Proximal Interacting Particle Langevin Algorithms

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Outline

Latent Variable Models (LVM)

Consider the following data-generating process

$$x \sim p_\theta(\cdot)$$
$$y \sim p_\theta(\cdot|x)$$

for some parameter $\theta \in \mathbb{R}^{d_\theta}$, where $x \in \mathbb{R}^{d_x}$ is a latent variable which cannot be observed.

Given a data point y we want to find $\theta_\star$ maximising the marginal log-likelihood

$$\log p_\theta(y) = \log \int_{\mathbb{R}^{d_x}} p_\theta(x, y) \mathrm{d}x,$$

where $p_\theta(x, y) = p_\theta(x) p_\theta(y|x)$.

Expectation Maximisation (EM)

E-step w.r.t. *latent variables* x: compute for fixed θ

$$Q(\theta|\theta^{(n)}) = \int_{\mathbb{R}^{d_x}} \log p_\theta(x, y) p_{\theta^{(n)}}(x|y) \mathrm{d}x,$$

with $p_{\theta^{(n)}}(x|y) = p_{\theta^{(n)}}(x, y)/p_{\theta^{(n)}}(y)$

M-step w.r.t. *parameters* θ: maximise $Q(\cdot|\theta^{(n)})$

An Optimisation Point of View

Our aim is to find $\theta_\star$ maximising

$$k(\theta) := p_\theta(y) = \int p_\theta(x, y)\mathrm{d}x = \int e^{-U(\theta,x)}\mathrm{d}x,$$

with $U(\theta, x) := -\log p_\theta(x, y)$.

This is a well-studied problem in optimisation, one solution is to find a **measure** which concentrates around $\theta_\star$ and use standard tools to **sample** from this measure.

E.g. **simulated annealing**, set $k(\theta)^N$ and let $N \to \infty$.

Simulated Annealing for LVM

The extended target

$$\pi^N(\theta, x_1, x_2, ..., x_N) \propto \exp\left(-\sum_{i=1}^{N} U(\theta, x_i)\right)$$

admits as θ-marginal

$$\pi_\Theta^N(\theta) \propto \int_{\mathbb{R}^{d_x}} ... \int_{\mathbb{R}^{d_x}} \exp\left(-\sum_{i=1}^{N} U(\theta, x_i)\right) \mathrm{d}x_1 \mathrm{d}x_2 ... \mathrm{d}x_N$$
$$= \left(\int_{\mathbb{R}^{d_x}} e^{-U(\theta,x)} \mathrm{d}x\right)^N = k(\theta)^N,$$

which as $N \to \infty$ concentrates on $\theta_\star$.

Outline

Langevin Dynamics

The Langevin diffusion

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2}\mathrm{d}W_t$$

has invariant measure $\pi \propto e^{-U}$.

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The diffusion

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2/\beta}\mathrm{d}W_t$$

has invariant measure $\pi_\beta \propto e^{-\beta U}$, where β is known as the *inverse temperature parameter*.
As $\beta \to \infty$, π_β concentrates around its modal points.

Interacting Particle Langevin Algorithm (IPLA)

To sample from our target measure we use the following interacting particle system (IPS) of N particles

$$\mathrm{d}\boldsymbol{\theta}_t^N = -\frac{1}{N}\sum_{j=1}^{N} \nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{j,N})\mathrm{d}t + \sqrt{\frac{2}{N}}\mathrm{d}\boldsymbol{B}_t^{0,N}, \tag{1}$$

$$\mathrm{d}\boldsymbol{X}_t^{i,N} = -\nabla_x U(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{i,N})\mathrm{d}t + \sqrt{2}\mathrm{d}\boldsymbol{B}_t^{i,N}, i = 1, 2, ..., N.$$

Although (1) is an IPS, we consider it a diffusion evolving on $\mathbb{R}^{d_x} \times (\mathbb{R}^{d_\theta})^N$ and use techniques from **Langevin-based algorithms**.

Algorithm

Euler–Maruyama discretisation of Langevin IPS with stepsize γ

$$\theta_{n+1}^N = \theta_n^N - \frac{\gamma}{N}\sum_{j=1}^N \nabla_\theta U(\theta_n^N, X_n^{j,N}) + \sqrt{\frac{2}{N}}\xi_{n+1}^{0,N}$$

$$X_{n+1}^{i,N} = X_n^{i,N} - \gamma \nabla_x U(\theta_n^N, X_n^{i,N}) + \sqrt{2}\,\xi_{n+1}^{i,N}$$

Assumptions

A1. (Lipschitz) Let $v = (\theta, x)$ and $v' = (\theta', x')$. We assume that there exist $L > 0$ such that

$$\|\nabla U(v) - \nabla U(v')\| \leq L\|v - v'\|.$$

A2. (Convexity) Let $v = (\theta, x)$. Then, there exists $\mu > 0$ such that

$$\left\langle v - v', \nabla U(v) - \nabla U(v') \right\rangle \geq \mu\|v - v'\|^2,$$

for all $v, v' \in \mathbb{R}^{d_\theta} \times \mathbb{R}^{d_x}$.

