that operate directly in continuous-time have attracted significant attention (Bouchard-Côté, Vollmer, and Doucet 2018; Bierkens et al. 2019). These samplers are irreversible, which has been shown to increase mixing speeds (Neal 2004), and allow for exact subsampling of data by exploiting the factor structure of product likelihoods, completely avoiding the bias of stochastic gradients; this subsampling operation can furthermore be done at constant cost in common cases (Bierkens et al. 2019). This article discusses continuous-time algorithms for simulating values, or sampling, from the posterior of Bayesian problems with only almost everywhere differentiable posteriors.

This broad class of distributions includes all log-concave posteriors, as well as posteriors that arise from a log-concave and nondifferentiable prior, and a differentiable likelihood. This latter class of distributions have a long history in convex optimization, where the nondifferentiable priors are used to ensure existence and regularity of solutions (Boyd and Vandenberghe 2004). The most widespread uses of nondifferentiable priors have been in the image analysis literature, for example in denoising (Rudin, Osher, and Fatemi 1992; Chambolle et al. 2010), deblurring (Babacan, Molina, and Katsaggelos 2008; Beck and Teboulle 2009), multiframe super resolution (Farsiu et al. 2004), and compressed sensing (Candès, Romberg, and Tao 2006; Babacan, Molina, and Katsaggelos 2009). Outside of image analysis, the Laplace, or double exponential, prior is used in Lasso regression and its Bayesian counterpart (Tibshirani 1996; Park and Casella 2008), in sparse regularization via the nuclear envelope (e.g., Nitanda 2014; Bauschke and Combettes 2011; see Parikh et al. 2014 for a review) to smooth the convex prior. The resulting regularized prior function is known as the Moreau-Yosida envelope (MYE) prior, and is everywhere continuously differentiable, in particular, the gradient is just a linear function of the proximal operator. The closeness of the MYE to the true underlying function is determined by a
single **envelope tightness parameter** \( \lambda \), and this parameter plays a key role in what follows. We will generically denote a posterior density that incorporates a MYE prior as \( \pi^\lambda \).

Recently, MCMC algorithms and computational resources have matured to a point where it is now feasible to carry out full posterior inference for high-dimensional instances of these models, rather than just maximum a posteriori (MAP) estimation as is done in optimization. Since its introduction to the sampling literature in the seminal paper of Pereyra (2016), the proximal operator and the MYE have been used to propose new gradient-based sampling methods for nondifferentiable distributions (Chaari et al. 2016; Durmus, Moulines, and Pereyra 2018; Salim, Kovalev, and Richtárik 2019). The use of these operators in sampling algorithms is, however, not without complications. As the gradient of the MYE is \( 1/\lambda \)-Lipschitz continuous (Durmus, Moulines, and Pereyra 2018, prop. 3.1) and simultaneously the accuracy of the posterior approximation is increased by decreasing \( \lambda \), the step-sizes one may take in the algorithms of Pereyra (2016) or Salim, Kovalev, and Richtárik (2019) need to scale at order \( O(\lambda) \) to ensure that the invariant distribution of the diffusion process is close to the target \( \pi^\lambda \). The unadjusted diffusions also introduce bias from both their discretization and the use of the MYE to approximate the target density, yet it is only possible to adjust for the bias via Metropolis–Hastings corrections if the proposal density is available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing. In mission-critical cases, such as calculating available in closed form. This correction also comes at the cost of slower mixing.

In Theorem 3 that one can asymptotically compute good approximations to the true expectations if the envelope tightness parameter \( \lambda \) is chosen small enough.

- A common thread for the Langevin-based algorithms presented in Pereyra (2016), Durmus, Moulines, and Pereyra (2018), and Salim, Kovalev, and Richtárik (2019) is that they all use first-order methods to discretize the Langevin SDE. As an extension to the existing literature, we show that the second-order unadjusted Underdamped Langevin Dynamics can be used to target the smooth posterior. Numerically, this can lead to better mixing 4.1. These dynamics require an extra momentum variable but come with provably faster convergence properties (Ma et al. 2019) at limited extra computational effort.

- We show that the recent class of continuous-time sampling algorithms (Bou-Rabee et al. 2017; Bouchard-Côté, Vollmer, and Doucet 2018; Bierkens et al. 2019, all based on Piecewise-deterministic Markov Processes (PDMP, originally introduced in Davis (1984), for a thorough overview, see Jacobsen 2006), can exactly sample from our class of nondifferentiable posteriors by only using the gradient at points of differentiability. It is therefore unnecessary to calculate the potentially costly MYE or proximal operator, and the samples are asymptotically exact draws from the correct posterior \( \pi \) rather than the approximate \( \pi^\lambda \).

- We provide numerical comparisons of these samplers in moderate to high-dimensional problems from Bayesian statistics and imaging, evaluate and compare the performance of the algorithms, and give clear recommendations for end users applying nondifferentiable priors. Notably, we carry out exact Bayesian inference on a nondifferentiable circular distribution, and in a nonconvex genomics model where proximal operators are inapplicable, recovering significant gene expressions in the latter. In the supplementary material B, we also provide new insight on the performance of PDMP methods in a challenging Bayesian imaging model in high dimension, and a matrix denoising example using Hamiltonian dynamics (Vemuri et al. 2017).

The article is organized as follows: In Section 2, we introduce the proximal operator and the Moreau–Yosida envelope (MYE), as well as giving an error estimate of the smooth target. In Section 3, we review the existing Langevin-based methods for a MYE-smoothed posterior, introduce a new second-order method, and discuss how to use PDMPs to exactly sampling the target. Section 4 compares the algorithms on a variety of examples, and Section 6 concludes. Long proofs can be found in Supplementary Material A, additional numerical experiments in supplementary material B.

