Optimizing the diffusion of overdamped Langevin dynamics

Régis SANTET

(CERMICS, École des Ponts & MATHERIALS Team, Inria Paris)

Joint work with: T. Lelièvre, G. Pavliotis, G. Robin, G. Stoltz

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I. Overdamped Langevin dynamics

- Computing average properties...
- ...using various diffusion coefficients...
- ...to accelerate convergence

II. Characterization of the optimal diffusion

- Establish a proper optimization problem...
- ...to obtain necessary conditions on the solution.
- Approximation using homogenization

III. Numerical results

- Approximate numerically the optimal diffusion...
- ...approximate the dynamics...
- to observe the efficiency gains

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Ergodic average

$$\mathbb{E}_\pi[f] \approx \frac{1}{N} \sum_{i=1}^{N} f(q^i)$$

with (q^i) samples from a trajectory solving (1)

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- invariance of the canonical measure: $\mathcal{L}^*\mathbf{1} = 0 \Leftrightarrow \mathcal{L}^\dagger\pi = 0$

$$\frac{d}{dt}\left[\mathbb{E}_\pi(\varphi(q_t))\right] = \frac{d}{dt}\left(\int_{\mathbb{T}^d} \mathrm{e}^{t\mathcal{L}}\varphi \, \mathrm{d}\pi\right) = \int_{\mathbb{T}^d} \mathcal{L}\left(\mathrm{e}^{t\mathcal{L}}\varphi\right) \mathrm{d}\pi = 0$$

where $\mathrm{e}^{t\mathcal{L}}\varphi(q_0) = \mathbb{E}_{q_0}[\varphi(q_t)]$

Diffusion matrix $\mathcal{D}(q) \in \mathcal{S}_d^+(\mathbb{R})$ (not necessarily definite)[1]

$$\mathrm{d}q_t = \left(-\mathcal{D}(q_t)\nabla V(q_t) + \beta^{-1}\,\mathrm{div}\,\mathcal{D}(q_t)\right)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\mathcal{D}^{1/2}(q_t)\,\mathrm{d}W_t$$

with $\mathrm{div}\,\mathcal{D}_i \equiv$ divergence of i-th column of $\mathcal{D}$ $\rightarrow$ **generator** $\mathcal{L}_{\mathcal{D}}$

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- $\mathcal{D} \equiv$ inverse of position-dependent mass tensor/metric (RMHMC)[2]

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Motivations

- Explore efficiently multimodal targets
- Compensate for anisotropic potential energy landscapes

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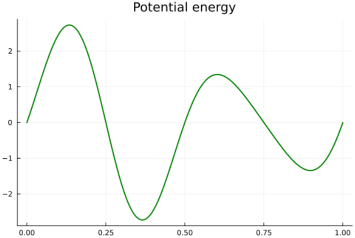
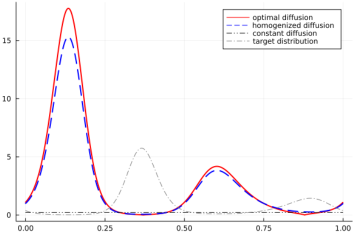
- Example with $V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$

$\mathcal{D}_{\mathrm{opt}}, \mathcal{D}_{\mathrm{exp}} = \mathrm{e}^{\beta V}, \mathcal{D}_{\mathrm{cst}} = a \in \mathbb{R}$ (all three normalized in $L^2(\pi)$)





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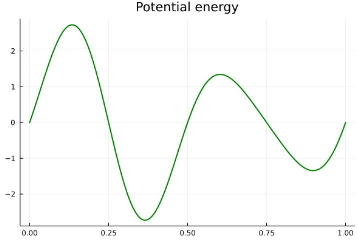

