Optimizing the diffusion for sampling with overdamped Langevin dynamics

Gabriel STOLTZ

(CERMICS, Ecole des Ponts & MATHERIALS team, Inria Paris)

In collaboration with Tony Lelièvre, Greg Pavliotis, Geneviève Robin and Régis Santet

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Outline

- **Overdamped Langevin dynamics**
  - General diffusion coefficients
  - Convergence rates

Characterization of the optimal diffusion
  - Normalization of the diffusion
  - Necessary conditions
  - Approximation in the homogenized limit

Numerical results
  - Numerical approximation of the optimal diffusion
  - Numerical integration of overdamped Langevin dynamics
  - Efficiency gains from optimized diffusions

T. Lelièvre, G. A. Pavliotis, G. Robin, R. Santet and G. Stoltz, Optimizing the diffusion of overdamped Langevin dynamics, *arXiv preprint* **2404.12087**

Overdamped Langevin dynamics

Computing average properties

Aim: Sample target measure $\mu(dq) = Z_\mu^{-1} \mathrm{e}^{-\beta V(q)} \, dq$ on $\mathcal{Q} = \mathbb{T}^d$
(assume $Z_\mu = 1$ in the remainder; configuration space = torus)

Main issue

Computation of high-dimensional integrals... Ergodic averages

$$\mathbb{E}_\mu(\varphi) = \lim_{t \to +\infty} \widehat{\varphi}_t, \qquad \widehat{\varphi}_t = \frac{1}{t} \int_0^t \varphi(q_s) \, ds$$

• One possible choice: overdamped Langevin dynamics
= Stochastic perturbation of gradient dynamics

$$dq_t = -\nabla V(q_t) \, dt + \sqrt{\frac{2}{\beta}} \, dW_t$$

• Other choices include Metropolis-like schemes

Properties of the standard overdamped Langevin dynamics

Generator $\mathcal{L} = -\nabla V(q) \cdot \nabla_q + \frac{1}{\beta}\Delta_q$

- elliptic generator hence irreducibility and ergodicity
- adjoints on $L^2(\mathcal{Q})$ versus $L^2(\mu)$

$$\int_{\mathcal{Q}} (\mathcal{L}f)\, g = \int_{\mathcal{Q}} f \left(\mathcal{L}^\dagger g\right), \qquad \int_{\mathcal{Q}} (\mathcal{L}f)\, g \, d\mu = \int_{\mathcal{Q}} f \left(\mathcal{L}^\star g\right) d\mu$$

- flat adjoint $\mathcal{L}^\dagger \varphi = \mathrm{div}_q \left((\nabla V)\varphi + \frac{1}{\beta}\nabla_q \varphi \right)$
- self-adjoint operator on $L^2(\mu)$, hence reversibility

$$\mathcal{L} = -\frac{1}{\beta}\nabla_q^\star \nabla_q = -\frac{1}{\beta}\sum_{i=1}^d \partial_{q_i}^\star \partial_{q_i} = \mathcal{L}^\star, \qquad \partial_{q_i}^\star = -\partial_{q_i} + \beta \partial_{q_i} V$$

Invariance of canonical measure encoded as $\mathcal{L}^\dagger \mu$ or $\mathcal{L}^\star \mathbf{1} = 0$

$$\frac{d}{dt}\left[\mathbf{E}_\mu\left(\varphi(X_t)\right)\right] = \frac{d}{dt}\left(\int_{\mathcal{Q}} \mathrm{e}^{t\mathcal{L}}\varphi \, d\mu\right) = \int_{\mathcal{Q}} \mathcal{L}\left(\mathrm{e}^{t\mathcal{L}}\varphi\right) d\mu = 0$$