### 1.1. Contributions

The contributions of this article are:

- The availability of the gradient through the proximal operator has in particular allowed for the use of Langevin dynamics (Roberts et al. 1996; Roberts and Rosenthal 1998), where the gradient of the MYE of the log-posterior is applied as the drift-function in a discretized stochastic differential equation (SDE). If this SDE is run unadjusted, that is, without a Metropolis–Hastings acceptance step, we shown
define $\ell(x) = \log \mathcal{L}(x)$, the log-likelihood. Since data is fixed, we subdue it in the notation from now on. By Bayes’ theorem, the posterior distribution of $x$ given data is then $\pi(x) \propto \mathcal{L}(x)\pi_0(x) \in C^0_{\text{non}}(\mathbb{R}^n, \mathbb{R})$. It will be convenient to work entirely in log-space, we subdue it in the notation from now on. By Bayes’ theorem, the posterior distribution of $x$ given data is then $\pi(x) \propto \mathcal{L}(x)\pi_0(x) \in C^0_{\text{non}}(\mathbb{R}^n, \mathbb{R})$.

The proximal operator is in fact a generalization of the Euclidean projection operator: let $g$ be a proper lower semicontinuous convex function, and let $\lambda$ be the optimization problem

$$
\text{prox}_g^\lambda(x) = \arg \min_u \{ g(u) + \frac{1}{2\lambda} \| x - u \|^2 \}. 
$$

The proximal operator is in fact a generalization of the Euclidean projection operator: let $g(x) = 0$ if $x \in A$, $g(x) = \infty$ otherwise, for some convex set $A \in \mathbb{R}^n$, then the resulting proximal operator is $\text{prox}_g(x) = \text{proj}_A(x)$ (Parikh et al. 2014). In addition, if $g \in C^1(\mathbb{R}^d)$, then the $\text{prox}_g^\lambda$ operator satisfies

$$
p = \text{prox}_g^\lambda(x) \iff x - p = \lambda \nabla g(p),
$$

or, if $g$ is convex but not differentiable, it still satisfies $p = \text{prox}_g^\lambda(x) \iff x - p = \lambda \partial g(p)$, where $\partial g(p)$ denotes the subdifferential relation $\partial g(p) = \{ u \in \mathbb{R}^n : \forall y \in \mathbb{R}^n, (y - p)^T u + g(p) \leq g(y) \}$.

### 2.2. The Moreau-Yosida Envelope

One can approximate a nondifferentiable and convex function $g$ with the Moreau-Yosida envelope (MYE) which is defined by

$$
g^\lambda(x) = \inf_z \left[ g(z) + \frac{1}{2\lambda} \| x - z \|^2 \right].
$$

The MYE is again a convex function by convexity of the infimum, and as the positivity of the quadratic term preserves minima. If $g$ furthermore is $L$-Lipschitz continuous, this envelope is close to the original function, as the following theorem from (Hosseini, Mordukhovich, and Uschmajew 2019, Proposition 3.4 with $\lambda = 1/r$) shows

**Theorem 1.** Let $g : \mathcal{X} \to [-\infty, \infty]$ be a proper lower semicontinuous convex function, and $L$-Lipschitz. Let $\lambda > 0$. Then for any $x \in \text{dom}(g)$,

$$
0 \leq g(x) - g^\lambda(x) \leq \frac{L^2\lambda}{2}.
$$

This characterizes the tradeoff between the precision parameter $\lambda$ and the Lipschitz constant of the gradient of $g$, such that $\lambda$ should be chosen of the order $O(L^{-2})$ to achieve tightness of the approximation. We note that the upper bound is often achieved, for example, for the example in Figure 1 for $\lambda = 0.25$ we have a Lipschitz constant $L = 1$, and for any $x$ with $|x| > \lambda$ we can easily check that $g(x) = g^\lambda(x) = \frac{1}{2}$. Additionally, the MYE is differentiable everywhere, and we can compute the derivative using the proximal operator defined in the previous section (Bauschke and Combettes 2011, Theo. 12.30):

**Theorem 2.** Let $g : \mathcal{X} \to [-\infty, \infty]$ be a proper lower semicontinuous convex function, and let $\lambda > 0$. Then $g^\lambda$ is Fréchet differentiable, and its gradient is $1/\lambda$-Lipschitz continuous, given by

$$
\nabla g^\lambda(x) = \frac{1}{\lambda} (x - \text{prox}_g^\lambda(x)).
$$

Rearranging the above equation reveals that iterative application of the proximal operator just corresponds to gradient descent of the MYE-smoothed version of $g$. In Figure 1, we
provide a simple visual aid that illustrates the behavior of both the MYE and proximal operator and the respective densities in a basic example, \( g(x) = |x| \) such that \( g \in C^0 \). The resulting MYE in this case is the Huber loss function. In general, we do not have access to closed-form solutions to either the MYE or the proximal operator, and the solution to either can be quite computationally expensive.

Having recalled these basic facts about the proximal operator, we now provide an easily verifiable bound on the precision achievable when using the MYE in sampling algorithms: Theorem 3 quantifies the error obtained if we compute (exactly) an expectation with respect to the smoothed target distribution versus the true (nondifferentiable) distribution in the sense that for suitably regular \( f : \mathcal{X} \to \mathbb{R} \), \( \mathbb{E}_\pi(f) \approx \mathbb{E}_\pi^\lambda(f) \). The benefit of the first inequality is that we can easily verify the right-hand side numerically and thus get an error bound estimate.