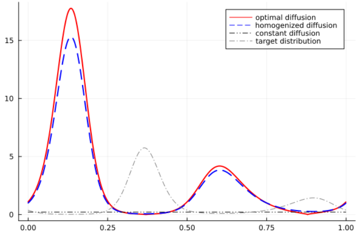

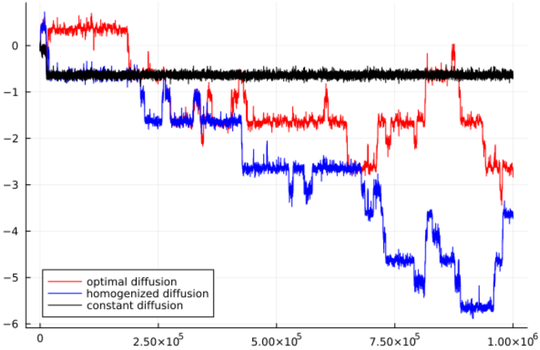

RWMH example trajectories (same noise)

- ‘Optimal’ $\mathcal{D}$ helps to **cross energy barriers** (if $V \uparrow$, then $\mathcal{D} \uparrow$)

Measuring convergence

- asymptotic variance in CLT
- convergence of the law at time t towards the target distribution
- average exit time of a mode

This work $\rightarrow$ second option in a $L^2(\pi)$ framework

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Main tool

Poincaré inequality satisfied by π

$$\forall \pi_0 \in L^2(\pi^{-1}), \qquad \int_{\mathbb{T}^d} \left(\frac{\pi_0}{\pi} - 1\right)^2 \mathrm{d}\pi \leqslant \frac{\beta}{\Lambda(\mathcal{D})} \int_{\mathbb{T}^d} \left|\nabla\left(\frac{\pi_0}{\pi}\right)\right|^2 \mathrm{d}\pi$$

$\Lambda(\mathcal{D})$: smallest nonzero eigenvalue of $-\beta\mathcal{L}_{\mathcal{D}}$: the **spectral gap**

Claim Poincaré inequality implies that

$$\forall \pi_0 \in L^2(\pi^{-1}), \qquad \left\| \frac{\pi_t}{\pi} - 1 \right\|_{L^2(\pi)} \leqslant \mathrm{e}^{-\beta^{-1}\Lambda(\mathcal{D})t} \left\| \frac{\pi_0}{\pi} - 1 \right\|_{L^2(\pi)}$$

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Conditions to obtain a Poincaré inequality

- bounded connected domains: equivalent to Lebesgue measure (Poincaré–Wirtinger inequality)
- Whole domain: conditions on the growth of V at infinity
- In general: Logarithmic Sobolev Inequalities

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

$$\Lambda(\mathcal{D}) = \inf_{u \in H_0^1(\pi) \setminus \{0\}} \frac{\displaystyle\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \mathcal{D} \nabla u \, \mathrm{d}\pi}{\displaystyle\int_{\mathbb{T}^d} u^2 \, \mathrm{d}\pi}$$

This work → **Maximize the spectral gap** $\Lambda(\mathcal{D})$ w.r.t. $\mathcal{D}$

Choices in the literature

- $\mathcal{D} = (\nabla^2 V)^{-1}$ for strictly convex potentials[2]
- $\mathcal{D} = \mathrm{e}^{\beta V}$ 'Langevin tempered algorithms' [3]

[2] Girolami/Calderhead (2011)

[3] Roberts/Stramer (2002)

Previous works available

- Optimizing the diffusion in the case of the uniform distribution[4]

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- Other choices to accelerate convergence, *e.g.* non-reversible drifts[6]

$$\mathrm{d}q_t = (-\nabla V(q_t) + b(q_t))\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t, \qquad \nabla \cdot (b\pi) = 0$$

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This work: staying in the realm of reversible dynamics

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- **Aim**: Estimation of $\mathbb{E}_\pi[f] = \int_{\mathbb{T}^d} f \, \mathrm{d}\pi, \quad \pi \propto \mathrm{e}^{-\beta V}$

with the estimator

$$\hat{I}_N := \frac{1}{N} \sum_{i=1}^{N} f(q^i), \qquad q^i \sim \pi$$

with q^i obtained from the integration of the overdamped Langevin dynamics

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• **Difficulty**: explore **anisotropic** potentials with **multiple minima**

• **Challenge**: **Find optimal diffusion coefficient $\mathcal{D}$ to accelerate convergence $\Rightarrow$ Maximize the spectral gap $\Lambda(\mathcal{D})$!**

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Need to set normalizing constraints on $\mathcal{D}$

- $\Lambda(a\mathcal{D}) = a\Lambda(\mathcal{D}) \xrightarrow[a\to+\infty]{} +\infty$: large $\mathcal{D}$ requires smaller time steps
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Open question: what is a good normalization ? Likely related to the numerics...

