Une méthode uniformément précise pour des dynamiques de Langevin évoluant au voisinage de variétés

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Contents

Reference of this talk:

- A. Laurent. A uniformly accurate scheme for the numerical integration of penalized Langevin dynamics. arXiv:2110.03222. To appear in SIAM J. Sci. Comput. (2022).

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The overdamped Langevin equation in molecular dynamics

Consider N particles moving in a fluid with positions $q(t)$ and velocities $p(t)$. The particles are submitted to

- a potential $V(q)$ and the associated force $-\nabla V(q)$,
- a friction force $-\gamma p$,
- a collision term $\sqrt{\frac{2\gamma}{\beta}}dW(t)$.

Then applying the fundamental principle of dynamics, we find the underdamped Langevin equation:

$$\begin{cases} dq(t) = p(t)dt, \\ dp(t) = (-\nabla V(q(t)) - \gamma p(t))dt + \sqrt{\frac{2\gamma}{\beta}}dW(t). \end{cases}$$

The overdamped Langevin equation in molecular dynamics

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In a high friction regime ($\gamma \to \infty$), we obtain the following simplified equation called the overdamped Langevin equation, where $f = -\nabla V$:

$$dX(t) = f(X(t))dt + \sigma dW(t), \quad X(0) = X_0 \in \mathbb{R}^d.$$

This is a stochastic differential equation (SDE). It means that X satisfies

$$X(t) = X(0) + \int_0^t f(X(s))ds + \int_0^t \sigma dW(s).$$

The overdamped Langevin equation in molecular dynamics

We consider the overdamped Langevin equation:

$$dX(t) = f(X(t))dt + \sigma dW(t),$$

where $f(x) = -\nabla V(x)$ and $\sigma > 0$.

Different types of convergence:

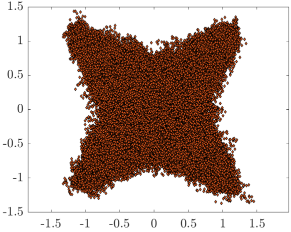
- Strong (approximation of a single trajectory for a realization of $W(t)$),
- Weak (approximation of the law of $X(t)$),
- Invariant measure (approximation of the law of $X(t)$ at equilibrium).

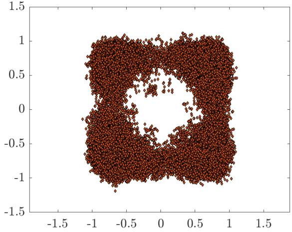
Example with a stiff potential

We consider the overdamped Langevin equation with $d = 2$

$$dX(t) = -\nabla V^\varepsilon(X(t))dt + \sigma dW(t), \quad V^\varepsilon(x) = \frac{1}{2\varepsilon}(|x|^2 - 1)^2 + 3(x_1^2 - x_2^2)^2.$$

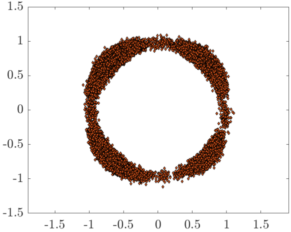
$\varepsilon = 1$

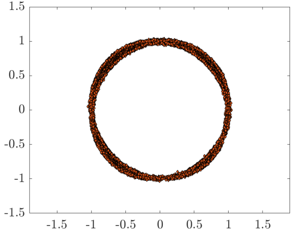




$\varepsilon = 0.1$

$\varepsilon = 0.01$





$\varepsilon = 0.001$

Constrained Langevin dynamics

Adding constraints $\zeta(X(t)) = 0$ with $\zeta \colon \mathbb{R}^d \to \mathbb{R}^q$ (e.g. strong covalent bonds between atoms, or fixed angles in molecules), the solution lies on the manifold $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$ and we get constrained Langevin dynamics:

$$dX(t) = \Pi_{\mathcal{M}}(X(t)) f(X(t)) dt + \sigma \Pi_{\mathcal{M}}(X(t)) \circ dW(t), \quad X(0) = X_0 \in \mathcal{M},$$

where $\Pi_{\mathcal{M}} : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ is the projection operator on the tangent bundle of $\mathcal{M}$.