**Theorem 3.** Let \( g = -\log \pi \) be the negative logarithm of a probability density function, with \( g \) being a proper lower semi-continuous convex function, and \( L \)-Lipschitz. Let \( g^\lambda \) be the Moreau-Yosida envelope to \( g \), and let \( \pi^\lambda(x) = \exp(-g^\lambda(x))/\int \exp(-g^\lambda(z))dz \) be a probability density function. Then for any \( \pi \) and \( \pi^\lambda \) integrable \( f : \mathcal{X} \to \mathbb{R} \)

\[
|\mathbb{E}_\pi(f) - \mathbb{E}_\pi^\lambda(f)| \leq (\exp(L^2\lambda) - 1)\mathbb{E}_\pi^\lambda(|f|) \tag{4}
\]

\[
|\mathbb{E}_\pi^\lambda(f) - \mathbb{E}_\pi(f)| \leq (\exp(L^2\lambda) - 1)\mathbb{E}_\pi(|f|). \tag{5}
\]

The same inequalities hold if \( g = g_1 + g_2 \) with a convex and Lipschitz-continuous \( g_1 \) and a differentiable (but not necessarily Lipschitz-continuous) \( g_2 \): In that case, one takes the MYE of \( g_1 \) only, resulting in the approximate pdf \( \pi^\lambda(x) = \exp(-g_1^\lambda(x) - g_2(x))/\int \exp(-g_1^\lambda(z) - g_2(z))dz \).

**Proof.** See Supplementary material A.1.

Choosing \( f(x) = \text{sgn}(\pi^\lambda(x) - \pi(x)) \) in this theorem allows to recover proposition 3.1 in Durmus, Moulines, and Pereyra (2018) by only considering a one-sided inequality in Equation (20) in the proof of the theorem, and can thus be viewed as a generalization thereof. Theorem 3 shows that for exact integral estimates, one wants to pick \( \lambda \) as small as possible. This, however, does come at a cost, as the gradients of the MYE approximated target grow as \( \lambda \to 0 \) such that one needs to take a smaller step size in the diffusion algorithms discussed in the next section. The relation between different approximation parameters and the size of the gradient is given by the next lemma.

**Lemma 1.** Let \( g : \mathcal{X} \to ]-\infty, \infty[ \) be a proper lower semi-continuous convex function, and let \( 0 < \lambda_1 \leq \lambda_2 \); then for the corresponding Moreau-Yosida envelopes \( g^{\lambda_1} \) and \( g^{\lambda_2} \), we have

\[
\|\nabla g^{\lambda_1}(x)\| \geq \|\nabla g^{\lambda_2}(x)\| \quad \forall x \in \mathcal{X}.
\]

**Proof.** See Supplementary material A.2.

### 3. Continuous-Time Stochastic Processes for Sampling From Nondifferentiable Posteriors

We now discuss ways of sampling from posteriors that are nondifferentiable. We will first discuss algorithms based on the Langevin equations and proximal operators, and introduce another Langevin-type method using underdamped, or second-order, Langevin dynamics. We will then discuss how samplers based on Piecewise-deterministic Markov processes can be used in the above-mentioned setting.

#### 3.1. Langevin Dynamics

##### 3.1.1. Overdamped Langevin Dynamics

The overdamped Langevin equation is defined as the stochastic differential equation given by

\[
dx_t = \nabla U(x_t)dt + \sqrt{2}dB_t, \tag{6}
\]

where \( U(x) \) is the log-posterior and \( B_t \) is a \( n \)-dimensional Brownian motion. The resulting invariant distribution of the semi-group associated to the Langevin equation is under smoothness assumptions proportional to \( \exp(-U(x)) \). This implies that Equation (6) can be simulated according to some discretization scheme, typically Euler-Maruyama, to generate samples that are distributed according to \( \pi \). The discretization of Equation (6) leads to bias that is typically corrected with a Metropolis–Hastings (M-H) step, leading to the popular Metropolis-adjusted Langevin Algorithm (MALA) (Roberts et al. 1996). Large-scale, data-intensive models has led to a notable increase in interest in unadjusted Langevin algorithms (ULA) Welling and Teh (2011), as no accept/reject step is applied. In this case, mixing is generally improved (Durmus, Moulines, and Pereyra 2018) and gradient evaluations are not wasted on rejected proposals. The step-size is also not forced to comply with theoretically-optimal acceptance rates (Roberts and Rosenthal 1998), rather, the step-size is chosen to be of the order of \( \lambda \) (Durmus, Moulines, and Pereyra 2018).

For a general nondifferentiable distribution \( \pi \) one may, as proposed in Pereyra (2016) and further studied in Durmus, Moulines, and Pereyra (2018), target the MYE-smoothed version \( \pi^{\lambda} \) instead. In particular, the gradient of Equation (6) is split into a likelihood derivative and an evaluation of the proximal operator via Theorem 2

\[
\nabla \log \pi^{\lambda}(x) = \nabla \ell(x) + \frac{1}{\lambda}(x - \text{prox}_{\lambda \ell^1}(x)) =: -\nabla U^\pi(x). \tag{7}
\]

The resulting sampler is known as proximal MALA (pMALA) or MY-ULA, depending on whether or not a Metropolis–Hastings step is included. In Pereyra, Mieles, and Zygalakis (2020), the authors used stabilized explicit integrators to simulate the diffusion 6, which allows accelerated sampling from the posterior. Such stabilized explicit integrators are especially strong for stiff PDEs, and the SK-ROCK algorithm from Pereyra, Mieles, and Zygalakis (2020) is included in our numerical comparisons where applicable.