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

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

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Proof ideas:

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

Settings: $p \in (1, +\infty)$, $|\cdot|_{\mathrm{F}} \equiv$ Frobenius norm, $a = 0$ and $b > 0$ 'small enough', continuity assumption for $\mathcal{D}^\star$ for $d = 1$

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Proof If not, write the Euler–Lagrange equation (perturbation theory)

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

where $-\beta\mathcal{L}_{\mathcal{D}^\star} u_{\mathcal{D}^\star} = \lambda(\mathcal{D}^\star) u_{\mathcal{D}^\star}$ so that
$\mathcal{D}^\star = \alpha \left|\mathcal{D}^\star\right|^{2-p} \mathrm{e}^{\beta(p-1)V} \nabla u_{\mathcal{D}^\star} \otimes \nabla u_{\mathcal{D}^\star} \to$ contradiction !

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Claim If $\mathcal{D}^\star$ is uniformly definite positive, then the eigenvalue $\Lambda(\mathcal{D}^\star)$ is degenerate

Proof If not, write the Euler–Lagrange equation (perturbation theory)

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

where $-\beta\mathcal{L}_{\mathcal{D}^\star} u_{\mathcal{D}^\star} = \lambda(\mathcal{D}^\star) u_{\mathcal{D}^\star}$ so that
$\mathcal{D}^\star = \alpha\, |\mathcal{D}^\star|^{2-p}\, \mathrm{e}^{\beta(p-1)V} \nabla u_{\mathcal{D}^\star} \otimes \nabla u_{\mathcal{D}^\star} \to$ contradiction !

Difficulty: the map $\mathcal{D} \mapsto \Lambda(\mathcal{D})$ may therefore not be differentiable at $\mathcal{D}^\star$, it cannot be used as is to characterize $\mathcal{D}^\star$

Smooth-maximum approach: $\sup_{\mathcal{D}\in\mathfrak{D}_p^{a,b}} f_\alpha(\mathcal{D})$ and let $\alpha \to +\infty$

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

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- Euler–Lagrange equation for f_α

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

where $G_\alpha = \sum_{i\geqslant 2} \mathrm{e}^{\alpha\lambda_{i,\alpha}}, H_\alpha = \sum_{i\geqslant 2} \lambda_{i,\alpha} \mathrm{e}^{\alpha\lambda_{i,\alpha}}$

- The limit depends on $\lim_{\alpha\to+\infty} \alpha(\lambda_{j,\alpha} - \lambda_{2,\alpha})$

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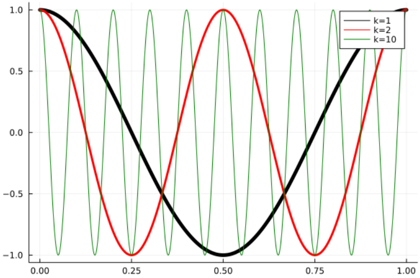
- The limit depends on $\lim_{\alpha\to+\infty}\alpha(\lambda_{j,\alpha} - \lambda_{2,\alpha})$
- Typical example: $d = 1$, degeneracy of order 2 for $\lambda_{2,\infty}$

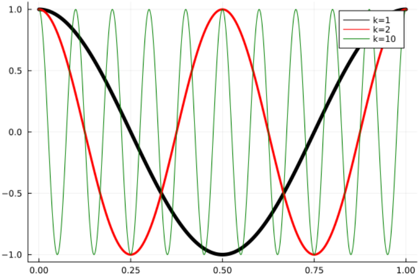
$$\mathcal{D}^{\star,\infty} = \gamma_\infty \mathrm{e}^{\beta V}\left(\left|e'_{2,\infty}\right|^2 + \frac{\mathrm{e}^\eta(1+\mathrm{e}^\eta+\eta)}{1+\mathrm{e}^\eta - \eta\mathrm{e}^\eta}\left|e'_{3,\infty}\right|^2\right)^{1/(p-1)}$$