Equivalent formulation, with $g = \nabla \zeta$:

$$dX(t) = f(X(t)) dt + \sigma dW(t) + g(X(t)) d\lambda_t, \quad \zeta(X(t)) = 0.$$

Constrained Langevin dynamics

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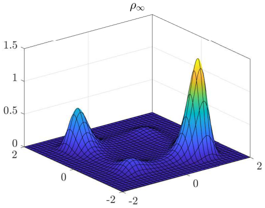
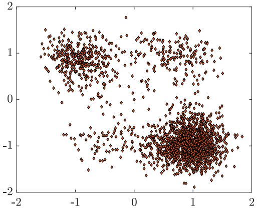
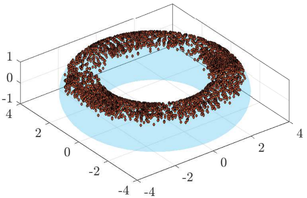
Ergodicity property:

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathcal{M}} \phi(y)\rho_\infty(y)d\sigma_{\mathcal{M}}(y) \quad \text{almost surely.}$$







Penalized Langevin dynamics

In practice, constraints are satisfied up to a parameter ε, and we obtain penalized Langevin dynamics:

$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

Penalized Langevin dynamics

Overdamped Langevin dynamics in $\mathbb{R}^d$:

$$dX = f(X)dt + \sigma dW.$$

Constrained overdamped Langevin equation on $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$:

$$dX^0 = f(X^0)dt + \sigma dW + g(X^0)d\lambda^0.$$

Penalized Langevin dynamics for simulating trajectories in the vicinity of the manifold $\mathcal{M}$, where $g = \nabla\zeta$ and $G = g^T g$:

$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

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$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

Theorem (Ciccotti, Lelièvre, Vanden-Eijnden, 2008)

Under technical assumptions, X^ε converges strongly to X^0, that is,

$$\sup_{t\leqslant T} \mathbb{E}\Big[\big|X^\varepsilon(t) - X^0(t)\big|^2 \Big] \leqslant C\varepsilon.$$

Moreover, $\zeta(X^\varepsilon(t))$ satisfies $\sup_{t\leqslant T} \mathbb{E}\Big[\big|\zeta(X^\varepsilon(t))\big|^2 \Big] \leqslant C\varepsilon.$

Penalized Langevin dynamics

Overdamped Langevin dynamics in $\mathbb{R}^d$:

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Question: can we create a numerical integrator for solving penalized dynamics, with the properties of

- accuracy and cost independent of ε?
- convergence to a consistent scheme on the manifold $\mathcal{M}$ when $\varepsilon \to 0$?

Contents

The Euler integrators in $\mathbb{R}^d$

We consider the penalized overdamped Langevin dynamics:

$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

The Euler-Maruyama method is given by

$$X_{n+1}^\varepsilon = X_n^\varepsilon + hf(X_n^\varepsilon) + \sigma\sqrt{h}\xi_n + h\frac{\sigma^2}{2}(G^{-1}g'g)(X_n^\varepsilon) - \frac{h}{\varepsilon}(gG^{-1}\zeta)(X_n^\varepsilon),$$

where h is the timestep and $\xi_n \sim \mathcal{N}(0, I_d)$ are independent Gaussian vectors.

Issue: the Euler scheme works for $\varepsilon = \mathcal{O}(1)$, but becomes unstable when $\varepsilon \to 0$.

The Euler integrators in $\mathbb{R}^d$

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Remark

Possible solution of the instability with the implicit Euler method?

$$X_{n+1}^\varepsilon = X_n^\varepsilon + hf(X_n^\varepsilon) + \sigma\sqrt{h}\xi_n + h\frac{\sigma^2}{2}(G^{-1}g'g)(X_n^\varepsilon) - \frac{h}{\varepsilon}(gG^{-1}\zeta)(X_{n+1}^\varepsilon),$$

Issue: stability does not guarantee accuracy.