Overdamped Langevin dynamics with multiplicative noise

Diffusion matrix $\mathcal{D}(q) \in \mathbb{R}^d$ (symmetric positive, not necessarily definite)

$$dq_t = \left(-\mathcal{D}(q_t)\nabla V(q_t) + \frac{1}{\beta}\mathrm{div}\mathcal{D}(q_t)\right) dt + \sqrt{\frac{2}{\beta}}\mathcal{D}^{1/2}(q_t)\, dW_t$$

with $\mathrm{div}\,\mathcal{D}$ the vector whose i-th component is the divergence of the i-th column of the matrix $\mathcal{D} = [\mathcal{D}_1, \ldots, \mathcal{D}_d]$

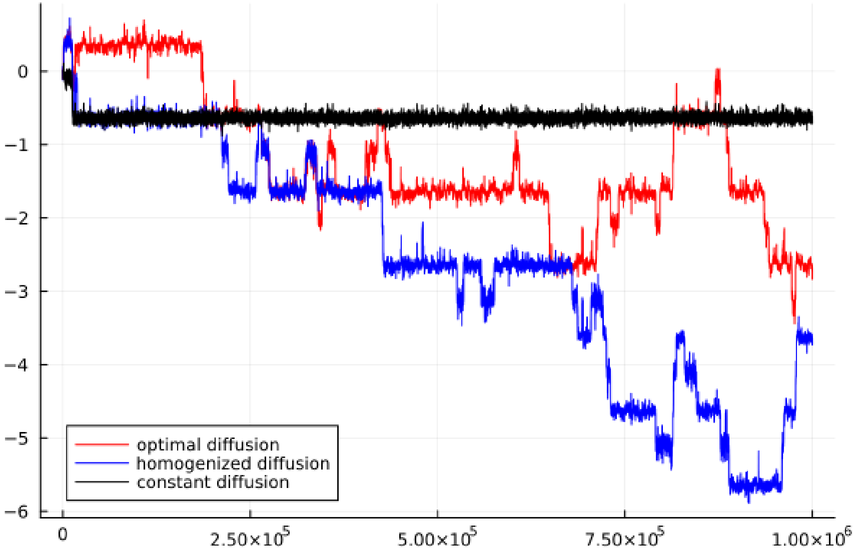
Two possible motivations:

- Compensate for anisotropic potential energy landscapes
- Reduce metastability

Generator still self-adjoint, invariant probability measure μ

$$\mathcal{L}_{\mathcal{D}} = -\frac{1}{\beta}\nabla^\star \mathcal{D}\nabla = -\frac{1}{\beta}\sum_{i,j=1}^{d} \partial_{q_j}^\star \mathcal{D}_{i,j}\partial_{q_i}$$

Behavior of overdamped Langevin dynamics for various $\mathcal{D}$



Convergence of overdamped Langevin dynamics

Various measures of convergence, for instance

- asymptotic variance in central limit theorem
- convergence of the law at time t to the stationary distribution
- average exit time of a metastable well

Here: second option, in a $L^2(\mu)$ framework

Law at time t written as $\psi(t) = f(t)\mu$, so that $f(t) = \mathrm{e}^{t\mathcal{L}_{\mathcal{D}}} f(0)$

$$\mathbf{E}_{\psi(0)}\left(\varphi(X_t)\right) = \int_{\mathcal{Q}} \varphi\, f(t)\, d\mu = \int_{\mathcal{Q}} \mathrm{e}^{t\mathcal{L}_{\mathcal{D}}}\varphi\, f(0)\, d\mu$$

Typical convergence result: exponential convergence rate for $\mathrm{e}^{t\mathcal{L}_{\mathcal{D}}}$

$$\|f(t) - \mathbf{1}\|_{L^2(\mu)} = \left\|\mathrm{e}^{t\mathcal{L}_{\mathcal{D}}}\left(f(0) - \mathbf{1}\right)\right\|_{L^2(\mu)} \leqslant \mathrm{e}^{-\Lambda(\mathcal{D})t/\beta}\|f(0) - \mathbf{1}\|_{L^2(\mu)}$$