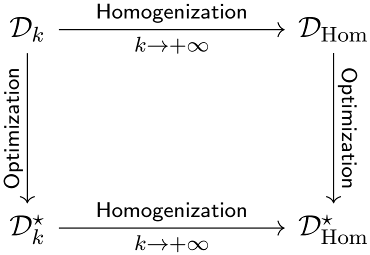

1.0
0.5
0.0
−0.5
−1.0
0.00
0.25
0.50
0.75
1.00
k=1
k=2
k=10

Goal: Obtain a good approximation of the optimal diffusion

• Idea 1: study the asymptotic behaviour of the optimal diffusion in the homogenized limit

• Idea 2: optimize the periodic homogenization limit





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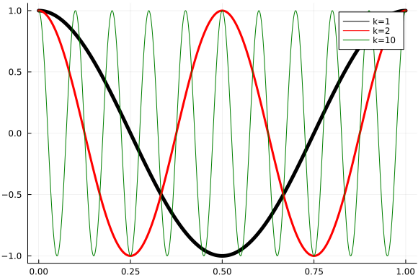

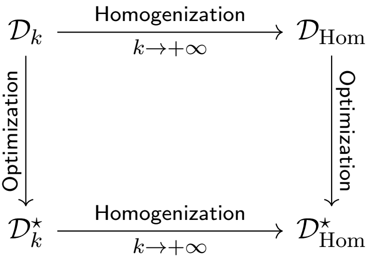

Commutation optimization/homogenization: maximize $\Lambda_{\mathrm{hom}}(\mathcal{D})$

$$\boxed{\mathcal{D}^\star_{\mathrm{hom}}(q) = \mathrm{e}^{\beta V(q)} \mathrm{I}_d}$$

Normalizing constraints on $\mathcal{D}$: our choice is

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

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Characterization of $\mathcal{D}^\star$

- possible degeneracy of the spectral gap $\Lambda(\mathcal{D}^\star)$ implies differentiability issues
- smooth-maximum approach adapted to $\mathcal{L}_\mathcal{D}$ (trace-class operator on $L^2(\pi)$)
- Can vanish on single points $\rightarrow$ ergodicity issues

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Homogenization theory: good approximation is

$$\mathcal{D}^\star_{\mathrm{Hom}}(q) = \mathrm{e}^{\beta V(q)} \mathrm{I}_d$$

I. Overdamped Langevin dynamics

- Computing average properties...
- ...using various diffusion coefficients...
- ...to accelerate convergence

II. Characterization of the optimal diffusion

- Establish a proper optimization problem...
- ...to obtain necessary conditions on the solution.
- Approximation using homogenization

III. Numerical results

- Approximate numerically the optimal diffusion...
- ...approximate the dynamics...
- to observe the efficiency gains

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- D isotropic, piecewise constant, on uniform mesh
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$$A(D)U_D = \lambda(D)BU_D, \qquad U_D^{\mathsf{T}}BU_D = \mathrm{I}_d$$

with

$$[A(D)]_{i,j} = \int_{\mathbb{T}^d} \nabla\varphi_j^{\mathsf{T}} D \nabla\varphi_i \,\mathrm{d}\pi, \qquad [B]_{i,j} = \int_{\mathbb{T}^d} \varphi_j\varphi_i \,\mathrm{d}\pi$$

$\to$ Generalized eigenvalue problem

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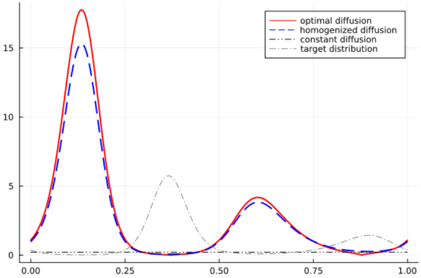
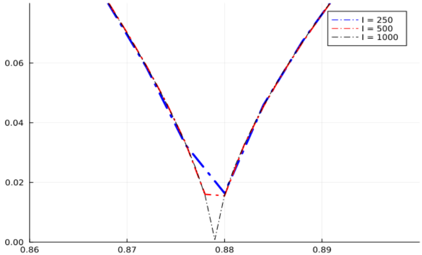
$\rightarrow$ Generalized eigenvalue problem

Only practical if $d \leqslant 3$!