Main Convergence Result

$$
\begin{aligned}
\mathbb{E}[\|\theta_n^N - \theta_\star\|^2]^{1/2} \leq & \sqrt{\frac{d_\theta}{N\mu}} \\
& + e^{-\mu n\gamma}\left(\mathbb{E}[\|Z_0^N - z_\star\|^2]^{1/2} + \left(\frac{d_x N + d_\theta}{N\mu}\right)^{1/2}\right) \\
& + C(1 + \sqrt{d_\theta/N + d_x})\gamma^{1/2},
\end{aligned}
$$

- $z_\star = (\bar{\theta}_\star, N^{-1/2}x_\star, \ldots, N^{-1/2}x_\star)$ and $(\bar{\theta}_\star, x_\star)$ is the minimiser of U
- Z_0^N is the initial condition
- $C > 0$ is a constant independent of $n, N, \gamma, d_\theta, d_x$

Proof Idea

We split the error of the algorithm as

$$W_2(\delta_{\theta_\star}, \mathcal{L}(\theta_n^N)) \leq W_2(\delta_{\theta_\star}, \pi_\Theta^N) + W_2(\pi_\Theta^N, \mathcal{L}(\boldsymbol{\theta}_{\gamma n})) + W_2(\mathcal{L}(\boldsymbol{\theta}_{\gamma n}), \mathcal{L}(\theta_n^N))$$

- $W_2(\delta_{\theta_\star}, \pi_\Theta^N)$ is the *concentration* of the invariant measure on $\theta_\star$
- $W_2(\pi_\Theta^N, \mathcal{L}(\boldsymbol{\theta}_{\gamma n}))$ is the *convergence* of the continuous time process to its invariant measure
- $W_2(\mathcal{L}(\boldsymbol{\theta}_{\gamma n}), \mathcal{L}(\theta_n^N))$ is error due to *time discretisation*

Toy Example

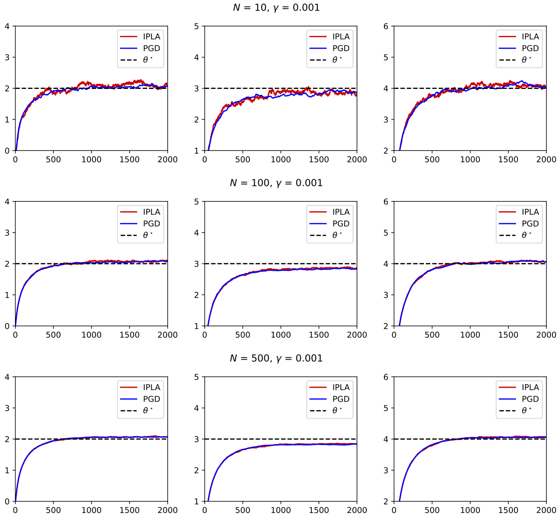
Bayesian logistic regression LVM where for $\theta \in \mathbb{R}^{d_\theta}$

$$p_\theta(x) = \mathcal{N}(x; \theta, \sigma^2 \mathrm{Id}_{d_x}),$$

$$p_\theta(y|x) = \prod_{j=1}^{d_y} s(v_j^T x)^{y_j}(1 - s(v_j^T x))^{1-y_j},$$

with $d_\theta = d_x$, $s(u) := e^u/(1+e^u)$ the logistic function and $\{v_j\}_{j=1}^{d_y} \in \mathbb{R}^{d_x}$ a set of covariates with corresponding binary responses $\{y_j\}_{j=1}^{d_y} \in \{0, 1\}$.

IPLA vs PGD



Outline

Non-differentiable Targets

Consider the case in which

$$U(\theta, x) = -\log p_\theta(x, y) = g_1(\theta, x) + g_2(\theta, x),$$

with $g_1 \in \mathcal{C}^1$ and g_2 not $\mathcal{C}^1$ but convex and lower semi-continuous.

- Lasso regularisation
- the elastic net
- total-variation norm

What's the need?