##### 3.1.2. Underdamped Langevin Dynamics

The dynamics of the overdamped Langevin equation are characterized by reversible, diffusive behavior. A generic way to alleviate these backtracking tendencies over short time-scales is to introduce persistence in the trajectories via a notion of velocity. We therefore augment our target space \( \mathcal{X} \) with \( \mathbb{R}^n \), and
on this space let $v$ be a $n$-dimensional vector of velocities drawn from $\mathcal{N}(0, u I_n)$. To this end, we now consider the underdamped Langevin diffusion on $(x, v) \in \mathbb{R}^{n \times n}$

$$\begin{align*}
    dx_i &= v_it dt \\
    dv_i &= -\gamma v_it dt + u\nabla U(x_i) dt + \sqrt{2\gamma u} dB_t,
\end{align*}$$

(8)

(9)

for $u > 0$ and $\gamma > 0$ a speed parameter. Under mild conditions, this process has an invariant distribution proportional to \( \exp(-U(x) - \|v\|^2 / (2u)) \), and thus the marginal distribution of $x$ is the desired target distribution $\pi(x) \propto \exp(-U(x))$. A second-order discretization scheme is provided in the Supplementary Material A.5. Recent theoretical advances have been made to elucidate nonasymptotic properties and the speed of convergence in probability metrics (KL-divergence, Wasserstein distance, etc.) for various formulations of Langevin-based algorithms, see, for example, Dalalyan (2017), Cheng et al. (2017), and Wibisono (2019). In the case where $U$ is $m$-strongly log-concave and Lipschitz-differentiable with parameter $L$, the number of samples required to achieve $\epsilon$ precision in Wasserstein-2 distance scales with $O(\sqrt{n})$, with $n$ the dimension of the model, compared to $O(n)$ for the overdamped dynamics (Cheng et al. 2017). A natural extension of the MY-ULA algorithm is therefore to use the more elaborate dynamics of the underdamped Langevin SDE to explore the smoothed target distribution $\pi^*$:

$$\begin{align*}
    dx_i &= v_it dt \\
    dv_i &= -\gamma v_it dt + u\nabla U(x_i) dt + \sqrt{2\gamma u} dB_t,
\end{align*}$$

(10)

(11)

As with MY-ULA, the convergence of a discretization of these dynamics depends on the Lipschitz constant of the gradient (Cheng et al. 2017), which implies that the trade-off between posterior accuracy and mixing speed remains with MY-UULA. In spite of this, the improved dimensional scaling of MY-UULA can provide significant improvements over MY-ULA, see, for example, Example 4.1.

### 3.2. Piecewise-Deterministic Markov Processes

Below we elucidate the two most popular types of PDMP samplers, the Bouncy Particle Sampler (BPS) (First introduced in statistical physics by Peters and de With 2012 and subsequently ported to statistics in Bouchard-Côté, Vollmer, and Doucet 2018) and the zig–zag Sampler (ZZS) (Bierkens et al. 2019). Both are augmented-variable methods that introduce a notion of velocity to accelerate exploration. PDMP-samplers explore the target with persistent, deterministic dynamics, interspersed with direction-changes at random times. For both types of samplers, the key quantity is, similarly to the diffusion-based methods, the gradient of the target density. In contrast, however, the computational cost of running the samplers is determined by bounds on the gradient, and it only enters the dynamics at select times through the jump-process that updates the velocities. To run the samplers under a.e. differentiability, note that the gradient is well-defined everywhere outside a Lebesgue-nullset

$$A_0 = \left\{ x \in \mathcal{X} \mid \exists i \text{ such that } \frac{\partial U}{\partial x_i} \text{ does not exist} \right\};$$

(12)

we will on that subset replace any undefined derivative with zero, detailed descriptions and proofs are given below. We begin with the ZZS, the BPS and its variations follows subsequently. We end this section with a short overview of how to simulate these processes in practice.

#### 3.2.1. Zig–Zag Sampler

We augment our space with a new random variable, which we will denote velocity. Let $v \in \{-1, 1\}^n$, and consider the uniform distribution over velocities $p(v) = U(v)$. The continuous-time process $(x_t, v_t)_{t \geq 0} = (x_t, v_t)$ associated with the ZZS targets the joint distribution $p(x, v) = \pi(x) U(v)$.

Consider an initial value $(x_0, v_0) \sim p_0(x_0, v_0)$. The deterministic flow of the ZZS between events is given as a solution to the ODE $(\dot{x}_i, \dot{v}_i) = (v_i, 0)$, which is just $(x_i, v_i) = (x_0 + v_0 \cdot t, 0)$, indicating that the flow of $x$ over time is a continuous but non-differentiable process in $x$. For each individual dimension of the problem, we associate an inhomogeneous Poisson process (IPP), and the rate at which a jump, a change in velocity, occurs for dimension $i$ is given by

$$\rho_{ZZ}^i(t) := \rho_{ZZ}(t; x, v) = \max \left\{ 0, \frac{\partial}{\partial x_i} U(x + v \cdot t) \cdot v_i \right\}$$

The rate at which jumps occur globally for the sampler is sub-sequently just $\rho_{ZZ}(t) = \sum_{i=1}^n \rho_{ZZ}^i(t)$. In the case of prior non-differentiability, define

$$B_x = \left\{ 1, 2, \ldots, n \mid \frac{\partial U}{\partial x_i}(x) \text{ does not exist.} \right\}, \quad \forall x \in A_0$$

with $A_0$ as in Equation (12), and subsequently set $\{\partial U/\partial x_i(x)\}_{i \in B_x}$ equal to zero. Intuitively, if the derivative of $U(x)$ with respect to a coordinate $i$ is of the same sign as the velocity $v_i$, then it implies that the particle is entering the tail of the density. As this accumulation continues, one of the rates will generate an event in an attempt to force a return to regions of higher probability. The rate that generated the event and the new event time $\tau$ are in practice found by

$$f^* = \arg \min_{j=1,2,\ldots,n} f_j^*, \quad \tau = \tau^f,$$

respectively, and for the particular dimension $f^*$, the flip operator $F_{f^*} v$ is applied

$$F_{f^*} v = \begin{cases} v_i = -1 \cdot v_i, & \text{if } i = f^* \\
v_k = v_k, & \text{else,} \end{cases}$$

which trivially preserves the volume of the extended target. In this sense, the ZZS is naturally localized across all dimensions, as each dimension depends only on the variables that interacts with the derivative with respect to that coordinate. The infinitesimal generator of the Markov process associated with the ZZS is

$$L_{ZZ}f(x, v) = \langle \nabla f(x, v), v \rangle + \sum_{i=1}^n \rho_{ZZ}^i(t) [f(x, F_{f^*} v) - f(x, v)].$$

(13)

**Lemma 2.** Consider a distribution $\pi(x) U(v)$ that is differentiable in $x$ outside of $A_0$. If $A_0$ is a Lebesgue null-set, the Zig–Zag process with generator given in Equation (13) has invariant distribution $\pi(x) U(v)$.