- Use approximation solution $\mathcal{D}^\star_{\mathrm{Hom}}$
- Use coordinate reaction/summary statistics $\xi : \mathbb{R}^d \rightarrow \mathbb{R}^m$, $m \in \{1, 2\}$

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





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

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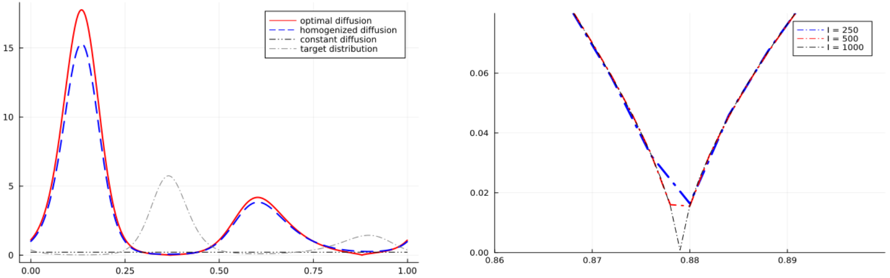
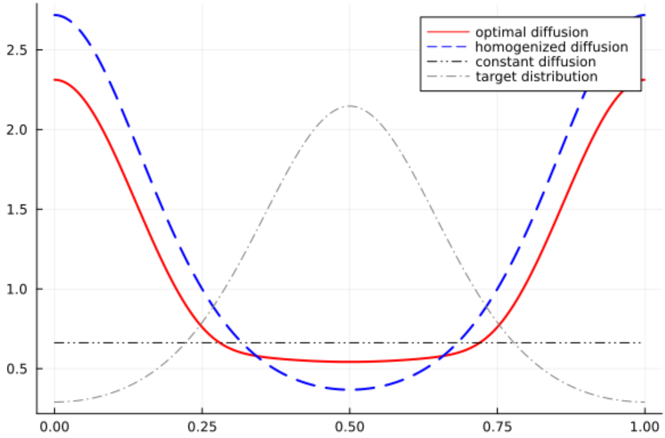


Spectral gaps: 0.81 (constant), 10.6 (homogenized), 11.2 (optimal)

Characterization: $\eta \approx -1.278$ kills the second term !

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

$$V(q) = \cos(2\pi q)$$



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

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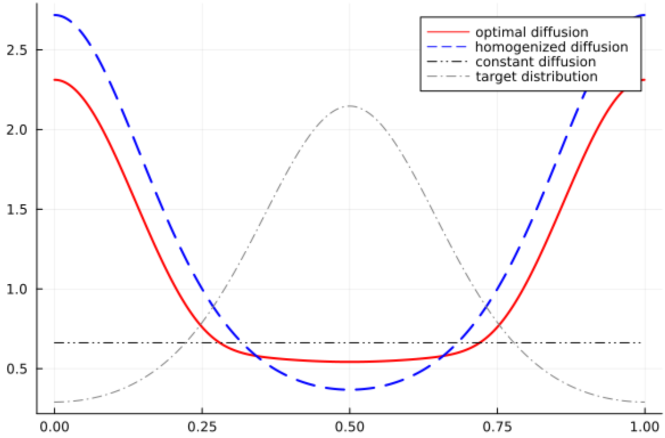
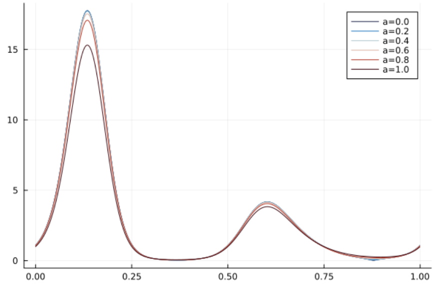
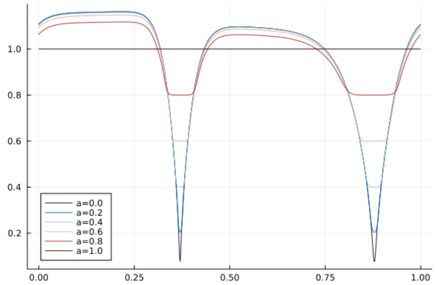