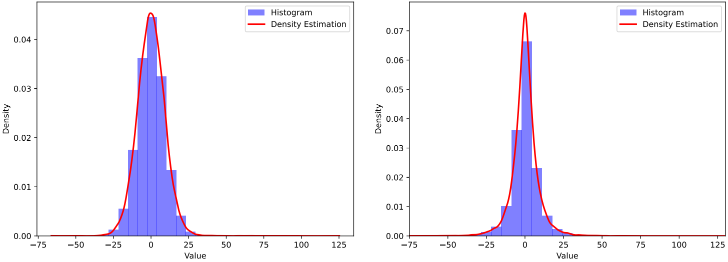


Figure: Normal vs Laplace prior. Histogram and density estimation of the weights of a BNN for a randomly chosen particle from the final (500 steps) cloud of 100 particles.

Proximity map

Proximity map

For U convex, proper and lower semi-continuous and $\lambda > 0$

$$\mathrm{prox}_U^{\lambda}(x) := \arg\min_{z \in \mathbb{R}^d} \left\{ U(z) + \|z - x\|^2/(2\lambda) \right\}.$$

Moves points in the direction of the minimum of U acting as a "gradient".

Moreau-Yosida envelope

Moreau-Yosida envelope

For any $\lambda > 0$, define the λ-Moreau-Yosida approximation of U as

$$U^{\lambda}(x) := \min_{z \in \mathbb{R}^d} \left\{ U(z) + \|z - x\|^2/(2\lambda) \right\}.$$

Take $\pi(x) \propto \exp(-U(x))$. We we define the λ-Moreau-Yosida approximation of π as the following density

$$\pi_{\lambda}(x) \propto \exp(-U^{\lambda}(x))$$

Moreau-Yosida envelope

Moreau-Yosida envelope

For any $\lambda > 0$, define the λ-Moreau-Yosida approximation of U as

$$U^{\lambda}(x) := \min_{z \in \mathbb{R}^d} \left\{ U(z) + \|z - x\|^2 / (2\lambda) \right\}.$$

Take $\pi(x) \propto \exp(-U(x))$. We we define the λ-Moreau-Yosida approximation of π as the following density

$$\pi_\lambda(x) \propto \exp(-U^{\lambda}(x))$$

- converge (pointwise, in TV, ...) to π as $\lambda \to 0$
- π_λ is continuously differentiable with $\nabla \log \pi_\lambda(x) = \lambda^{-1}(x - \mathrm{prox}_U^{\lambda}(x))$

Moreau-Yosida envelope

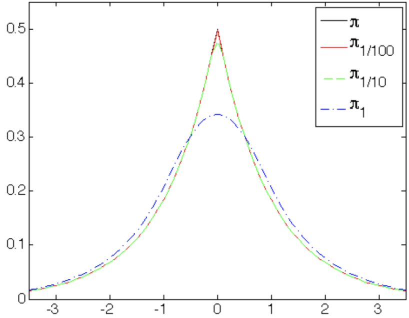


Figure: Moreau-Yoshida envelope for the Laplace distribution $\pi(x) \propto \exp(-|x|)$ (Pereyra, 2016).

Moreau-Yosida Langevin Dynamics

Since $\pi_\lambda \propto e^{-U^\lambda}$ is now continuously differentiable, we can write the Langevin diffusion

$$\mathrm{d}X_{\lambda,t} = -\nabla U^\lambda(X_{\lambda,t})\mathrm{d}t + \sqrt{2}\mathrm{d}B_t,$$

or, equivalently,

$$\mathrm{d}X_{\lambda,t} = \lambda^{-1}(\mathrm{prox}_U^\lambda(X_{\lambda,t}) - X_{\lambda,t})\mathrm{d}t + \sqrt{2}\mathrm{d}B_t.$$

The resulting algorithm is known as MY-ULA (Durmus et al., 2018; Pereyra, 2016).

Proximal Interacting Particle Langevin SDE

We consider as target measure π_N^λ, the Moreau-Yosida envelope of π_N and obtain

$$
\begin{aligned}
\mathrm{d}\boldsymbol{\theta}_t^N &= -\frac{1}{N}\sum_{j=1}^{N} \nabla_\theta U^\lambda(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{j,N})\mathrm{d}t + \sqrt{\frac{2}{N}}\mathrm{dB}_t^{0,N} \\
\mathrm{d}\boldsymbol{X}_t^{i,N} &= -\nabla_x U^\lambda(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{i,N})\mathrm{d}t + \sqrt{2}\mathrm{dB}_t^{i,N}.
\end{aligned}
$$

For regular enough U this SDE approaches the IPLA SDE as $\lambda \to 0$.