**Proof.** See Supplementary material A.3. \(\square\)
3.2.2. Bouncy Particle Sampler

Given our variable of interest \( x \in \mathbb{R}^n \), we again augment the state space with an additional \( n \)-dimensional component \( v \) and assume that in stationarity \( v \sim N(0, I_n) \). With the same flow as the zig–zag sampler, the particle continues along a trajectory until an event occurs, and the rate at which these jumps of the velocity occur is determined by the rate function of a single iPP:

\[
\rho_{\text{BPS}}(t) := \rho(t; x, v) = \max(0, (v, \nabla U(x + v \cdot t))),
\]

where we recall that \( U(x) \) is the negative log-probability of the posterior distribution. Whenever an event occurs, all velocities are updated globally via the deterministic transition operator

\[
\mathcal{R}_x v = v - 2 \frac{(v, \nabla U(x))}{\|\nabla U(x)\|^2} \nabla U(x),
\]

which corresponds to a reflection in the hyperplane orthogonal to the gradient at \( x \). As both the rate and the reflection operator is undefined on \( A_0 \), we set \( \nabla U(x) = 0, \forall x \in A_0 \). In some cases, the BPS has been observed to be reducible (Deligianni et al. 2019). To avoid this degenerate behavior, velocity refreshments are introduced: at some rate \( \phi > 0 \) we draw a new velocity from the stationary distribution \( N(0, I_n) \); we denote this independent kernel by \( Q(v^\prime) \). The infinitesimal generator of the BPS with refreshment is then

\[
\mathcal{L}_{\text{BPS}} f(x, v) = \langle \nabla_x f(x), v \rangle + \rho_{\text{BPS}}(x,v) [f(x, \mathcal{R}_x v) - f(x, v)] + \phi \int_{\mathbb{R}^n} [f(x, v^\prime) - f(x, v)] Q(v^\prime) dv^\prime
\]

for all \( f \in D(\mathcal{L}) \), the domain of \( \mathcal{L} \).

**Lemma 3.** Consider a distribution \( \pi(x)N(0; 0, I_n) \) that is differentiable in \( x \) outside of \( A_0 \). If \( A_0 \) is a Lebesgue null-set, the bouncy particle sampler with generator given in Equation (13) has invariant distribution \( \pi(x)N(0; 0, I_n) \).

*Proof.* See Supplementary material A.4. \( \square \)

For high-dimensional problems, the BPS will without refreshments remain on a single contour of \( U \) and another contour of \( \log p(v) \) since \( \|v\| = c \) for some \( c > 0 \), in fact, the limiting dynamics correspond to those of the randomized Hamiltonian Monte Carlo algorithm, see Deligianni et al. (2018). To circumvent this issue, it is in general necessary to exploit some factor structure of the posterior potential

\[
U(x) = \sum_i U_i(x),
\]

where each \( U_i \) can depend on any number of dimensions of \( x \). The BPS extends easily to this case, as the individual factors can run as fully local bouncy particle samplers. With subscript \( i \) on variables denoting restriction to the components in factor \( i \), the event-times are now determined by local rate functions \( \rho_{i}\text{BPS}(t) := \max(0, (v_i, \nabla U_i(x_i + v_i \cdot t))) \), and the actual reflection event time is, as it is for the ZZS, just the minimum over all event times, \( \tau_e = \min_i \tau_i \). Accordingly, the reflection operator for each factor instead only uses the gradient of the reflecting factor, and only updates the corresponding subset \( v_i \) of the velocity vector via

\[
\mathcal{R}_i v_i = v_i - 2 \frac{(v_i, \nabla U_i(x_i))}{\|\nabla U_i(x_i)\|^2} \nabla U_i(x_i).
\]

We denote the factorized version the local BPS (LBPS), in contrast with the standard global version. In the supplement, Section A.6, we include an extended version with Hamiltonian dynamics (Vanetti et al. 2017).

3.2.3. Simulation

Since the flow of the basic PDMP models is trivial to calculate, the computational burden of simulation is on the generation of the arrival times of the iPP(s) that determines the changes in velocity. Given that the velocity component is either Gaussian or uniform, the burden entirely depends on having tight bounds on the gradient. By the Markov property the process renews at each event, so we only need to consider the generation of the first event time \( \tau_1 \). For some arbitrary initial \( (x_0, v_0) \), define \( \varrho(t) = \int_0^t \rho(x_0 + s \cdot v_0) ds \), where \( \rho \) is the rate function of the chosen PDMP. For an iPP, the probability of no arrivals in \([0, t]\) is then given by

\[
\mathbb{P}(\tau_1 > t) = \exp \left\{ - \varrho(t) \right\} = \exp \left\{ - \int_0^t \rho(x_0 + s \cdot v_0) ds \right\}.
\]

