Learning Rate Free Sampling in Constrained Domains

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1. Introduction

Problem & Motivation

- We are interested in sampling from an unnormalised probability distribution $\pi(\mathrm{d}x)$ on some constrained domain $\mathcal{X} \subset \mathbb{R}^d$, with density

$$\boxed{\pi(x) \propto e^{-U(x)}}.$$

- Many existing methods such as mirrored Langevin dynamics (MLD) [1] and mirrored Stein variational gradient descent (MSVGD) [2] depend on a learning rate or step size γ.
- The learning rate needs to be carefully tuned to ensure convergence to the target distribution π at a suitable rate.

Contributions

- We introduce a general perspective of constrained sampling as a mirrored optimisation problem on the space of probability measures.
- Based on this perspective, we introduce a unifying framework for several existing constrained sampling algorithms, including MLD and MSVGD.
- We then propose mirrored coin sampling, a suite of new particle-based algorithms for sampling on constrained domains which are entirely learning-rate free.
- We illustrate the performance of our approach on a range of numerical examples. Our method achieves comparable performance to existing constrained sampling algorithms with no need to tune a learning rate.

2. Constrained Sampling as Optimisation

We can view the constrained sampling problem as a mirrored optimisation problem on the space of probability measures.

- Let $\phi : \mathcal{X} \to \mathbb{R} \cup \{\infty\}$ be a convex function of Legendre type. We call $\nabla\phi : \mathcal{X} \to \mathbb{R}^d$ the mirror map and $\nabla\phi(\mathcal{X}) = \mathbb{R}^d$ the dual space.
- Using the mirror map, we can define the mirrored target $\nu = (\nabla\phi)_{\#}\pi$, with $\pi = (\nabla\phi^*)_{\#}\nu$.
- We can then view the constrained target π as the solution of the mirrored optimisation problem

$$\boxed{\pi = (\nabla\phi^*)_{\#}\nu, \quad \nu = \underset{\eta \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\, \mathcal{F}(\eta)}, \tag{1}$$

where $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty]$ is a dissimilarity functional uniquely minimised at the mirrored target $\nu = (\nabla\phi)_{\#}\pi$.

One solution is to find a continuous process which transports samples from $\eta_0 := (\nabla\phi)_{\#}\mu_0$ to ν, and thus via the mirror map also from μ_0 to π, according to

$$\boxed{\frac{\partial \eta_t}{\partial t} + \nabla \cdot (w_t \eta_t) = 0 \quad , \quad \mu_t = (\nabla\phi^*)_{\#}\eta_t},$$

where $(w_t)_{t\geq 0}$ should ensure convergence of η_t to ν. The canonical choice is $w_t = -\nabla_{W_2}\mathcal{F}(\eta_t)$, in which case we call this the mirrored Wasserstein gradient flow (MWGF) of $\mathcal{F}$.

- We can view several existing constrained sampling algorithms as special cases of the MWGF, including MLD [1] and MSVGD [2].
- We can also use this framework to design new constrained sampling algorithms, e.g., mirrored kernel Stein discrepancy descent (MKSDD).

3. Mirrored Coin Sampling

Any algorithm derived as a discretisation of the MWGF (e.g., MLD, MSVGD), will depend on an appropriate choice of learning rate γ.

We propose an alternative approach, based on coin sampling [3], leading to algorithms which are entirely learning-rate free.

Let's first review the general coin betting framework, and how it can be used to solve convex optimisation problems of the form $x^* = \arg\min_{x\in\mathbb{R}^d} f(x)$:

- Consider a gambler who bets on a series of adversarial coin flips.
- The gambler starts with initial wealth $w_0 > 0$, and bets on the outcomes of coin flips $c_t \in \{-1, 1\}$, where $+1$ denotes heads and -1 denotes tails.
- The gambler bets $x_t \in \mathbb{R}$, where $\mathrm{sign}(x_t) \in \{-1, 1\}$ denotes whether the bet is on heads or tails, and $|x_t| \in \mathbb{R}$ denotes the size of the bet.
- The wealth w_t of the gambler thus accumulates as

$$w_t = w_0 + \sum_{s=1}^{t} c_s x_s.$$

- We will assume the gambler's bets satisfy $x_t = \beta_t w_{t-1}$, where $\beta_t \in [-1, 1]$ is a signed betting fraction. We here assume that $\beta_t = t^{-1}\sum_{s=1}^{t-1} c_s$.
- The sequence of bets made by the gambler is thus given by

$$x_t = \frac{\sum_{s=1}^{t-1} c_s}{t}\left(w_0 + \sum_{s=1}^{t-1} c_s x_s\right).$$

Remarkably, if we consider a betting game in which $c_t = -\nabla f(x_t)$, then $f(\frac{1}{T}\sum_{t=1}^{T} x_t) \to f(x^*)$ at a rate determined by the betting strategy [4]. This approach is completely learning-rate free!

