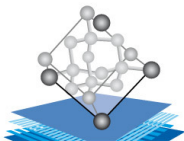




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Optimizing the diffusion for sampling with overdamped Langevin dynamics

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Workshop *Monte Carlo sampling: beyond the diffusive regime*, Newton Institute

- **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 $\mu(dq) = Z_\mu^{-1} e^{-\beta V(q)} dq$ 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

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

- 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 $L^2(\mu)$

$$\int_{\mathcal{Q}} (\mathcal{L}f) g = \int_{\mathcal{Q}} f (\mathcal{L}^\dagger g), \quad \int_{\mathcal{Q}} (\mathcal{L}f) g d\mu = \int_{\mathcal{Q}} f (\mathcal{L}^* g) d\mu$$

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

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

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

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

Overdamped Langevin dynamics with multiplicative noise

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

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

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

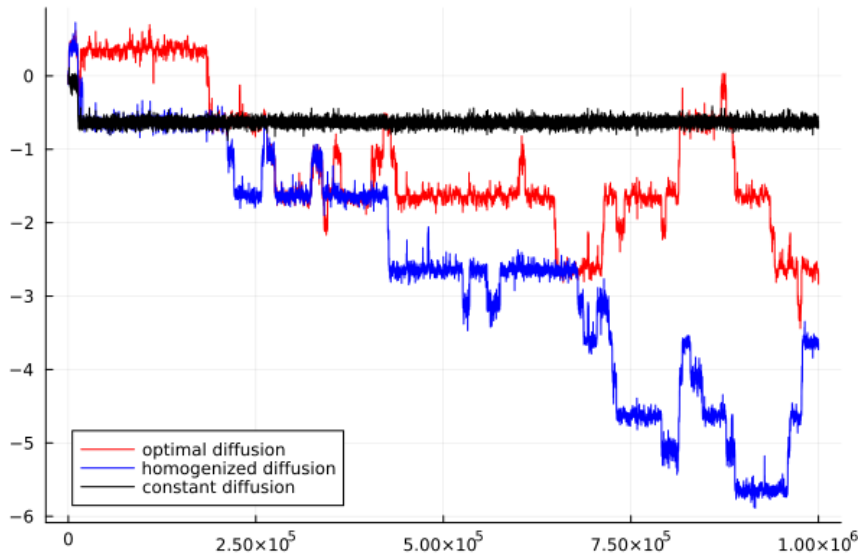
Two possible motivations:

- Compensate for **anisotropic** potential energy landscapes
- Reduce **metastability**

Generator still self-adjoint, **invariant probability measure** μ

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

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 $f(t) = e^{t\mathcal{L}_{\mathcal{D}}} f(0)$

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

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

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

Implies bounds on the asymptotic variance

Obtaining an exponential rate of convergence

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

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

Desired inequality follows from a **Gronwall estimate** and

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

Criterion to choose \mathcal{D}

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

Possible choices:

- $\mathcal{D} = (\nabla^2 V)^{-1}$ for strongly convex potentials [Girolami/Calderhead 2011]
- $\mathcal{D} = e^{\beta V}$ [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: $L_V^p(\mathbb{T}^d, \mathcal{M}_{a,b})$ (note $\mathcal{Q} = \mathbb{T}^d$), with associated norm

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

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

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

Matrix norm compatible with order on symmetric positive matrices

Maximization performed on

$$\mathfrak{D}_p^{a,b} = \left\{ \mathcal{D} \in L_V^\infty(\mathbb{T}^d, \mathcal{M}_{a,b}) \mid \int_{\mathbb{T}^d} |\mathcal{D}(q)|_{\mathbb{F}}^p e^{-\beta p V(q)} dq \leq 1 \right\}$$

Well posedness of the maximization problem

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

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

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

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^ lead to degenerate eigenvalues*

Precise statement:

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

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

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

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

so that $\mathcal{D}_p^* = \alpha_p |\mathcal{D}_p^*|_{\mathbb{F}}^{2-p} e^{\beta(p-1)V} \nabla u_{\mathcal{D}_p^*} \otimes \nabla u_{\mathcal{D}_p^*}$, contradicting $\mathcal{D}_p^*(q) \geq c \text{Id}_d$

Characterization of positive optimal diffusions (2/2)