Implies bounds on the asymptotic variance

Obtaining an exponential rate of convergence

Spectral gap on $H_0^1(\mu) = \left\{ u \in H^1(\mu) \,\middle|\, \int_{\mathbb{T}^d} u(q)\,\mu(q)\,dq = 0 \right\}$

$$\Lambda(\mathcal{D}) = \inf_{u \in H_0^1(\mu)\setminus\{0\}} \frac{\displaystyle\int_{\mathbb{T}^d} \nabla u(q)^\top \mathcal{D}(q) \nabla u(q)\,\mu(q)\,dq}{\displaystyle\int_{\mathbb{T}^d} u(q)^2 \mu(q)\,dq}$$

Desired inequality follows from a Gronwall estimate and

$$\frac{d}{dt}\left(\frac{1}{2}\left\|\mathrm{e}^{t\mathcal{L}_\mathcal{D}}\varphi\right\|^2_{L^2(\mu)}\right) = \left\langle \mathrm{e}^{t\mathcal{L}_\mathcal{D}}\varphi, \mathcal{L}_\mathcal{D}\,\mathrm{e}^{t\mathcal{L}_\mathcal{D}}\varphi \right\rangle_{L^2(\mu)} \leqslant -\frac{\Lambda(\mathcal{D})}{\beta}\left\|\mathrm{e}^{t\mathcal{L}_\mathcal{D}}\varphi\right\|^2_{L^2(\mu)}$$

Criterion to choose $\mathcal{D}$

Maximize the spectral gap $\Lambda(\mathcal{D})$

Possible choices:

- $\mathcal{D} = \left(\nabla^2 V\right)^{-1}$ for strongly convex potentials [Girolami/Calderhead 2011]
- $\mathcal{D} = \mathrm{e}^{\beta V}$ [Roberts/Stramer 2002, Ghimenti/van Wijland/... 2023]

Characterization of the optimal diffusion

Need for normalization

Motivation: $\Lambda(\alpha\mathcal{D}) = \alpha\Lambda(\mathcal{D})$ and large $\mathcal{D}$ require smaller timesteps

L^∞ bounds trivial (saturate the constraint)

Chosen normalization: $L^p_V(\mathbb{T}^d, \mathcal{M}_{a,b})$ (note $\mathcal{Q} = \mathbb{T}^d$), with associated norm

$$\|\mathcal{D}\|_{L^p_V} = \left(\int_{\mathbb{T}^d} |\mathcal{D}(q)|_{\mathrm{F}}^p \, \mathrm{e}^{-\beta p V(q)} \, dq \right)^{1/p}$$

and requirement $\mathrm{e}^{-\beta V}\mathcal{D} \in \mathcal{M}_{a,b}$ with (for $a, b \geqslant 0$)

$$\mathcal{M}_{a,b} = \left\{ M \in \mathcal{S}_d^+ \,\middle|\, \forall \xi \in \mathbb{R}^d, \ a|\xi|^2 \leqslant \xi^\top M \xi \leqslant \frac{1}{b}|\xi|^2 \right\}$$

Matrix norm compatible with order on symmetric positive matrices

Maximization performed on

$$\mathfrak{D}_p^{a,b} = \left\{ \mathcal{D} \in L^\infty_V(\mathbb{T}^d, \mathcal{M}_{a,b}) \,\middle|\, \int_{\mathbb{T}^d} |\mathcal{D}(q)|_{\mathrm{F}}^p \, \mathrm{e}^{-\beta p V(q)} \, dq \leqslant 1 \right\}$$

Well posedness of the maximization problem

Existence of maximizer for $p \in [1, +\infty)$: For any $a \in [0, |\mathrm{Id}_d|_{\mathrm{F}}^{-1}]$ and $b > 0$ such that $ab \leqslant 1$, there exists $\mathcal{D}_p^\star \in \mathfrak{D}_p^{a,b}$ such that

$$\Lambda(\mathcal{D}_p^\star) = \sup_{\mathcal{D} \in \mathfrak{D}_p^{a,b}} \Lambda(\mathcal{D})$$

Moreover, for any open set $\Omega \subset \mathbb{T}^d$, there exists $q \in \Omega$ such that $\mathcal{D}_p^\star(q) \neq 0$.