Moreau-Yosida Interacting Particle Langevin Algorithm (MYIPLA)

If $U = g_1 + g_2$, we can take $U^\lambda = g_1 + g_2^\lambda$ so that

$$\nabla U^\lambda(v) = \nabla g_1(v) + \lambda^{-1}(v - \mathrm{prox}_{g_2}^\lambda(v))$$

and obtain

$$\mathrm{d}\boldsymbol{\theta}_t^N = \frac{1}{N}\sum_{j=1}^N \left(-\nabla_\theta g_1(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{j,N}) + \lambda^{-1}(\mathrm{prox}_{g_2}^\lambda(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{j,N})_\theta - \boldsymbol{\theta}_t^N)\right)\mathrm{d}t + \sqrt{\frac{2}{N}}\mathrm{dB}_t^{0,N}$$

$$\mathrm{d}\boldsymbol{X}_t^{i,N} = \left(-\nabla_x g_1(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{i,N}) + \lambda^{-1}(\mathrm{prox}_{g_2}^\lambda(\boldsymbol{\theta}_t^N, \boldsymbol{X}_t^{i,N})_x - \boldsymbol{X}_t^{i,N})\right)\mathrm{d}t + \sqrt{2}\mathrm{dB}_t^{i,N}.$$

Algorithm

Euler–Maruyama discretisation of proximal Langevin IPS with stepsize γ

$$\theta_{n+1}^N = \Big(1 - \frac{\gamma}{\lambda}\Big)\theta_n^N + \frac{\gamma}{N}\sum_{i=1}^N \Big(- \nabla_\theta g_1(\theta_n^N, X_n^{i,N}) + \frac{1}{\lambda}\operatorname{prox}_{g_2}^{\lambda}(\theta_n^N, X_n^{i,N})_\theta \Big) + \sqrt{\frac{2\gamma}{N}}\xi_{n+1}^{0,N}$$

$$X_{n+1}^{i,N} = \Big(1 - \frac{\gamma}{\lambda}\Big)X_n^{i,N} - \gamma \nabla_x g_1(\theta_n^N, X_n^{i,N}) + \frac{\gamma}{\lambda}\operatorname{prox}_{g_2}^{\lambda}(\theta_n^N, X_n^{i,N})_x + \sqrt{2\gamma}\, \xi_{n+1}^{i,N}$$

Assumptions – g_1

A1. (Lipschitz) Let $v = (\theta, x)$ and $v' = (\theta', x')$. We assume that there exist $L > 0$ such that

$$\|\nabla g_1(v) - \nabla g_1(v')\| \leq L\|v - v'\|.$$

A2. (Convexity) Let $v = (\theta, x)$. Then, there exists $\mu > 0$ such that

$$\left\langle v - v', \nabla g_1(v) - \nabla g_1(v') \right\rangle \geq \mu\|v - v'\|^2,$$

for all $v, v' \in \mathbb{R}^{d_\theta} \times \mathbb{R}^{d_x}$.

Assumptions – g_2

A3. g_2 is proper, convex, lower semi-continuous and lower bounded.

A4. Let $v = (\theta, x)$ and $v' = (\theta', x')$. We assume that

$$\|g_2(v) - g_2(v')\| \leq \|g_2\|_{\text{Lip}} \|v - v'\|.$$

Main Convergence Result

$$
\begin{aligned}
\mathbb{E}[\|\theta_n^N - \theta_\star\|^2]^{1/2} \leq & \frac{\lambda}{\mu}\Big(\frac{\|g_2\|_{\mathrm{Lip}}^2}{2} A + B\Big) + \sqrt{\frac{d_\theta}{N\mu}} \\
& + e^{-\mu n \gamma}\left(\mathbb{E}[\|Z_0^N - z_\star\|^2]^{1/2} + \Big(\frac{d_x N + d_\theta}{N\mu}\Big)^{1/2}\right) \\
& + C(1 + \sqrt{d_\theta/N + d_x})\gamma^{1/2},
\end{aligned}
$$

- $z_\star = (\bar{\theta}_\star, N^{-1/2}x_\star, \ldots, N^{-1/2}x_\star)$ and $(\bar{\theta}_\star, x_\star)$ is the minimiser of U^λ
- Z_0^N is the initial condition
- $A, B, C > 0$ is a constant independent of $n, N, \gamma, \lambda, d_\theta, d_x$

Proof Idea

Overall, we split the error of the algorithm as

$$W_2(\delta_{\theta_\star}, \mathcal{L}(\theta_n^N)) \leq \|\theta_\star - \theta_{\star,\lambda}\| + W_2(\delta_{\theta_{\star,\lambda}}, \mathcal{L}(\theta_n^N))$$