Difficulty: Cannot **directly** rely on Euler–Lagrange equation

Strategy: $\max_{\mathcal{D} \in \mathcal{D}_p^{a,b}} f_\alpha =$ regularize using **softmax** and pass to the limit¹

$$f_\alpha(\mathcal{D}) = \frac{\text{Tr}_{L^2(\mu)}(\mathcal{L}_{\mathcal{D}} e^{\alpha \mathcal{L}_{\mathcal{D}}})}{\text{Tr}_{L^2(\mu)}(e^{\alpha \mathcal{L}_{\mathcal{D}}}) - 1} = \frac{N_2 \lambda_2 + \sum_{i \geq 3} N_i \lambda_i e^{\alpha(\lambda_i - \lambda_2)}}{N_2 + \sum_{i \geq 3} N_i e^{\alpha(\lambda_i - \lambda_2)}} \xrightarrow{\alpha \rightarrow +\infty} \lambda_2$$

Can write Euler–Lagrange condition for f_α using spectral calculus

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

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

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

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

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

¹Thank you Danny Perez for suggesting this!!

Approximation by homogenization theory

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

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

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

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

$$\bar{\mathcal{D}} = \int_{\mathbb{T}^d} \mathcal{D}(q) (1 - w'_{\mathcal{D}}(q)^2) \mu(q) dq, \quad \left[e^{-\beta V} \mathcal{D} (1 + w'_{\mathcal{D}}) \right]' = 0$$

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

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

Numerical results

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

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

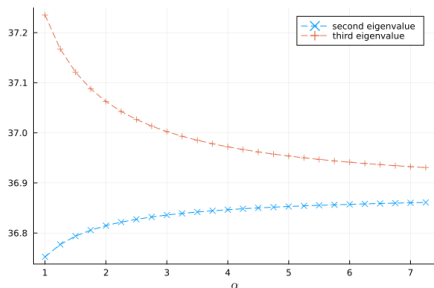
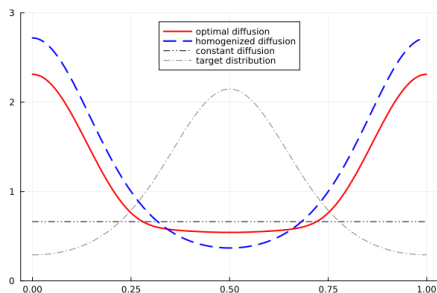
Discretization of the SDE

- use **Metropolis** acceptance/rejection to ensure unbiased sampling
- rejection probability $O(\sqrt{\Delta t})$ for proposals based on naive Euler–Maruyama discretization
- lowered to $O(\Delta t^{3/2})$ with dedicated (**implicit**) HMC algorithms²

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

Optimal diffusion / case $\eta \in (0, \eta^*)$

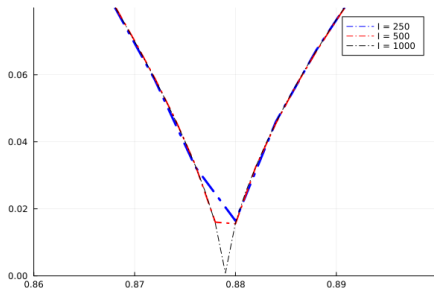
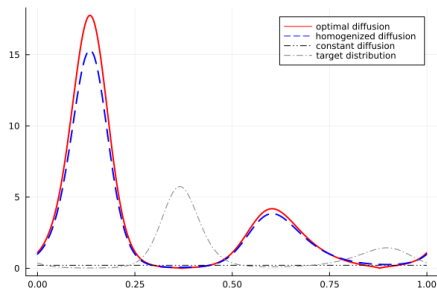
Potential $V(q) = \cos(2\pi q)$ $\eta \approx 0.51$



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

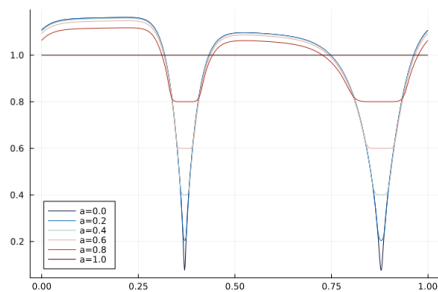
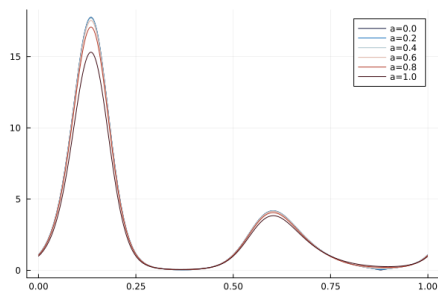
Optimal diffusion / case $\eta = \eta^*$