Main arguments/properties:

- Λ is bounded (Poincaré inequality)
- Λ is concave (sup of linear functions in $\mathcal{D}$)
- Λ is upper semicontinuous for the weak-* L_V^∞ topology $(b > 0)$
- the set $\mathfrak{D}_p^{a,b}$ is compact for the weak-* L_V^∞ topology

Characterization of positive optimal diffusions (1/2)

Uniformly positive optimal diffusions $\mathcal{D}_p^\star$ lead to degenerate eigenvalues

Precise statement:

- Frobenius norm $|\cdot|_{\mathrm{F}}$, Lebesgue exponent $p \in (1,+\infty)$ and $a = 0$
- assume that there exists a maximizer $\mathcal{D}_p^\star$ of Λ on $\mathfrak{D}_p^{a,b}$, with $\mathcal{D}^\star(q)\,\mathrm{e}^{-V(q)} \leqslant \frac{1}{b_+}\,\mathrm{Id}_d$ for $b_+ > b$
- additionally $\mathcal{D}_p^\star \in C^0(\mathbb{T},\mathbb{R}_+)$ when $d = 1$

If $\mathcal{D}_p^\star \geqslant c\mathrm{Id}_d$, then $\Lambda(\mathcal{D}_p^\star)$ is a degenerate eigenvalue of $-\beta\mathcal{L}_{\mathcal{D}_p^\star}$.

Idea of proof: Proceed by contradiction and assume that the eigenvalue is simple. From the Euler–Lagrange equation (regular perturbation theory)

$$\int_{\mathbb{T}^d} \delta\mathcal{D}(q) : \left(\nabla u_{\mathcal{D}_p^\star} \otimes \nabla u_{\mathcal{D}_p^\star}\right) \mu(q)\,dq = p\gamma \int_{\mathbb{T}^d} \left|\mathcal{D}_p^\star(q)\right|_{\mathrm{F}}^{p-2} \mathcal{D}_p^\star(q) : \delta\mathcal{D}(q)\,\mathrm{e}^{-\beta p V(q)}\,dq,$$

so that $\mathcal{D}_p^\star = \alpha_p \left|\mathcal{D}_p^\star\right|_{\mathrm{F}}^{2-p} \mathrm{e}^{\beta(p-1)V} \nabla u_{\mathcal{D}_p^\star} \otimes \nabla u_{\mathcal{D}_p^\star}$, contradicting $\mathcal{D}_p^\star(q) \geqslant c\mathrm{Id}_d$

Characterization of positive optimal diffusions (2/2)

Difficulty: Cannot directly rely on Euler–Lagrange equation

Strategy: $\max_{\mathcal{D}\in\mathfrak{D}_p^{a,b}} f_\alpha$ = regularize using softmax and pass to the limit[1]

$$f_\alpha(\mathcal{D}) = \frac{\mathrm{Tr}_{L^2(\mu)}(\mathcal{L}_\mathcal{D}\mathrm{e}^{\alpha\mathcal{L}_\mathcal{D}})}{\mathrm{Tr}_{L^2(\mu)}(\mathrm{e}^{\alpha\mathcal{L}_\mathcal{D}})-1} = \frac{N_2\lambda_2 + \sum_{i\geqslant 3} N_i\lambda_i\mathrm{e}^{\alpha(\lambda_i-\lambda_2)}}{N_2 + \sum_{i\geqslant 3} N_i\mathrm{e}^{\alpha(\lambda_i-\lambda_2)}} \xrightarrow[\alpha\to+\infty]{} \lambda_2$$