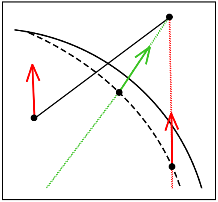
The Euler integrators for constrained Langevin dynamics

Langevin dynamics on manifold $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$

$$dX(t) = \Pi_{\mathcal{M}}(X(t))f(X(t))dt + \sigma\Pi_{\mathcal{M}}(X(t)) \circ dW(t).$$

Equivalent formulation with Lagrange multipliers

$$dX(t) = f(X(t))dt + \sigma dW(t) + g(X(t))d\lambda_t, \quad \zeta(X(t)) = 0.$$



Example (Euler integrators)

Two widely used integrators are the Euler scheme with explicit projection direction, where $g = \nabla\zeta$

$$X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\xi_n + \lambda g(X_n), \quad \zeta(X_{n+1}) = 0,$$

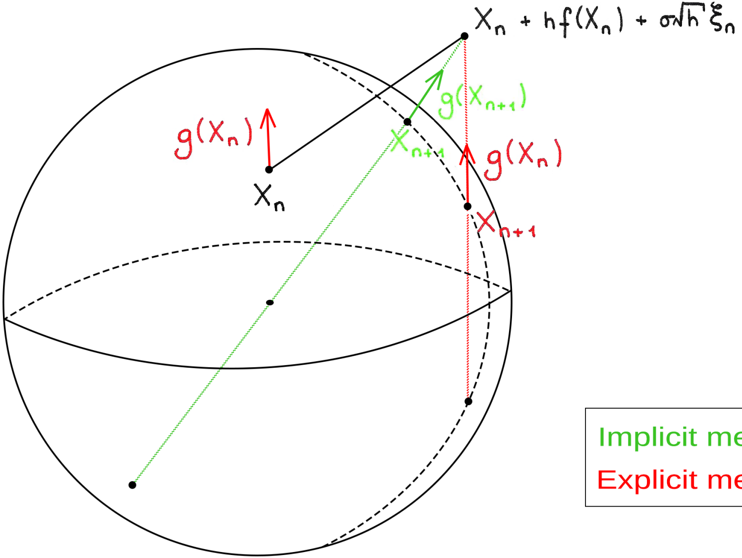
and alternatively the Euler scheme with implicit projection direction

$$X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\xi_n + \lambda g(X_{n+1}), \quad \zeta(X_{n+1}) = 0.$$

References: Ciccotti, Kapral, Vanden-Eijnden, 2005; Lelièvre, Le Bris, Vanden-Eijnden, 2008; Lelièvre, Rousset, Stolz, 2010; ...

Issue: The schemes work for $\varepsilon \to 0$, but become inaccurate when $\varepsilon = \mathcal{O}(1)$.

The Euler integrators for constrained Langevin dynamics



Implicit method
Explicit method

Standard integrators for penalized Langevin

Penalized Langevin dynamics:

$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

Euler-Maruyama integrator in $\mathbb{R}^d$ - accurate when $h \ll \varepsilon$, blow-up when $\varepsilon \to 0$:

$$X_{n+1} = X_n + \sqrt{h}\sigma\xi + hf(X_n) + h\frac{\sigma^2}{2}(G^{-1}g'g)(X_n) - \frac{h}{\varepsilon}(gG^{-1}\zeta)(X_n).$$

Constrained Euler scheme on $\mathcal{M}$ - accurate when $\varepsilon \to 0$, inaccurate else:

$$X^0_{n+1} = X^0_n + \sqrt{h}\sigma\xi + hf(X^0_n) + g(X^0_n)\lambda^0, \quad \zeta(X^0_{n+1}) = 0.$$

Standard integrators for penalized Langevin

Penalized Langevin dynamics:

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$$X^0_{n+1} = X^0_n + \sqrt{h}\sigma\xi + hf(X^0_n) + g(X^0_n)\lambda^0, \quad \zeta(X^0_{n+1}) = 0.$$

Question: is it possible to create a consistent integrator with an accuracy independent on ε?

$$\begin{array}{ccc} \text{integrator } (X^\varepsilon_n)_n \text{ in } \mathbb{R}^d & \xrightarrow{\varepsilon\to 0} & \text{integrator } (X^0_n)_n \text{ on } \mathcal{M} \\ \Big\downarrow{\scriptstyle h\to 0} & & \Big\downarrow{\scriptstyle h\to 0} \\ \text{penalized dynamic } X^\varepsilon(t) \text{ in } \mathbb{R}^d & \xrightarrow{\varepsilon\to 0} & \text{constrained dynamic } X^0(t) \text{ on } \mathcal{M} \end{array}$$