- $\|\theta_\star - \theta_{\star,\lambda}\|$ distance between the minimiser of $p_\theta(y)$ and that of its MY envelope
- $W_2(\delta_{\theta_\star}, \mathcal{L}(\theta_n^N))$ combines concentration, convergence and time discretisation error

Toy Example

Bayesian logistic regression LVM where for $\theta \in \mathbb{R}^{d_\theta}$

$$p_\theta(x) = \prod_{i=1}^{d_x} \text{Laplace}(x_i|\theta, 1),$$

$$p_\theta(y|x) = \prod_{j=1}^{d_y} s(v_j^T x)^{y_j}(1 - s(v_j^T x))^{1-y_j},$$

with $d_\theta = d_x$, $s(u) := e^u/(1 + e^u)$ the logistic function and $\{v_j\}_{j=1}^{d_y} \in \mathbb{R}^{d_x}$ a set of covariates with corresponding binary responses $\{y_j\}_{j=1}^{d_y} \in \{0, 1\}$.

Toy Example: Results

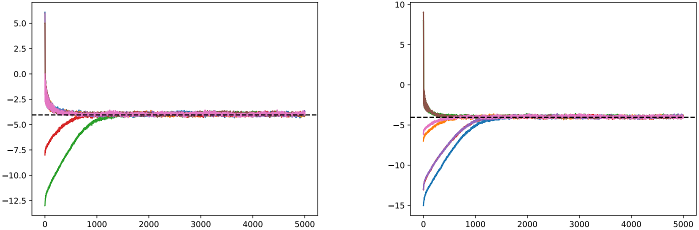


Figure: MYIPLA. Approximate vs Iterative solver for prox.

Bayesian Neural Network: Laplace prior

Bayesian two-layer neural network to classify MNIST images.
The latent variables are the weights, $w \in \mathbb{R}^{d_w := 40 \times 784}$, of the input layer and those, $v \in \mathbb{R}^{d_v := 2 \times 40}$, of the output layer.

$$
\begin{aligned}
p(l|f, x) &\propto \exp\left(\sum_{j=1}^{40} v_{lj} \tanh\left(\sum_{i=1}^{784} w_{ji} f_i\right)\right) \\
p_\alpha(w) &= \prod_i \mathrm{Laplace}(w_i | 0, e^{2\alpha}) \\
p_\beta(v) &= \prod_i \mathrm{Laplace}(v_i | 0, e^{2\beta})
\end{aligned}
$$

with $\theta = (\alpha, \beta)$.

Bayesian Neural Network: Laplace prior

Prior	% of zero weights		Thresholds		Error (%)	LPD
	Layer 1	Layer 2	Layer 1	Layer 2		
Laplace	74	48	0.2	0.2	7	-0.23
Normal	74	48	0.5	1.1	15	-0.74
	16	15	0.2	0.2	16	-0.78

Bayesian Neural Network: Laplace prior

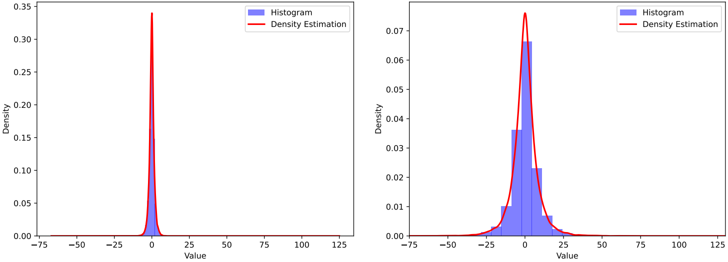


Figure: MYIPLA vs IPLA prior. Histogram and density estimation of the weights of a BNN with Laplace prior for a randomly chosen particle from the final (500 steps) cloud of 100 particles.

Conclusions I

We propose a family of algorithms to find the MLE in LVM which exploits

- scaling of Langevin diffusions
- optimisation perspective
- combines expectation and maximisation steps
- allows for non-differentiable prior/likelihoods
- returns approximations of both $\theta_\star$ and $p_{\theta_\star}(x|y)$

Conclusions II

There's more to do!

- other algorithms to sample from π^N can be constructed
- for ProxIPLA other discretisations exists (as well as a PGD equivalent)
- it should be possible to extend the analysis to the non-convex case

Both papers are on arXiv:

- IPLA `https://arxiv.org/abs/2303.13429`
- ProxIPLA `https://arxiv.org/abs/2406.14292`

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Thank you!

Bibliography I

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