Can write Euler–Lagrange condition for f_α using spectral calculus

$$\mathcal{D}^\star_{p,\alpha} = \gamma_{p,\alpha}\left|\mathcal{D}^\star_{p,\alpha}\right|_{\mathrm{F}}^{2-p}\mathrm{e}^{\beta(p-1)V}\sum_{k\geqslant 2}\left[\frac{G_\alpha(1+\alpha\lambda_{k,\alpha})-\alpha H_\alpha}{G_\alpha^2}\mathrm{e}^{\alpha\lambda_{k,\alpha}}\right]\nabla e_{k,\alpha}\otimes\nabla e_{k,\alpha}$$

with $G_\alpha = \sum_{j\geqslant 2} N_j\mathrm{e}^{\alpha\lambda_{j,\alpha}}$, $H_\alpha = \sum_{j\geqslant 2} N_j\lambda_j\mathrm{e}^{\alpha\lambda_{j,\alpha}}$; limit depends on $\lim_{\alpha\to+\infty}\alpha(\lambda_{j,\alpha}-\lambda_{2,\alpha})$

Typical example: $d=1$, degeneracy of order 2 of first non zero eigenvalue

$$\mathcal{D}^\star_{p,\infty}(q) = \tilde{\gamma}_{p,\infty}\mathrm{e}^{\beta V(q)}\left(\left|e'_{2,\infty}(q)\right|^2 + \frac{\mathrm{e}^\eta(1+\mathrm{e}^\eta+\eta)}{1+\mathrm{e}^\eta-\eta\mathrm{e}^\eta}\left|e'_{3,\infty}(q)\right|^2\right)^{1/(p-1)}$$

Second term vanishes for a value $\eta^\star \approx 1.27$

[1] Thank you Danny Perez for suggesting this!!

Approximation by homogenization theory

Diffusive time rescaling $\varepsilon q_{t/\varepsilon^2} \Rightarrow \overline{\mathcal{D}}^{1/2} B_t$ for effective diffusion $\overline{\mathcal{D}}$

Homogenized limit: for fixed $\mathcal{D}$,

- decrease the period: $\mathcal{D}_{\#,k}(q) = \mathcal{D}(kq)$ and $V_{\#,k}(q) = V(kq)$
- associated spectral gap

$$\Lambda_{\#,k}(\mathcal{D}) = \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\displaystyle\int_{\mathbb{T}^d} \nabla u^\top \mathcal{D}_{\#,k} \nabla u \, \mathrm{e}^{-\beta V_{\#,k}}}{\displaystyle\int_{\mathbb{T}^d} u^2 \, \mathrm{e}^{-\beta V_{\#,k}}} \,\middle|\, \int_{\mathbb{T}^d} u \, \mathrm{e}^{-\beta V_{\#,k}} = 0 \right\}$$

- converges to $\Lambda_{\mathrm{hom}}(\mathcal{D})$, spectral gap of $-\mathcal{L}_{\overline{\mathcal{D}}}$ on $L^2(\mathbb{T}^d)$ with (1D case)

$$\overline{\mathcal{D}} = \int_{\mathbb{T}^d} \mathcal{D}(q) \left(1 - w_{\mathcal{D}}'(q)^2\right) \mu(q) \, dq, \qquad \left[\mathrm{e}^{-\beta V} \mathcal{D}(1 + w_{\mathcal{D}}')\right]' = 0$$

Commutation optimization/homogenization: maximize $\Lambda_{\mathrm{hom}}(\mathcal{D})$

$$\mathcal{D}_{\mathrm{hom}}^\star(q) = \mathrm{e}^{\beta V(q)}$$

Numerical results

Numerical discretization

Maximization of the spectral gap

- D piecewise constant, on uniform mesh
- finite element approximation of test functions/eigenfunctions
- Sequential Least Squares Quadratic Programming algorithm for nonlinear eigenvalue problem with constraints