Sampling of \( \tau_1 \) can then be carried out by transforming the rate of the iPP to a homogeneous PP of rate 1, simulating an event-time of this process, and transforming the event-time back to the desired rate function via \( \tau_1 = \int_0^{\varrho^{-1}(u)} du \), where \( u \sim U(0, 1) \). Unfortunately, this iPP version of inversion sampling is only available in simple cases and instead, in the PDMP literature, the thinning method of Lewis and Shedler (1979) is used. To apply thinning, consider a fixed look-ahead \( \theta > 0 \). On \([0, \theta]\), we need the bound \( \bar{\rho} = \max_{t \in [0, \theta]} \rho(x_t, v_t) + \gamma \), for some \( \gamma > 0 \). For log-concave functions the maximum is attained at the endpoint of the interval, \( \bar{\rho} = \rho(x_\theta, \theta v_\theta, v_\theta) + \gamma \). The next event-time is then just simulated via \( \tau \sim \exp(\bar{\rho}) \), and accepted or rejected with probability \( \rho(\tau)/\bar{\rho} \). Evaluation of the empirical rejection probability provides a direct measure of the efficiency of the bounding procedure. If \( \tau > \theta \), instead update the look-ahead, calculate a new bound and generate a new event-time. Note that while \( \theta \) might appear similar to a step-size, it is purely a computational parameter, and does not affect the mixing of the PDMP algorithms. It is also worth noting that the trajectory length is directly correlated to the runtime, and as such does not contain any new information; yet it may provide a simple surrogate to the effective sample size and can also be helpful in planning the time needed for a simulation for a target Monte Carlo error.

4. Examples

In this section we compare the performance of the Langevin-based and the PDMP-based samplers in a number of numerical examples. They all illustrate that PDMPs can be used for exact sampling when using nondifferentiable priors. We also show that relaxing exactness (via MYE-based methods) does not necessarily lead to enhanced mixing compared to PDMP based approaches.
4.1. Anisotropic Laplace

We consider here an anisotropic distribution inspired by (Bouchard-Côté, Vollmer, and Doucet 2018, Exam. 4.4) on $\mathcal{X} = \mathbb{R}^{100}$ given by $\pi(x) \propto \exp\{-\beta^T |x|\}$, where $\beta = (1, 2, \ldots, 99, 100)^T$ is a vector of integers, $|\cdot|$ is applied element-wise, and superscript $T$ indicates transpose. These types of distributions generally prove challenging for MCMC samplers, as it is difficult to find a global stepsize that ensures efficient exploration across all dimensions. We approximate the potential $U(x) = \beta^T |x|$ by its Moreau-Yosida envelope with $\lambda = 10^{-5}$, giving us our smoothed target $\pi^\lambda$ with a very tight envelope.

We compare the performances of the Moreau-Yosida unadjusted Langevin algorithm (MY-ULA; Durmus, Moulines, and Pereyra 2018), our Moreau-Yosida unadjusted underdamped Langevin algorithm (MY-UULA), SK-ROCK as introduced in Pereyra, Mieles, and Zygalakis (2020), the proximal Metropolis-adjusted Langevin algorithm (pMALA; Pereyra 2016), the bouncy particle sampler (BPS; Bouchard-Côté, Vollmer, and Doucet 2018), and the zig-zag Sampler (ZZS; Bierkens et al. 2019). We let the algorithms run for an equivalent amount of wall clock time.

Figure 2 shows four relevant marginal empirical densities for the six different samplers. We set the stepsize for MY-ULA to $\delta = \lambda/2$, the stepsize for SK-ROCK to $\delta = 10^{-3}$, as in Pereyra, Mieles, and Zygalakis (2020). For pMALA, we set $\delta = 2\lambda_p$, where $\lambda_p = 2 \times 10^{-5}$ is tuned to achieve an acceptance ratio of around 55%. We observe that MY-ULA mixes very slowly in the most diffused marginal. Note that this is partly due to overdamped Langevin methods struggling with weakly log-concave distributions, see Durmus and Moulines (2019), another challenge in this example is the anisotropy:

![Figure 2](image-url).

Figure 2. The first three rows correspond to the approximate algorithms, the last three are asymptotically exact. The first four are based on discretizations of the Langevin diffusions, the last two rows correspond to the ZZS and BPS samplers. Each column corresponds to histograms of the first, second, fifth, and hundredth dimension of the anisotropic Laplace, the underlying orange line shows the true marginals. All algorithms were given the same clock time for a fair comparison. After this time expired, some algorithms have not yet mixed well, explaining the difference between the true distribution and the histograms, despite the last three algorithms being asymptotically exact.
while the algorithm mixes fast for the narrow marginals, it mixes slowly in the wide ones. Choosing a larger stepsize will result in faster mixing in these wide components, however, it will also lead to the narrow marginals not being captured properly. We also note that the resulting behavior is not a consequence of the tightness of the envelope: if, instead, \( \lambda \) was of the order \( 10^{-1} \) or \( 10^{-2} \), corresponding to much less tight envelopes, MY-ULA and MY-UULA suffer similarly. There is in general no way to adjust for anisotropy with methods using a step size outside of preconditioning, which requires extensive knowledge of the target distribution in general. Moving on to the asymptotically exact algorithms, pMALA shows slightly worse mixing behaviour compared to MY-ULA. Neither BPS nor ZZS degenerate in this scenario. The ZZS with its natural localization, provides very accurate estimates of the marginal densities across all dimensions. Due to the distribution factorizing into independent Laplace distributions, the BPS performs a bit worse than the ZZS in estimating marginals, as the latter makes use of the independence structure explicitly while the BPS is implemented naively in its global form. The BPS also requires roughly one refreshment in twenty reflections, or suffers from similar problems as the original BPS on Gaussian targets (Bouchard-Côté, Vollmer, and Doucet 2018). We emphasize here that a localized implementation of the BPS is possible in this example, and from our experience in this work gives better results than the global BPS. In Table 1 we see that SK-ROCK decorrelates very quickly for the narrow dimension (recall, however, that it fails to accurately capture the marginal), but for the most difficult wide dimension the ZZS outperforms SK-ROCK by a factor of four while targeting the correct invariant.