Standard integrators for penalized Langevin

Penalized Langevin dynamics:

$$dX^\varepsilon = f(X^\varepsilon)dt + \sigma dW + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt,$$

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Constrained Euler scheme on $\mathcal{M}$ - accurate when $\varepsilon \to 0$, inaccurate else:

$$X^0_{n+1} = X^0_n + \sqrt{h}\sigma\xi + hf(X^0_n) + g(X^0_n)\lambda^0, \quad \zeta(X^0_{n+1}) = 0.$$

Related works on multiscale problems:

- Highly-oscillatory problems: $\partial_t u = \frac{i}{\varepsilon}\Delta u + F(u)$ (Chartier, Lemou, Méhats, Vilmart, 2020; Chartier, Lemou, Trémant, 2020; Laurent, Vilmart, 2020; Almuslimani, Chartier, Lemou, Méhats, 2020; ...)
- Kinetic PDEs: $\partial_t u + \frac{1}{\varepsilon}a(v)\nabla_x u = \dots$ (Crouseilles, Hivert, Lemou, 2015; Bréhier, Rakotonirina-Ricquebourg, 2020; ...)

Contents

A new uniformly accurate integrator

New method

$$X_{n+1}^\varepsilon = X_n^\varepsilon + \sqrt{h}\sigma\xi_n + hf(X_n^\varepsilon) + \frac{(1-e^{-h/\varepsilon})^2}{2}(\zeta^2 G^{-2} g'g)(X_n^\varepsilon)$$
$$+ \frac{\sigma^2\varepsilon}{4}(1-e^{-2h/\varepsilon})(G^{-1}g'g)(X_n^\varepsilon) + g(X_n^\varepsilon)\lambda^\varepsilon,$$
$$\zeta(X_{n+1}^\varepsilon) = e^{-h/\varepsilon}\zeta(X_n^\varepsilon) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^\varepsilon)\xi_n$$
$$+ \varepsilon(1-e^{-h/\varepsilon})(g^T f + \frac{\sigma^2}{2}G^{-1}g^T g'g + \frac{\sigma^2}{2}\operatorname{div}(g))(X_n^\varepsilon).$$

This discretization solves with uniform accuracy the penalized Langevin dynamics:

$$dX^\varepsilon = \sigma dW + f(X^\varepsilon)dt + \frac{\sigma^2}{2}(G^{-1}g'g)(X^\varepsilon)dt - \frac{1}{\varepsilon}(gG^{-1}\zeta)(X^\varepsilon)dt.$$

Idea: project a modified step of the Euler method on a modified manifold $\mathcal{M}^\varepsilon$ that is close to $\mathcal{M}$ when $\varepsilon \to 0$.

A new uniformly accurate integrator

New method

$$
\begin{aligned}
X_{n+1}^\varepsilon &= X_n^\varepsilon + \sqrt{h}\sigma\xi_n + hf(X_n^\varepsilon) + \frac{(1-e^{-h/\varepsilon})^2}{2}(\zeta^2 G^{-2} g' g)(X_n^\varepsilon) \\
&\quad + \frac{\sigma^2\varepsilon}{4}(1-e^{-2h/\varepsilon})(G^{-1}g'g)(X_n^\varepsilon) + g(X_n^\varepsilon)\lambda^\varepsilon, \\
\zeta(X_{n+1}^\varepsilon) &= e^{-h/\varepsilon}\zeta(X_n^\varepsilon) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^\varepsilon)\xi_n \\
&\quad + \varepsilon(1-e^{-h/\varepsilon})(g^T f + \frac{\sigma^2}{2}G^{-1}g^T g' g + \frac{\sigma^2}{2}\operatorname{div}(g))(X_n^\varepsilon).
\end{aligned}
$$

Theorem (L., 2021)

Under technical assumptions, the new integrator (X_n^ε) is a consistent uniformly accurate approximation of the penalized Langevin dynamic $X^\varepsilon(t)$, that is,

$$
|\mathbb{E}[\phi(X_n^\varepsilon)] - \mathbb{E}[\phi(X^\varepsilon(nh))]| \leqslant C\sqrt{h}, \quad n = 0, 1, \dots, N,
$$

where C is independent of ε.