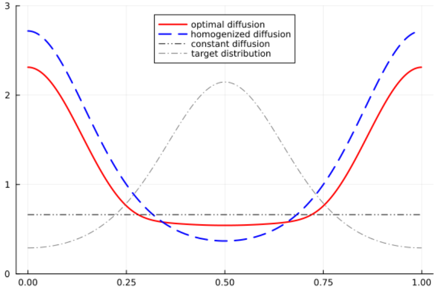
$$A(D)U_D = \lambda(D)BU_D, \qquad U_D^\top BU_D = \mathrm{Id}$$

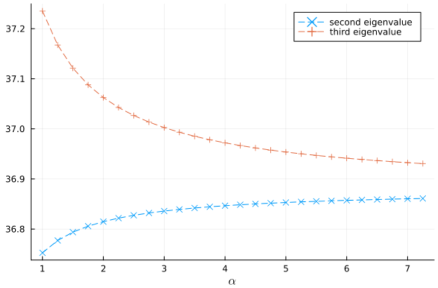
Discretization of the SDE

- use Metropolis acceptance/rejection to ensure unbiased sampling
- rejection probability $\mathrm{O}(\sqrt{\Delta t})$ for proposals based on naive Euler–Maruyama discretization
- lowered to $\mathrm{O}(\Delta t^{3/2})$ with dedicated (implicit) HMC algorithms[2]

[2] Noble/De Bortoli/Durmus (2022), Lelièvre/Santet/Stoltz (2023)

Potential $V(q) = \cos(2\pi q)$ $\qquad \eta \approx 0.51$

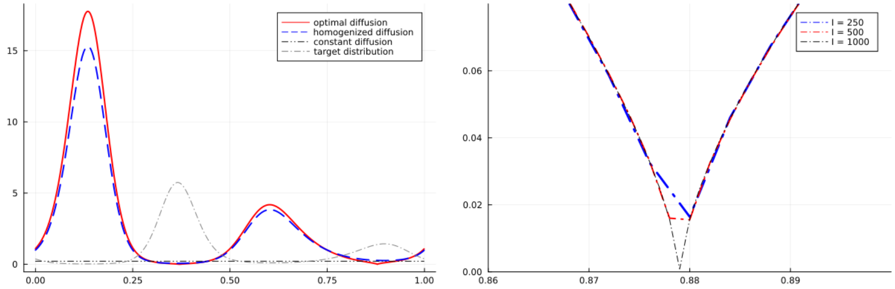




Spectral gaps: 30.47 (constant), 32.43 (homogenized), 36.75 (optimal)

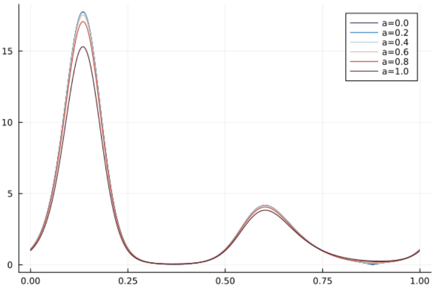
Optimal diffusion / case $\eta = \eta^\star$

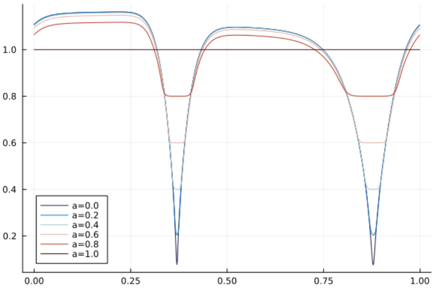
Potential $V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$



Spectral gaps: 0.81 (constant), 10.6 (homogenized), 11.2 (optimal)