### 4.2. Sparse Bayesian Logistic Regression

Gene selection via sparse estimation has been subject of significant attention in the medical statistics literature, see, for example, Shevade and Keerthi (2003) and Cawley and Talbot (2006), with a particular emphasis on the application of convex regularizers. The interpretation of frequentist regularizers in generalized linear models as negative log-priors has, however, had limited success: while the posterior mode coincides with the MLE, expected parameter values under a full posterior are significantly nonsparse due to the integral dependence on the posterior shape. To remedy this, scale-mixtures (Carvalho, Polson, and Scott 2010; Bhattacharya et al. 2015; Hosseini 2019) that combine significant mass near zero with heavy tails have seen widespread application. The resulting priors, however, are not log-concave, induce multimodality of the posterior, and often only satisfy a.e. differentiability. It is therefore not possible to apply MYE-based Langevin dynamics for this class of models as the Moreau-Yosida envelope is not well-defined due to the fact that the optimization problem (3) might have multiple solutions. The resulting posteriors are typically sampled using custom Gibbs samplers, we here show the general applicability of PDMPs to target such distributions. In particular, we consider a sparse Bayesian logistic regression model with a Bessel–K prior, see Hosseini (2019) for details on this prior specification. We let \( y \in \{-1,1\}^d \) be a binary vector, \( Z \in \mathbb{R}^n \times \mathbb{R}^d \) a matrix of covariates, and \( x \in \mathbb{R}^d \) a parameter vector. For each observation \( i \) we model the outcome as a Bernoulli trial with probability of success given by logistic \((Z_i^\top x)\), where \( Z_i \) is the \( i \)th column and \( \text{logistic}(z) = 1/(1 + \exp(-z)) \). The Bessel-K prior with parameters \((p, \epsilon)\) is given by \( p(x) \propto |x + \epsilon|^{(p-2)K_{p-\frac{1}{2}}(|x| + \epsilon)} \), where \( K_i \) is the modified Bessel function of the second kind with order \( \alpha \), an illustration is given in Figure 3, top-left. As the factor graph is dense, the BPS and variations are not a suitable choice in this case. The ZZS, however, is more amenable to models that feature a fully connected factor graph. We will use constant bounds, which, while overly conservative, alleviate the dominant computational cost of running the ZZS, calculating local bounds, with an operation of order \( O(1) \).

We will use a dataset derived from Golub et al. (1999), which consists of \( n = 7129 \) gene expressions with associated parameters \( x_j, j = 1,2,\ldots,7129 \), of \( d = 72 \) individuals with either acute myeloid or acute lymphoblastic leukemia. Rather than classification of tumor type, our aim is to discover expressions that significantly contribute to the classification and warrant further scrutiny, and we therefore pool the test and training set. Based on the discussion in Hosseini (2019), we let \( p = 0.002 \) and \( \epsilon = 0.05 \), generated \( 10^5 \) samples and discarded the first \( 10^4 \). Trace plots of parameters and the log-energy indicate the sampler mixed well. Bhattacharya et al. (2015) applied a sequential 2-means cluster procedure to estimate the number of sparse parameters for a similar problem, we instead post-hoc subset some percentile of the largest absolute posterior means of \( x \). If we subset the 0.2\% percent largest values, the 16 resulting expressions results in a perfect prediction on the pooled set, see top right in Figure 3, but include none of the ones found in Cawley and Talbot (2006); the second percentile of the largest absolute components of \( x \), 144 in total, include 10 of the 11 gene expressions found by the algorithm of Cawley and Talbot (2006) via leave-one-out cross-validation. This indicates that the model successfully recovers novel and relevant genetic expressions not found via standard coordinate descent methods. The low number of observations implies that the effect size is limited, subsequently the 90\% credible intervals all include zero; if the dataset was larger we would expect the credible intervals to concentrate more strongly around the contributing genes expressions. We plot the posterior median and means of success given by logistic \((Z_i^\top x)\), where \( Z_i \) is the modified Bessel function of the second kind with order \( \alpha \), an illustration is given in Figure 3, top-left. As the factor graph is dense, the BPS and variations are not a suitable choice in this case. The ZZS, however, is more amenable to models that feature a fully connected factor graph. We will use constant bounds, which, while overly conservative, alleviate the dominant computational cost of running the ZZS, calculating local bounds, with an operation of order \( O(1) \).

### 4.3. Circular Bayesian Statistics

Circular statistics addresses inference from periodic data such as angles and rotations, for example, when analyzing the direction ants move in when responding to an evenly illuminated black

| Algorithm | MY-ULA | MY-UULA | SK-ROCK | pMALA | BPS | ZZS |
|-----------|--------|---------|---------|-------|-----|-----|
| \( \beta = 1 \) | 2.0 | 2.3 | 6.0 | 1.7 | 3.0 | 24.9 |
| \( \beta = 100 \) | 50.5 | 218.3 | 4197.4 | 182.9 | 755.5 | 2037.4 |

NOTE: Recall that the first three algorithms are asymptotically biased, while the last three are asymptotically exact.
target (Jander 1957), this can be modeled by an asymmetric wrapped Laplace distribution (Fernández-Durán 2004). This example illustrates the applicability of PDMPs when dealing with circular, nondifferentiable, and multi-modal posteriors. Here again, the MYE is not well-defined, precluding the use of the samplers based on the MYE-approximation.