A new uniformly accurate integrator

New method

$$X_{n+1}^{\varepsilon} = X_n^{\varepsilon} + \sqrt{h}\sigma\xi_n + hf(X_n^{\varepsilon}) + \frac{(1-e^{-h/\varepsilon})^2}{2}(\zeta^2 G^{-2} g' g)(X_n^{\varepsilon})$$
$$+ \frac{\sigma^2 \varepsilon}{4}(1-e^{-2h/\varepsilon})(G^{-1} g' g)(X_n^{\varepsilon}) + g(X_n^{\varepsilon})\lambda^{\varepsilon},$$
$$\zeta(X_{n+1}^{\varepsilon}) = e^{-h/\varepsilon}\zeta(X_n^{\varepsilon}) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^{\varepsilon})\xi_n$$
$$+ \varepsilon(1-e^{-h/\varepsilon})(g^T f + \frac{\sigma^2}{2} G^{-1} g^T g' g + \frac{\sigma^2}{2}\operatorname{div}(g))(X_n^{\varepsilon}).$$

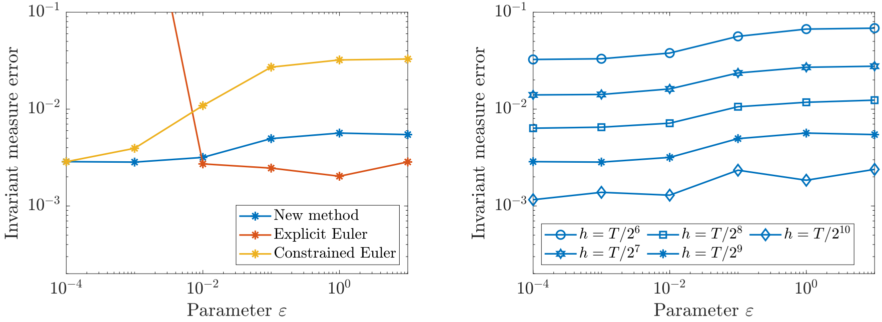
Theorem (L., 2021)

Under technical assumptions, the integrator $(X_n^{\varepsilon})_n$ *lies on the manifold when* $\varepsilon \to 0$ *and converges strongly to the constrained Euler scheme given by*

$$X_{n+1}^0 = X_n^0 + \sqrt{h}\sigma\xi + hf(X_n^0) + g(X_n^0)\lambda^0, \quad \zeta(X_{n+1}^0) = 0.$$

Numerical experiments - Invariant measure on the torus

We approximate $\int_{\mathbb{R}^d} \phi(x)\rho_\infty^\varepsilon(x)dx$ with the estimator $J = \frac{1}{M}\sum_{m=1}^M \phi(X_N^{(m)})$ when $\mathcal{M}$ is a torus in $\mathbb{R}^3$, and with the constraint $\zeta(x) = (|x|^2 + 8)^2 - 36(x_1^2 + x_2^2)$, the map $f(x) = -25(x_1 - 2, x_2, x_3)$, and $M = 10^7$ trajectories.



We observe the uniform accuracy of the new method and the loss of accuracy of the Euler schemes in $\mathbb{R}^d$ and on the manifold.

Numerical experiments - Orthogonal group

We compute the weak error when $\mathcal{M}$ is the orthogonal group

$$O(m) = \{M \in \mathbb{R}^{m\times m}, M^T M = I_m\},$$

with the potential $V(x) = 50|x - I_{m^2}|^2$, the map $f = -\nabla V$, $M = 10^6$ trajectories, the stiff parameter $\varepsilon = 0.005$ and the timestep $h = 2^{-7} \approx \varepsilon$.

m	$\dim(\mathcal{M})$	q	$J(m)$	error for $\bar{J}_{UA}$	error for $\bar{J}_{EC}$
2	1	3	2.00934	$3.1 \cdot 10^{-3}$	$1.8 \cdot 10^{-2}$
3	3	6	3.01458	$6.4 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$
4	6	10	4.02050	$1.1 \cdot 10^{-2}$	$7.2 \cdot 10^{-2}$
5	10	15	5.02669	$1.8 \cdot 10^{-2}$	$1.1 \cdot 10^{-1}$

Remark: the Euler scheme in $\mathbb{R}^d$ blows up for the chosen parameters.