Influence of the lower bound

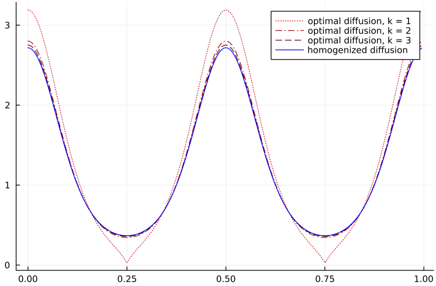


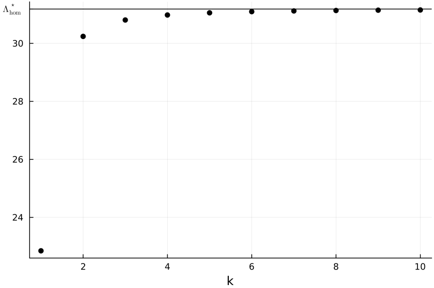


Spectral gap for various lower bounds a

Lower bound a	0.0	0.2	0.4	0.6	0.8	1.0
Spectral gap	11.227	11.226	11.208	11.145	10.983	10.572

Approximation by homogenized limit

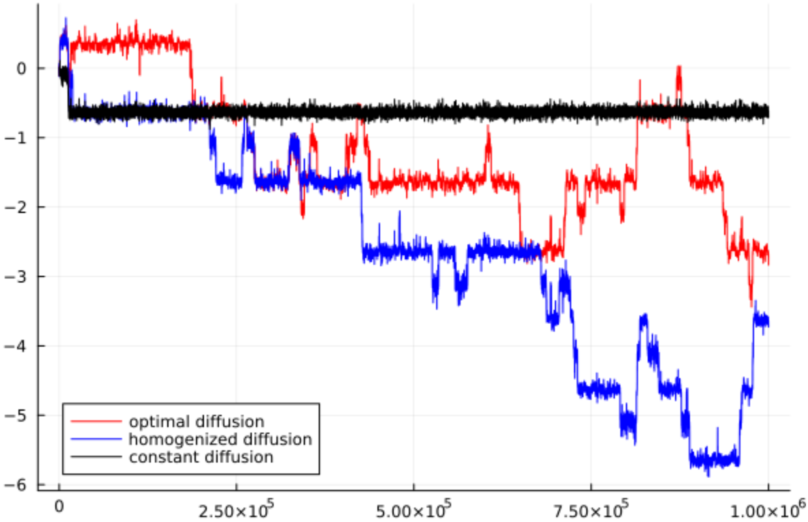




Positive diffusion when periodizing

Fast convergence to the homogenized limit

Simulation of overdamped Langevin dynamics



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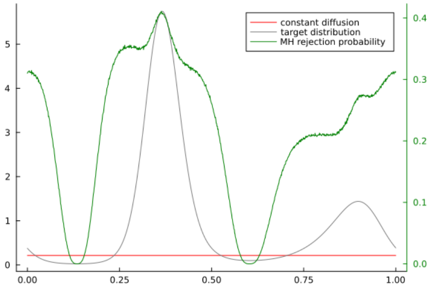
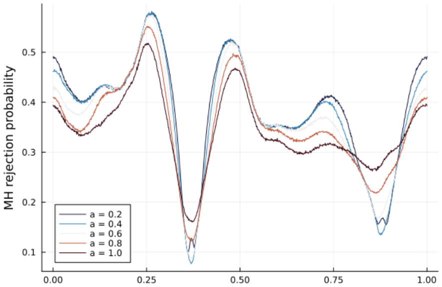
Potential $V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$





Rejection probabilities for constant diffusion mostly where V maximal

Rejection probabilities for optimized diffusion mostly where V minimal

Conclusion and perspectives

Extensions

Normalization: numerical criterion (e.g. Metropolis rejection probability)

Scaling with dimension:[3] diffusion depending only on some metastable degrees of freedom, e.g.

$$D(q) = P_\xi^\perp(q) + a(\xi(q))P_\xi(q), \qquad P_\xi = \frac{\nabla\xi \otimes \nabla\xi}{\|\nabla\xi\|^2}$$

where $\xi : \mathbb{R}^d \to \mathbb{R}^k$ (with $k \ll d$) is a collective variable

Underdamped Langevin dynamics:

- no variational framework
- optimization of constant diffusion[4]

[3] Lelièvre/Santet/Stoltz (2024)

[4] Chak/Kantas/Pavliotis/Lelièvre (2021)