We can use an extension of this approach to solve the mirrored optimisation problem over $\mathcal{P}_2(\mathbb{R}^d)$ in (1). Let $x_0 \sim \mu_0 \in \mathcal{P}_2(\mathcal{X})$, and set $y_0 = \nabla\phi(x_0) \sim (\nabla\phi)_{\#}\mu_0 := \eta_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Then, writing $\eta_t = \mathrm{Law}(y_t)$, update

$$y_t - y_0 = -\frac{\sum_{s=1}^{t-1} \nabla_{W_2}\mathrm{KL}(\eta_s|\nu)(y_s)}{t}\left(w_0 - \sum_{s=1}^{t-1}\langle \nabla_{W_2}\mathrm{KL}(\eta_s|\nu)(y_s), y_s - y_0\rangle\right) \tag{2}$$

$$x_t = \nabla\phi^*(y_t) \tag{3}$$

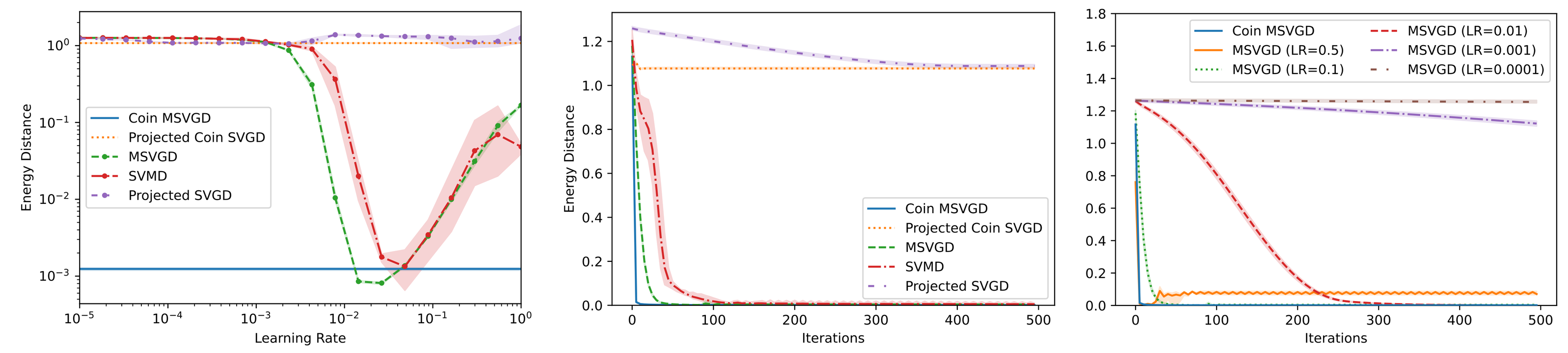
Under certain conditions, we can then show that $\mathrm{KL}(\frac{1}{T}\sum_{t=1}^{T}\mu_t|\pi) \to 0$, where $\mu_t = \mathrm{Law}(x_t) = (\nabla\phi^*)_{\#}\eta_t$.

Coin MSVGD. To obtain an implementable algorithm, replace $\nabla_{W_2}\mathrm{KL}(\eta|\nu)$ by $P_\eta \nabla_{W_2}\mathrm{KL}(\eta|\nu) = \int k(\cdot, z)\nabla_{W_2}\mathrm{KL}(\eta|\nu)(z)\eta(\mathrm{d}z)$, and approximate (2) - (3) using a particle-based approximation:

$$\boxed{y_t^i - y_0^i = -\frac{\sum_{s=1}^{t-1} P_{\eta_s^N}\nabla_{W_2}\mathrm{KL}(\eta_s^N|\nu)(y_s^i)}{t}\left(w_0^i - \sum_{s=1}^{t-1}\langle P_{\eta_s^N}\nabla_{W_2}\mathrm{KL}(\eta_s^N|\nu)(y_s^i), y_s^i - y_0^i\rangle\right)}$$