Conclusion and outlook

Summary:

- We introduced a new integrator for the approximation of penalized Langevin dynamics with uniform accuracy.
- The scheme is a projection method with a modified constraint.
- We obtain weak consistency, and the method converges strongly to the Euler scheme on $\mathcal{M}$ when $\varepsilon \to 0$. The integrator and its analysis work for problems of any dimension and codimension.

Outlooks and future works:

- High order UA integrators for penalized Langevin dynamics.
- Generalized unified class of Runge-Kutta methods for approximating Langevin dynamics in $\mathbb{R}^d$, on manifolds and in the vicinity of manifolds.
- Work in progress (with H. Munthe-Kaas, J. Stava, G. Vega-Molino): Lie-group methods for Langevin dynamics.
- Work in progress (with I. Almuslimani): UA integrator for SDEs with fast stochastic oscillation.

UA integrator in arbitrary codimension

UA method

$$X_{n+1}^{\varepsilon} = X_n^{\varepsilon} + \sqrt{h}\sigma\xi_n + hf(X_n^{\varepsilon}) + \frac{(1-e^{-h/\varepsilon})^2}{2}(g'(gG^{-1}\zeta)G^{-1}\zeta)(X_n^{\varepsilon})$$
$$+ \frac{\sigma^2\varepsilon}{8}(1-e^{-2h/\varepsilon})\nabla \ln(\det(G))(X_n^{\varepsilon}) + g(X_n^{\varepsilon})\lambda^{\varepsilon},$$

$$\zeta(X_{n+1}^{\varepsilon}) = e^{-h/\varepsilon}\zeta(X_n^{\varepsilon}) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^{\varepsilon})\xi_n$$
$$+ \varepsilon(1-e^{-h/\varepsilon})\Big(g^T f + \frac{\sigma^2}{4}g^T\nabla \ln(\det(G)) + \frac{\sigma^2}{2}\operatorname{div}(g)\Big)(X_n^{\varepsilon})$$
$$+ \sigma^2\left(\varepsilon(1-e^{-h/\varepsilon}) - \sqrt{\frac{\varepsilon h}{2}(1-e^{-2h/\varepsilon})}\right)$$
$$\times \sum_{i=1}^{d}[((g'(gG^{-1}g^T e_i))^T gG^{-1}g^T e_i)(X_n^{\varepsilon}) - ((g'(e_i))^T gG^{-1}g^T e_i)(X_n^{\varepsilon})].$$

Idea of the proof - Change of coordinate

- Assume there exists a smooth change of coordinate

$$\psi(x) = \begin{pmatrix} \varphi(x) \\ \zeta(x) \end{pmatrix}, \quad \text{with} \quad \varphi' g = 0.$$

- In these coordinates, the penalized Langevin dynamics rewrite into

$$\begin{aligned} d\varphi(X^\varepsilon) &= (\varphi' f)(X^\varepsilon)dt + \sigma\varphi'(X^\varepsilon)dW + \frac{\sigma^2}{4}(\varphi'(\nabla \ln(\det(G))))(X^\varepsilon)dt \\ &\quad + \frac{\sigma^2}{2}\Delta\varphi(X^\varepsilon)dt, \\ d\zeta(X^\varepsilon) &= (g^T f)(X^\varepsilon)dt + \sigma g^T(X^\varepsilon)dW + \frac{\sigma^2}{2}(G^{-1}g^T g' g)(X^\varepsilon)dt \\ &\quad + \frac{\sigma^2}{2}\operatorname{div}(g)(X^\varepsilon)dt - \frac{1}{\varepsilon}\zeta(X^\varepsilon)dt. \end{aligned}$$

Idea of the proof - Change of coordinate

- Assume there exists a smooth change of coordinate

$$\psi(x) = \begin{pmatrix} \varphi(x) \\ \zeta(x) \end{pmatrix}, \quad \text{with} \quad \varphi' g = 0.$$