Spectral gaps: 30.47 (constant), 32.43 (homogenized), 36.75 (optimal)

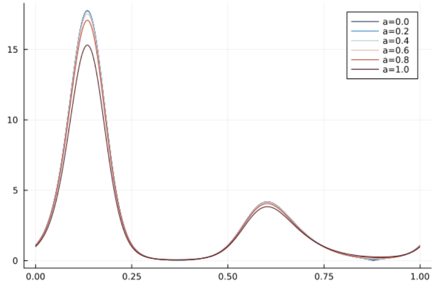
Characterization: $\eta \approx -0.51 \to \mathcal{D}^\star$ is uniformly definite positive



Optimal diffusions



Normalized by $\mathcal{D}^{\star}_{\mathrm{Hom}}$



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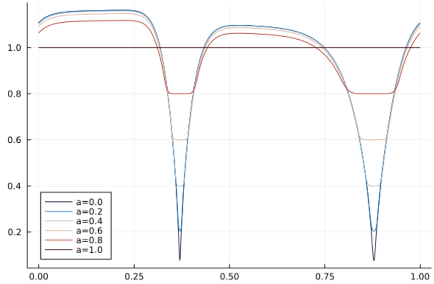

Normalized by $\mathcal{D}^\star_{\mathrm{Hom}}$

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

Discretization of the SDE

- **Random Walk** with 'guided variance', using Euler–Maruyama scheme

$$q^{i+1} = q^i + \sqrt{2\beta^{-1}\Delta t}\,\mathcal{D}^{1/2}(q^i)\,\mathrm{G}^{i+1}$$

- use Metropolis acceptance/rejection to ensure unbiased sampling

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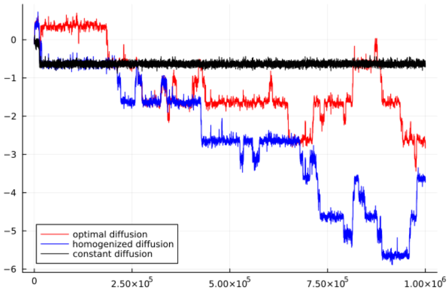
- rejection probability $\mathrm{O}(\Delta t^{1/2})$ for proposals based on naive Euler–Maruyama discretization of the continuous SDE[7]
- lowered to $\mathrm{O}(\Delta t^{3/2})$ with dedicated (implicit) HMC algorithms[8]
  RMHMC algorithm:

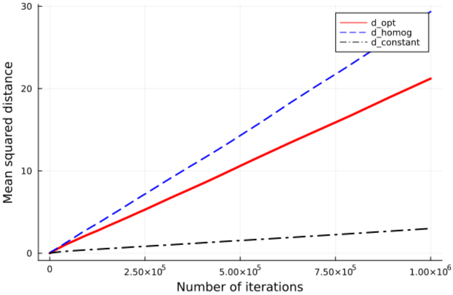
$$H(q,p) = V(q) - \frac{1}{2}\ln\det\mathcal{D}(q) + \frac{1}{2}p^{\mathsf{T}}\mathcal{D}(q)p$$

[7] Fathi/Stoltz (2017)

[8] Noble/De Bortoli/Durmus (2022), Lelièvre/RS/Stoltz (2023)

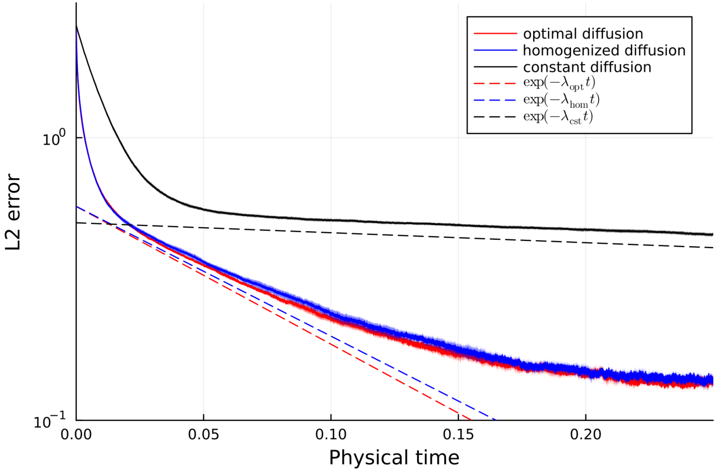
$$V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$$