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



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

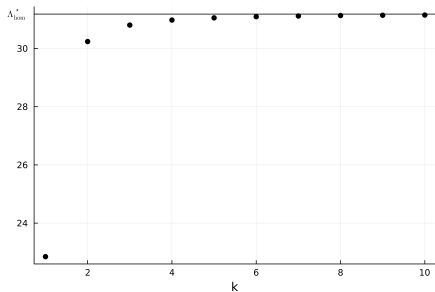
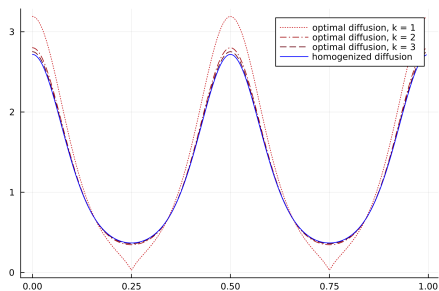
Influence of the lower bound



Spectral gap for various lower bounds a

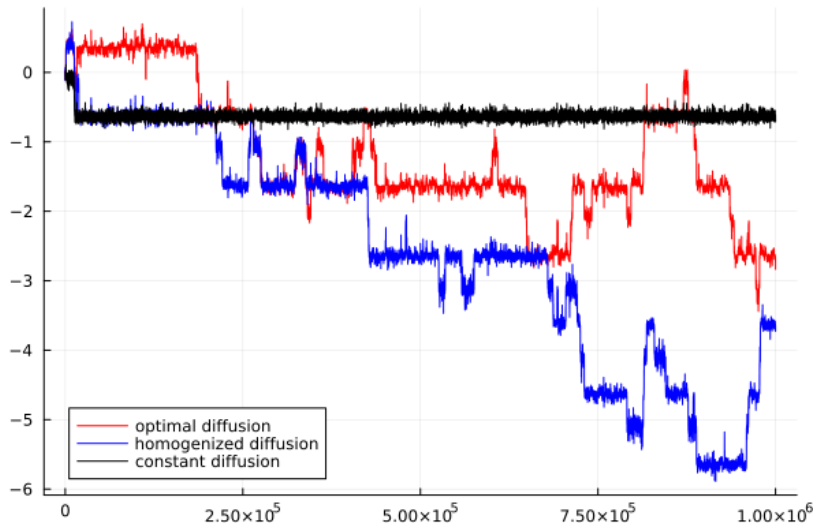
Lower bound a	0.0	0.2	0.4	0.6	0.8	1.0
Spectral gap	11.227	11.226	11.208	11.145	10.983	10.572

Approximation by homogenized limit



Positive diffusion when periodizing
Fast convergence to the homogenized limit

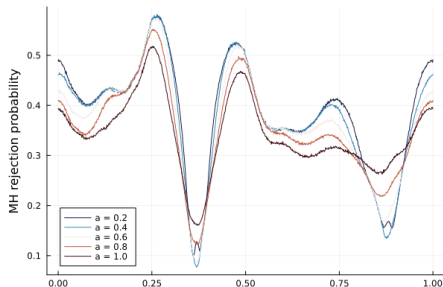
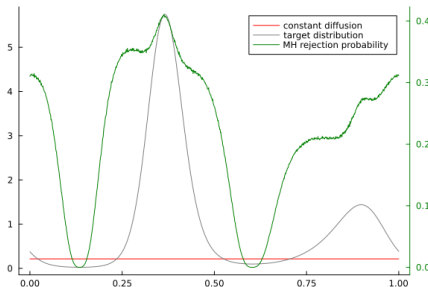
Simulation of overdamped Langevin dynamics



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

Metropolis rejection probabilities

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



Rejection probabilities for **constant** diffusion mostly where V **maximal**

Rejection probabilities for **optimized** diffusion mostly where V **minimal**

Conclusion and perspectives

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

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

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

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

Underdamped Langevin dynamics:

- **no variational** framework
- optimization of constant diffusion⁴

³Lelièvre/Santet/Stoltz, *arXiv preprint 2410.00525* (2024)

⁴Chak/Kantas/Pavliotis/Lelièvre (2021)