In Jander (1957), the author studies which direction ants walk in when being placed in the middle of an evenly illuminated arena with two black discs on the side. These directions were observed for 253 ants, the observations are summarized in Figure 4. For the one-disc example, Fernández-Durán (2004) showed that the wrapped Laplace distribution is a good fit to the
observations. For the two-disc model, we thus assume a mixture of two wrapped Laplace distributions with means $\mu_i \in [0, 2\pi)$, scale parameters $\lambda_i > 0$, and skew parameters $\kappa_i > 0$, $i \in \{1, 2\}$. The likelihood of a data point $y \in [0, 2\pi)$ given the mixture component is calculated by
\[
L(y|\mu_i, \lambda_i, \kappa_i) = \frac{\lambda_i \kappa_i}{1 + \kappa_i^2} \left( e^{-\lambda_i \kappa_i^2} + e^{\lambda_i \kappa_i^2} \right),
\]
where the definition of the auxiliary variable $\theta$ handles the periodic extension due to the shift by the mean. The prior on the $\mu_i$ are uniform distributions on $[0, 2\pi]$, the ones on the $\lambda_i$ are Exponential(1) distributions, the one on the $\kappa_i$ are Gamma(2,1/2) distributions, and the one on the mixture parameter $\rho$ is a Beta(100, 100) distribution. Figure 4 shows the posterior distribution for $\mu_i$ as estimated by the BPS.

The reader should in particular note the multi-modality of the distribution, which especially the BPS samples from effectively: Table 2 summarizes the effective sample size per second for the BPS, the ZZS, and a random walk Metropolis–Hastings Sampler.

## 5. Discussion

Both PDMPs and diffusion-based samplers have been shown to work in various examples, albeit differently well. This discussion aims to provide the reader with an understanding of the strengths and weaknesses of the respective methods, and to guide the practitioner as to which algorithm to use. In the following, we discuss the key aspects one needs to consider.

**Dimensionality:** PDMPs perform worse as the dimension increases: The ZZS requires at least $d$ events to completely change the direction of the velocity vector, and for each of these event the gradient in the respective direction needs to be reevaluated, which (depending on the problem) can become prohibitively expensive. The BPS is known to suffer in high-dimensions too, with problems arising even when targeting isotropic Gaussians (Bouchard-Côté, Vollmer, and Doucet 2018) requiring many refreshments. If the problem is localizable (such as in Example B.3), the local version of the BPS can alleviate these issues by reducing the problem size to multiple smaller problems. An interesting direction for future research would be to parallelize the dynamics of these smaller problems, which would be a strong argument for PDMPs in high-dimensional settings, as discussed in Example B.3. The smoothing by the MYE always results in a nonlocalizable target, such that the computation of the proximal operator cannot be broken down into smaller problems. Furthermore, in the large data regime, data subsampling is straightforward for the PDMP samplers.

**Anisotropic targets:** As illustrated in Example 4.1, and similarly in (the everywhere differentiable) Example B.1 in the appendix, especially the ZZS is able to adapt to highly anisotropic targets. The diffusion-based samplers would improve if one has a preconditioner available, but if this is not the case, they struggle: A tight envelope results in small step sizes such that mixing in the “slow mixing components” takes very long. However, if one chooses a rather crude approximation, the approximation error in the “fast mixing components” grows. This is graphically visible in Figure 2 and Supplementary Figure 5.

**Log-concavity:** The MYE is only well-defined for log-concave targets, and as illustrated in Examples 4.2 and 4.3, PDMPs allow targeting these nondifferentiable posteriors, while the diffusion-based algorithms rely on the MYE to be well-defined. In weakly log-concave settings such as Example 4.1 when the gradient of the target is not Lipschitz continuous, a very tight envelope is needed to ensure a good approximation: This however, results in small step sizes and thus slow mixing. Furthermore, the samplers based on the overdamped Langevin diffusion struggle in this setting as the gradients do not grow when $|x|$ diverges.

In strongly log-concave targets, such as Examples B.2 and B.3, the tuning guidance in Pereyra, Mieles, and Zygalakis (2020) and Durmus, Moulines, and Pereyra (2018) ensured reasonable approximations while at the same time facilitating fast mixing. In summary, for strongly log-concave targets the diffusion-based algorithms are often preferable, while PDMPs are a viable option when the MYE is not well-defined.

**Exact Sampling:** The PDMPs are inherently asymptotically exact samplers, while the unadjusted diffusion-based samplers are not. However, it is possible to incorporate a Metropolis–Hastings correction step in MY-ULA to account for this, giving the proximal Metropolis-adjusted Langevin algorithm (pMALA; Pereyra 2016). pMALA is recommended to be tuned such that one achieves around 50%-70% acceptances, which may result in slower mixing in comparison to the unadjusted algorithms.

**Proximal Operators and Event Rates:** The proximal operators for some functions are available in closed form (see, e.g., Polson et al. 2015), however often the minimization problems need to be solved numerically, in which case the evaluation becomes expensive. On the other end, the PDMPs will perform significantly worse if one can’t find good bound on the event rates, as in that case one needs to evaluate the gradients more often.

## 6. Conclusion

We have in this work shown that sampling algorithms based on PDMPs allow exact sampling from a range of nondifferentiable target distributions. In particular, we exploit gradients if they exist almost everywhere, which is a common scenario in many real-world applications using nondifferentiable priors. This has particular relevance in cases like cancer tumor classification Golub et al. (1999) where accuracy is at a premium, and in situations where the proximal operator is prohibitively expensive to calculate. In comparison to gradient-based methods,
PDMPs can naturally handle anisotropy of the posterior without preconditioning, and furthermore be localized whenever the distribution is of product-form. In contrast, the unadjusted diffusion algorithms perform well in cases where low accuracy of the envelope is acceptable and when the posterior exhibits strong log-concavity. Using second-order information in the MY-UULA algorithm can prove beneficial to mixing. Furthermore, we have illustrated efficient sampling of nonconvex posteriors where Moreau-Yosida methods are not applicable. In conclusion, we have shown that PDMPs are a very able tool whenever accurate posterior inference is required in complex non-differentiable scenarios, and discussed which distribution characteristics suggest one or the other class of algorithms to be preferable.

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**Supplementary Materials**

Supplementary Material A contains the proofs that are not included in the main article, as well as details on the implementations of some algorithms used. Supplementary Material B provides three additional numerical examples, which inform the discussion in Section 5.

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