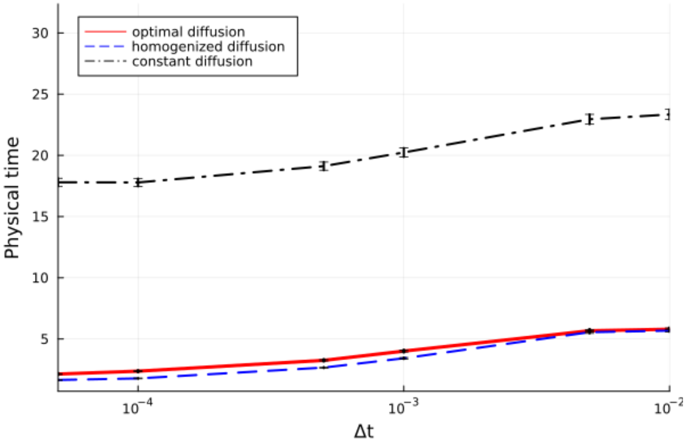
Mean square distance

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



L^2 error between empirical and target distributions

Settings: $\Delta t = 10^{-6}$, 10^4 samples generated uniformly on $\mathbb{T}$, 100 bins to approximate the L^2 norm, results averaged over 10 simulations



Transition times between the two wells, $N_{\text{transitions}} = 10^5$

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Efficiency

- Faster convergence
- Better mode exploration

Extensions

Normalization: numerical criterion ? *e.g.* Metropolis rejection probability

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Scaling with dimension

- using reaction coordinates/summary statistics, *e.g.*

$$\mathcal{D}(q) = D_0 \mathrm{e}^{\beta F(\xi(q))}, \qquad F = V - TS$$

- genuine diffusion matrix: beyond isotropic diffusions

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Underdamped Langevin dynamics

- No variational framework
- optimization of constant diffusion (optimal friction matrix)[9]
  $\rightarrow$ Generalized HMC

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

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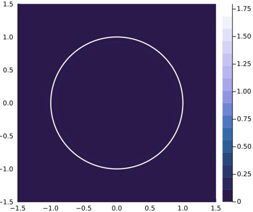
Thank you !

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

- Anisotropic diffusion coefficient $\mathcal{D}_{\mathsf{Tan}}(q) = \varepsilon \mathrm{I}_2 + \tilde{q}\tilde{q}^\mathsf{T}/\|q\|^2,\ \tilde{q} = (-y\ x)^\mathsf{T}$
- Isotropic diffusion coefficient $\mathcal{D}_{\mathsf{One}} \equiv (1+\varepsilon)\mathrm{I}_2, \quad \varepsilon = 0.1$



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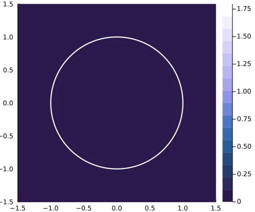
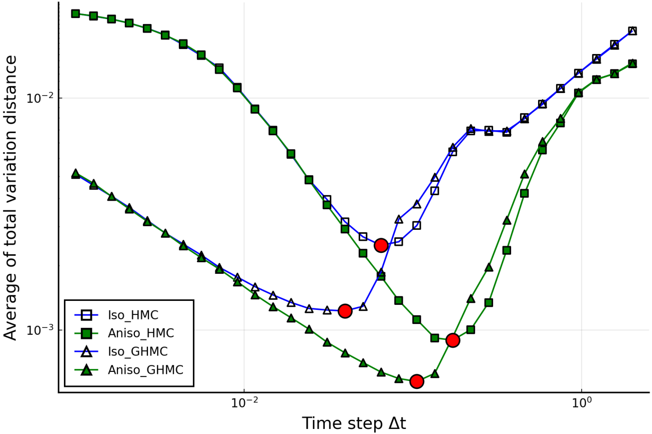
Computing: after fixed number of iterations, distance to the invariant measure of the angle distribution (uniform on $[0, 2\pi]$)