- In these coordinates, the penalized Langevin dynamics rewrite into

$$\begin{aligned} d\varphi(X^\varepsilon) &= (\varphi' f)(X^\varepsilon)dt + \sigma\varphi'(X^\varepsilon)dW + \frac{\sigma^2}{4}(\varphi'(\nabla \ln(\det(G))))(X^\varepsilon)dt \\ &\quad + \frac{\sigma^2}{2}\Delta\varphi(X^\varepsilon)dt, \\ d\zeta(X^\varepsilon) &= (g^T f)(X^\varepsilon)dt + \sigma g^T(X^\varepsilon)dW + \frac{\sigma^2}{2}(G^{-1}g^T g' g)(X^\varepsilon)dt \\ &\quad + \frac{\sigma^2}{2}\operatorname{div}(g)(X^\varepsilon)dt - \frac{1}{\varepsilon}\zeta(X^\varepsilon)dt. \end{aligned}$$

- The variation of constants formula yields

$$\begin{aligned} \zeta(X^\varepsilon(t)) &= e^{-t/\varepsilon}\zeta(X^\varepsilon(0)) + \sigma\int_0^t e^{(s-t)/\varepsilon} g^T(X^\varepsilon(s))dW \\ &\quad + \int_0^t e^{(s-t)/\varepsilon}\Big[g^T f + \frac{\sigma^2}{2}G^{-1}g^T g' g + \frac{\sigma^2}{2}\operatorname{div}(g)\Big](X^\varepsilon(s))dt, \end{aligned}$$

Idea of the proof - Change of coordinate

UA method

$$X_{n+1}^\varepsilon = X_n^\varepsilon + \sqrt{h}\sigma\xi_n + hf(X_n^\varepsilon) + \frac{(1-e^{-h/\varepsilon})^2}{2}(\zeta^2 G^{-2} g' g)(X_n^\varepsilon)$$
$$+ \frac{\sigma^2\varepsilon}{4}(1-e^{-2h/\varepsilon})(G^{-1}g'g)(X_n^\varepsilon) + g(X_n^\varepsilon)\lambda^\varepsilon,$$
$$\zeta(X_{n+1}^\varepsilon) = e^{-h/\varepsilon}\zeta(X_n^\varepsilon) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^\varepsilon)\xi_n$$
$$+ \varepsilon(1-e^{-h/\varepsilon})(g^T f + \frac{\sigma^2}{2}G^{-1}g^T g' g + \frac{\sigma^2}{2}\operatorname{div}(g))(X_n^\varepsilon).$$

- The variation of constants formula yields

$$\zeta(X^\varepsilon(t)) = e^{-t/\varepsilon}\zeta(X^\varepsilon(0)) + \sigma\int_0^t e^{(s-t)/\varepsilon} g^T(X^\varepsilon(s))dW$$
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Idea of the proof - Uniform weak expansion

Proposition

The solution of the penalized Langevin dynamics satisfies the uniform weak expansion

$$\left|\mathbb{E}[\phi(X^\varepsilon(h))] - \mathbb{E}[\phi(x + \sqrt{h}A_h^\varepsilon(x) + hB_h^\varepsilon(x))]\right| \leqslant C(1+|x|^K)h^{3/2},$$

where

$$A_h^\varepsilon = \sigma\xi + \frac{e^{-h/\varepsilon}-1}{\sqrt{h}}gG^{-1}\zeta + \sigma\left(\sqrt{\frac{\varepsilon}{2h}(1-e^{-2h/\varepsilon})}-1\right)gG^{-1}g^T\xi$$

Idea of the proof - Uniform weak expansion

Proposition

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UA method

$$X_{n+1}^\varepsilon = X_n^\varepsilon + \sqrt{h}\sigma\xi_n + h[\dots] + g(X_n^\varepsilon)\lambda^\varepsilon,$$

$$\zeta(X_{n+1}^\varepsilon) = e^{-h/\varepsilon}\zeta(X_n^\varepsilon) + \sigma\sqrt{\frac{\varepsilon}{2}(1-e^{-2h/\varepsilon})}g^T(X_n^\varepsilon)\xi_n$$

$$+ \varepsilon(1-e^{-h/\varepsilon})(g^Tf + \frac{\sigma^2}{2}G^{-1}g^Tg'g + \frac{\sigma^2}{2}\operatorname{div}(g))(X_n^\varepsilon).$$