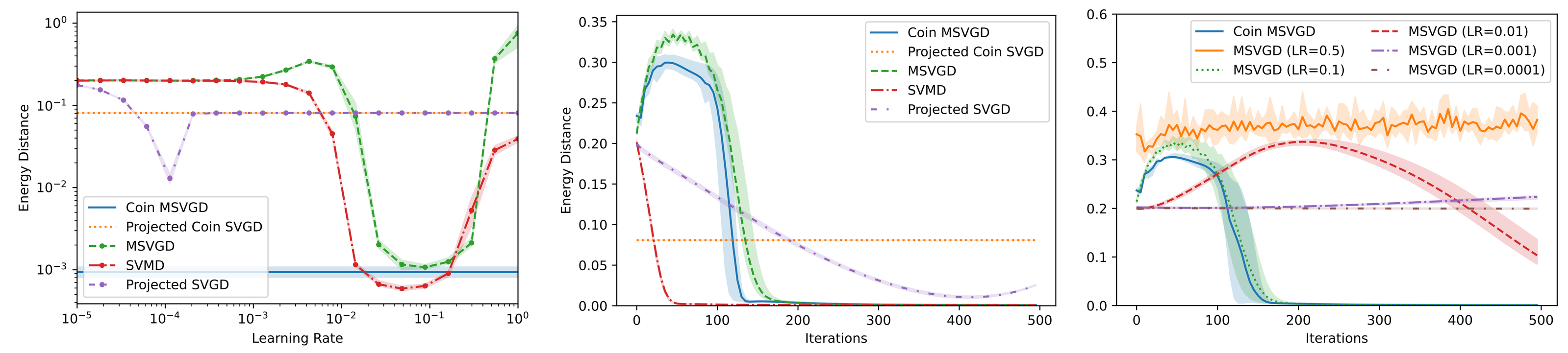
$$\boxed{x_t^i = \nabla\phi^*(y_t^i)}.$$

4. Numerical Experiments



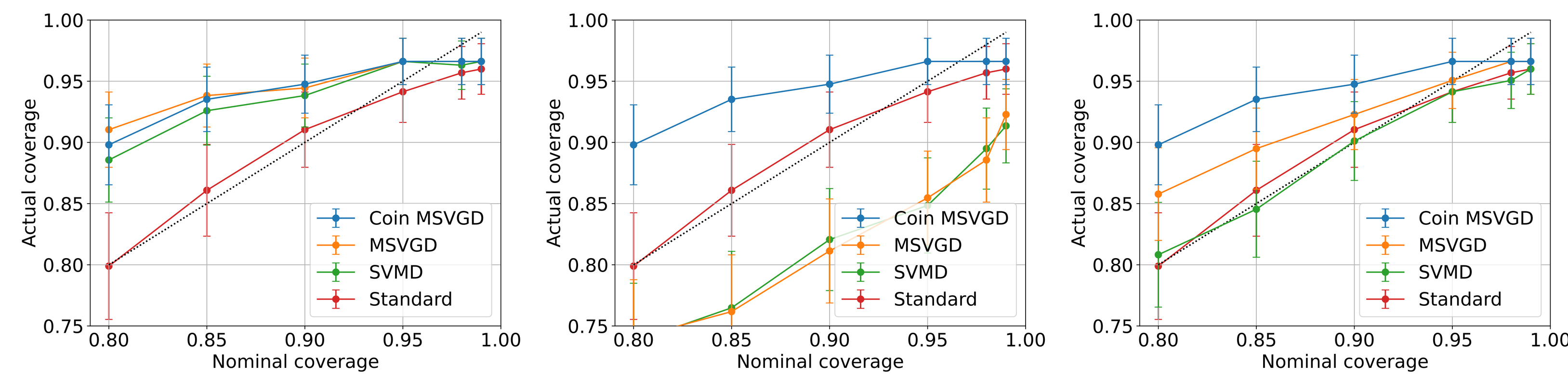
(a) Energy Dist. vs LR. (b) Energy Dist. vs T. (c) Energy Dist. vs T.

Fig 1. Sparse Dirichlet Target.