...using various diffusion coefficients... (Bonus 1/1)

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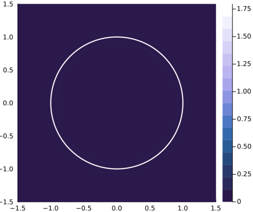

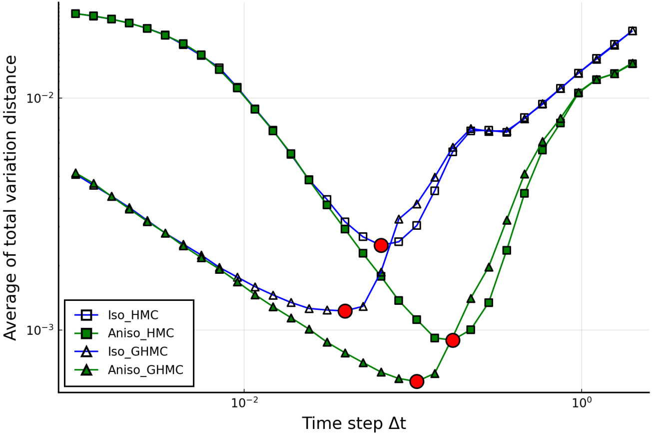

⇒ Compromise: small/large time steps (exploration vs rejection)

Definition [H-convergence]

A sequence $(\mathcal{A}^k)_{k\geqslant 1} \subset L^\infty(\mathbb{T}^d, \mathcal{M}_{a,b})$ H-converges to $\overline{\mathcal{A}} \in L^\infty(\mathbb{T}^d, \mathcal{M}_{a,b})$ if, for any $f \in H^{-1}(\mathbb{T}^d)$ such that $\langle f, \mathbf{1} \rangle_{H^{-1},H^1} = 0$, the sequence $(u^k)_{k\geqslant 1} \subset H^1(\mathbb{T}^d)$ of solutions to

$$\begin{cases} -\operatorname{div}\left(\mathcal{A}^k \nabla u^k\right) = f \quad \text{on } \mathbb{T}^d, \\ \displaystyle\int_{\mathbb{T}^d} u^k(q)\mathrm{d}q = 0 \end{cases}$$

satisfies in the limit $k \to +\infty$,

$$\begin{cases} u^k \rightharpoonup u & \text{weakly in } H^1(\mathbb{T}^d), \\ \mathcal{A}^k \nabla u^k \rightharpoonup \overline{\mathcal{A}} \nabla u & \text{weakly in } L^2(\mathbb{T}^d)^d, \end{cases}$$

where $u \in H^1(\mathbb{T}^d)$ is the solution of the homogenized problem

$$\begin{cases} -\operatorname{div}\left(\overline{\mathcal{A}} \nabla u\right) = f \quad \text{on } \mathbb{T}^d, \\ \displaystyle\int_{\mathbb{T}^d} u(q)\mathrm{d}q = 0 \end{cases}$$

Definition [Correctors]

If $\mathcal{A} = \mathcal{D}\exp(-\beta V)$, $(w_i)_{1\leqslant i\leqslant d} \subset H^1(\mathbb{T}^d)$ is the family of unique solutions to the problem

$$\begin{cases} -\operatorname{div}(\mathcal{A}(e_i + \nabla w_i)) = 0, \\ \displaystyle\int_{\mathbb{T}^d} w = 0 \end{cases}$$

Then for any $\xi \in \mathbb{R}^d$,

$$\xi^{\mathsf{T}}\overline{D}\xi = \xi^{\mathsf{T}}\left(\int_{\mathbb{T}^d}\mathcal{D}(q)\mathrm{d}\pi\right)\xi - \int_{\mathbb{T}^d}\nabla w_\xi^{\mathsf{T}}\mathcal{D}\nabla w_\xi\mathrm{d}\pi.$$