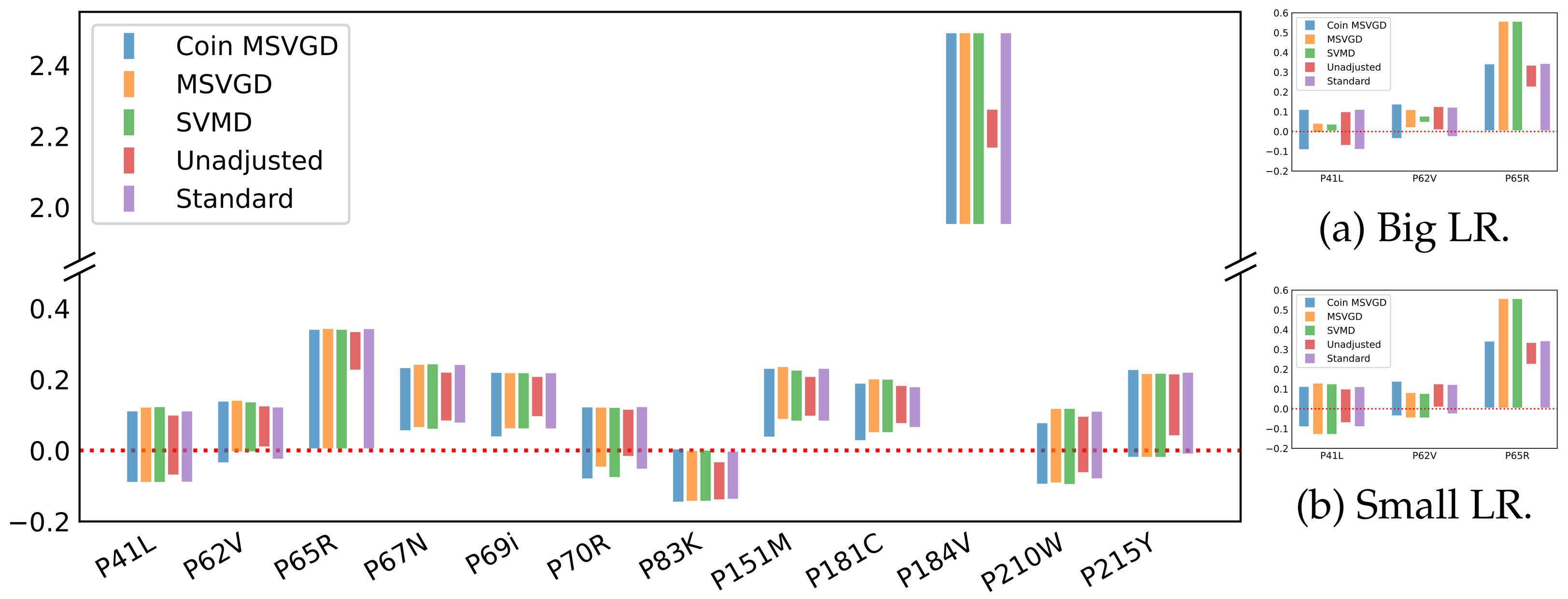
(a) Energy Dist. vs LR. (b) Energy Dist. vs T. (c) Energy Dist. vs T.

Fig 2. Quadratic Simplex Target.



(a) Optimal LR. (b) Small LR. (b) Large LR.

Fig 3. Post-Selection Inference. Coverage of post-selection confidence intervals for regression coefficients selected using the randomised Lasso.



(a) Big LR.

(b) Small LR.

Fig 4. Post-Selection Inference. Confidence intervals for mutations selected by randomised Lasso as candidates for HIV-1 drug resistance.

5. References

[1] Ya-Ping Hsieh, Ali Kavis, Paul Rolland, and Volkan Cevher. Mirrored Langevin Dynamics. In *NeurIPS 2018*.
[2] Jiaxin Shi, Chang Liu, and Lester Mackey. Sampling with Mirrored Stein Operators. In *ICLR 2022*.
[3] Louis Sharrock and Christopher Nemeth. Coin Sampling: Gradient-Based Bayesian Inference without Learning Rates. In *ICML 2023*.
[4] Francesco Orabona and David Pal. Coin Betting and Parameter-Free Online Learning. In *NeurIPS 2016*.

6. Code

Code and more results available on GitHub: