Optimizing the diffusion for overdamped Langevin dynamics

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

(Non)equilibrium Molecular Dynamics: Algorithms, Analysis, and Application

Diffusion dependent Overdamped Langevin dynamics

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

with the estimator

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

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- **Solution**: Position dependent pos. def. sym. matrix $\mathcal{D}$[1]

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

[1] Bou-Rabee/Donev/Vanden-Eijnden (2014)

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- **Challenge**: Find optimal diffusion coefficient $\mathcal{D}$ to accelerate convergence

[1] Bou-Rabee/Donev/Vanden-Eijnden (2014)

Quantify convergence rate

- Related to the spectral gap of the dynamics' generator $\mathcal{L}_{\mathcal{D}}$:

$$\mathcal{L}_{\mathcal{D}}\varphi = \left(-\mathcal{D}\nabla V + \beta^{-1}\operatorname{div}\mathcal{D}\right)\cdot\nabla\varphi + \beta^{-1}\mathcal{D} : \nabla^2\varphi$$

Then for any initial distribution π_0, the law π_t of the process q_t satisfies[2]

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

$\Lambda(\mathcal{D})$: spectral gap of $-\beta\mathcal{L}_{\mathcal{D}} \geqslant 0$

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- **Examples**: Approach mainly used in Bayesian Inference[3]: $\mathcal{D} \equiv (\nabla^2 V)^{-1}$

Other works[4] suggest $\mathcal{D} \propto \mathrm{e}^{\beta V}\mathrm{I}_d$

[2] Lelièvre/Nier/Pavliotis (2013)

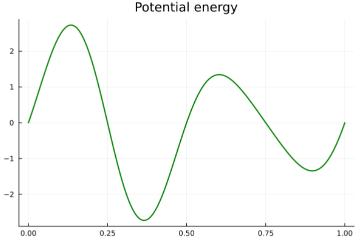
[3] Girolami/Calderhead (2011)

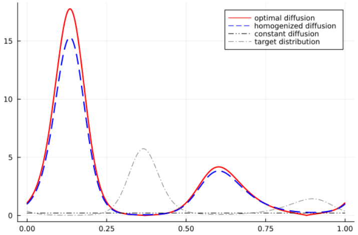
[4] Roberts/Stramer (2002), Lelièvre/Pavliotis/Robin/Santet/Stoltz (In prep.)

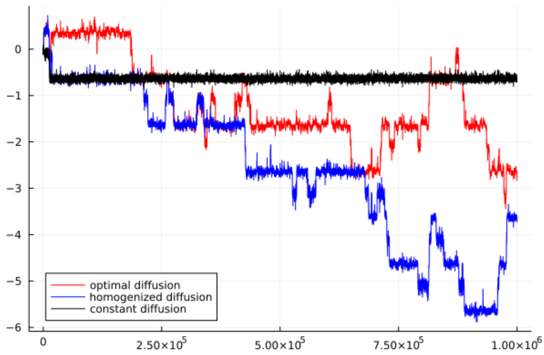
Which diffusion coefficient? Metastability case

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

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







RWMH example trajectories (same noise)

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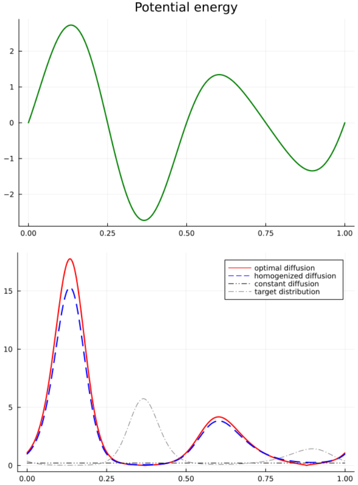

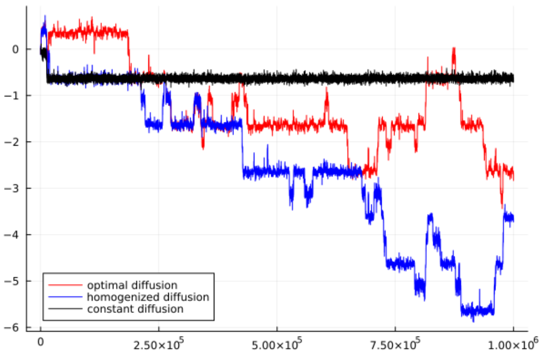

RWMH example trajectories (same noise)

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

Formulation of the optimization problem

- Using $\mathcal{L}_{\mathcal{D}} = -\beta^{-1}\nabla^\star\mathcal{D}\nabla$ on $L^2(\pi)$, the spectral gap of $-\beta\mathcal{L}_{\mathcal{D}}$ is

$$\Lambda(\mathcal{D}) = \min_{u\in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T}\mathcal{D}\nabla u\,\mathrm{d}\pi}{\int_{\mathbb{T}^d} u^2\,\mathrm{d}\pi} \,\middle|\, \int_{\mathbb{T}^d} u\,\mathrm{d}\pi = 0 \right\}$$

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- L^p constraint on $\mathcal{D}$: $\mathcal{D} \in L^p_\pi\left(\mathbb{T}^d, \mathcal{M}_{a,b}\right)$ for $1 \leqslant p \leqslant +\infty$, $a, b \geqslant 0$ if

$$\mathrm{e}^{-\beta V(q)}\mathcal{D}(q) \in \mathcal{M}_{a,b} = \left\{ M \in \mathcal{S}_d^+ \,\middle|\, \forall \xi \in \mathbb{R}^d, a\,|\xi|^2 \leqslant \xi^{\mathsf{T}} M \xi \leqslant b^{-1}\,|\xi|^2 \right\} \text{ a.e.}$$

endowed with

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

$$\mathfrak{D}_p^{a,b} = \left\{ \mathcal{D} \in L^\infty_\pi(\mathbb{T}^d, \mathcal{M}_{a,b}) \,\middle|\, \|\mathcal{D}\|_{L^p_\pi} \leqslant 1 \right\}$$

Theoretical analysis of the optimization problem

- $V \in \mathcal{C}^\infty(\mathbb{T}^d)$, V and π bounded on $\mathbb{T}^d$
- π satisfies a Poincaré inequality
- $\mathfrak{D}_p^{a,b}$ weakly closed for L^p_π
- $\mathcal{D} \mapsto \Lambda(\mathcal{D})$ concave

Theorem [Existence of a maximizer]

For any $p \in [1, +\infty)$, there exists

$$\boxed{\mathcal{D}_p^\star = \underset{\mathcal{D} \in \mathfrak{D}_p^{a,b}}{\arg\max}\, \Lambda(\mathcal{D})}$$

The maximizer is such that

- $\|\mathcal{D}\|_{L^p_\pi} = 1$;
- For any open set $\Omega \subset \mathbb{T}^d$, there exists $q \in \Omega$ such that $\mathcal{D}_p^\star(q) \neq 0$

Maximizer characterization: Euler–Lagrange equation

- Differentiability issues when $\Lambda(\mathcal{D}_p^\star)$ is degenerate (which is expected)

$\rightarrow$ smooth-maximum approach

$$f_\alpha(x_1, \ldots, x_n) = \frac{\sum_{i=1}^n x_i \mathrm{e}^{\alpha x_i}}{\sum_{i=1}^n \mathrm{e}^{\alpha x_i}} \xrightarrow[\alpha \to +\infty]{} \max_{1 \leqslant i \leqslant n} x_i.$$

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Euler–Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}t} f_\alpha\left(\mathcal{L}_{\mathcal{D}_p^\star + t\delta\mathcal{D}}\right)\Big|_{t=0} + \gamma\,\frac{\mathrm{d}}{\mathrm{d}t}\left\|\mathcal{D}_p^\star + t\delta\mathcal{D}\right\|_{L^p_\pi}^p\Big|_{t=0} = 0$$

and formal limit when $\alpha\to+\infty$ leads to

$$\boxed{\mathcal{D}_p^\star(q) = \gamma_p\left|\mathcal{D}_p^\star(q)\right|_{\mathrm{F}}^{2-p}\mathrm{e}^{\beta(p-1)V(q)}\sum_{i=1}^{N_2}\nabla u^i_{\mathcal{D}_p^\star}(q)\otimes\nabla u^i_{\mathcal{D}_p^\star}(q)}$$

with $\left(u^i_{\mathcal{D}_p^\star}\right)_{1\leqslant i\leqslant N_2}$ eigenvectors associated to $\Lambda(\mathcal{D}^\star)$.

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with $\left(u_{\mathcal{D}_p^\star}^i\right)_{1\leqslant i\leqslant N_2}$ eigenvectors associated to $\Lambda(\mathcal{D}^\star)$.

- Discussion about positivity (ergodicity issues ?)

Numerical approximation of the optimization problem

- For simplicity, $\mathcal{D}(q) = \mathscr{D}(q)\mathrm{I}_d$
- Piecewise constant approximation for $\mathscr{D}$ on $\mathbb{T}^d$
- $\mathbb{P}_1$ Finite Elements approximation to compute $(\Lambda(\mathcal{D}), u_{\mathcal{D}})$:

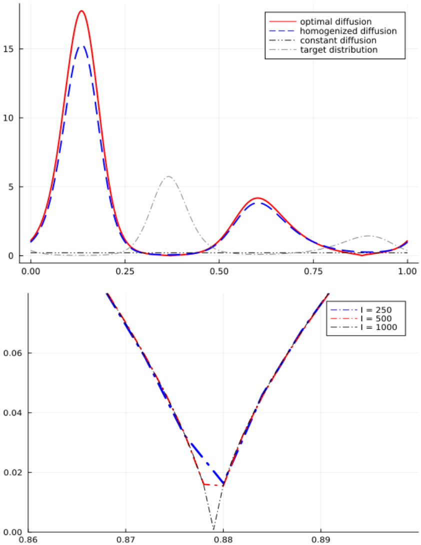
$$\boxed{A(\mathcal{D})u_{\mathcal{D}} = \Lambda(\mathcal{D})Bu_{\mathcal{D}}}$$

with

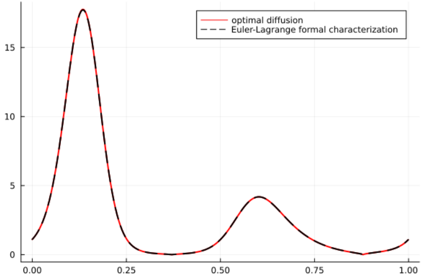
$$A_{i,j}(\mathcal{D}) = \int \nabla\varphi_j^{\mathsf{T}}\mathcal{D}\nabla\varphi_i \,\mathrm{d}\pi, \qquad B_{i,j} = \int \varphi_j\varphi_i \,\mathrm{d}\pi$$

- Generalized eigenvalue problem: A sym., B pos. def. sym.

Numerical results - 1

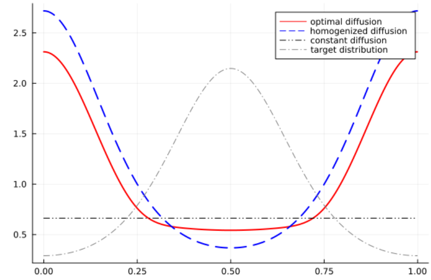


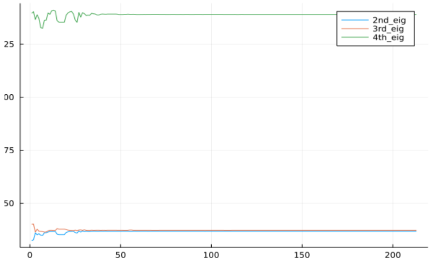
$$V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$$



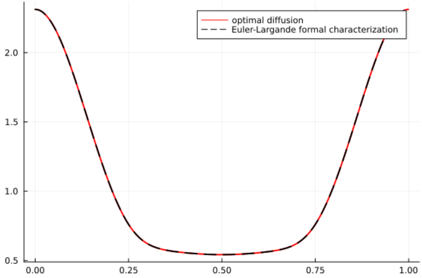
Non-degenerate eigenvalue

Numerical results - 2





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

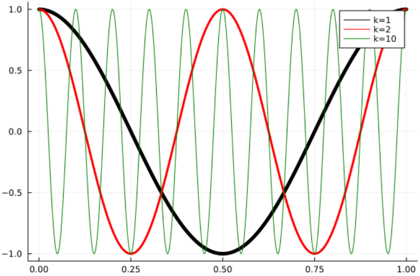


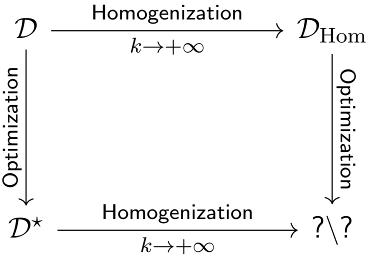
Degenerate eigenvalue

- Previous procedure only helpful in low dimensions
- Need to solve a high-dimensional generalized eigenvalue problem

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





- Decrease the period: $(\mathbb{Z}/k)^d$-periodic functions $V_{\#,k}(q) = V(kq)$ and $\mathcal{D}_{\#,k}(q) = \mathcal{D}(kq)$
- Write the spectral gap problem:

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

[5] See for instance Allaire, *Shape Optimization by the Homogenization Method* (2002)

Periodic homogenization procedure

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• Use **H-convergence**:[5] $\exists \overline{\mathcal{D}} \in \mathfrak{D}_p^{a,b}$, $\Lambda_{\#,k}(\mathcal{D}) \xrightarrow[k \to +\infty]{} \Lambda_{\mathrm{Hom}}(\mathcal{D})$ with

$$\boxed{\Lambda_{\mathrm{Hom}}(\mathcal{D}) := \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \overline{\mathcal{D}} \nabla u}{\int_{\mathbb{T}^d} u^2} \,\middle|\, \int_{\mathbb{T}^d} u = 0 \right\}}$$

• $\overline{\mathcal{D}}$ can be expressed using $\mathcal{D}$ and corrector functions appearing in the H-convergence procedure

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Optimization of the homogenized limit

$$\mathcal{D} \xrightarrow[k\to+\infty]{\text{Hom.}} \mathcal{D}_{\text{Hom}} \xrightarrow{\text{Opt.}} \mathcal{D}^\star_{\text{Hom}}$$

Goal: compute

$$\boxed{\Lambda^\star_{\text{Hom}} = \sup_{\mathcal{D}\in\mathfrak{D}_p^{a,b}} \Lambda_{\text{Hom}}(\mathcal{D})}$$

Theorem [Analytic expression]

- Linear constraint: For a fixed $M \in \mathcal{S}_d^{++}$, under the constraint, $\int_{\mathbb{T}^d} \mathcal{D}\,\mathrm{d}\pi = M$,

$$\boxed{\mathcal{D}^\star_{\text{Hom}}(q) = M/\pi(q)}$$

is a maximizer.

- L^p_π constraint, $d = 1$: Under the constraint $\|\mathcal{D}\|_{L^p_\pi} \leqslant 1$,

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

is a maximizer.

Homogenization of the optimal diffusion

Goal: optimize for a given $k \geqslant 1$, then let $k \to +\infty$

- Recall the oscillating potential $V_{\#,k}(q) = V(kq)$. Let $\mathfrak{D}^{a,b}_{\#,k,p} \equiv \mathfrak{D}^{a,b}_{p}$ but defined with $V_{\#,k}$ instead of V.
- Let

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Lemma

There exists a maximizer $\mathcal{D}^{k,\star} \in \mathfrak{D}^{a,b}_{p}$ such that, denoting by $\mathcal{D}^{k,\star}_{\#,k}(q) = \mathcal{D}^{k,\star}(kq)$,

$$\Lambda^k(\mathcal{D}^{k,\star}_{\#,k}) = \Lambda^{k,\star}$$

Commutation between Homogenization and Optimization

$$\begin{array}{ccc} \Lambda(\mathcal{D}) & \xrightarrow[k\to+\infty]{\text{Hom.}} & \Lambda_{\mathrm{Hom}}(\mathcal{D}) \\ \Big\downarrow{\scriptstyle \text{Opt.}} & & \Big\downarrow{\scriptstyle \text{Opt.}} \\ \Lambda^{k,\star} & \xrightarrow[k\to+\infty]{\text{Hom.}} & \Lambda^{\star}_{\mathrm{Hom}} \end{array}$$

Theorem

The sequence $(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^{\star}_{\mathrm{Hom}} := \Lambda(\mathcal{D}^{\star}_{\mathrm{Hom}})$.

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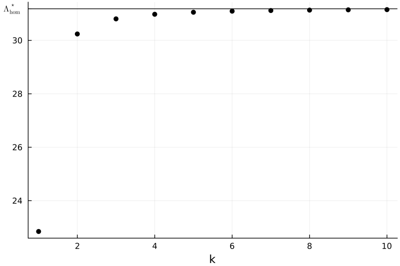
Theorem

The sequence $(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^{\star}_{\mathrm{Hom}} := \Lambda(\mathcal{D}^{\star}_{\mathrm{Hom}})$.

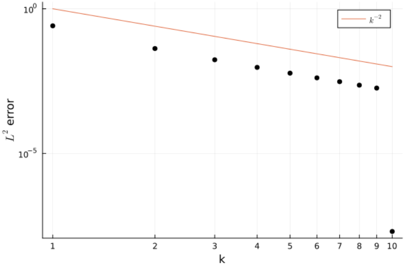
- This implies that a good proxy $(d=1)$ is $\mathcal{D}^{\star}_{\mathrm{Hom}} = \mathrm{e}^{\beta V}$
- In this case, $\overline{\mathcal{D}} = \left(\int_{\mathbb{T}} \mathrm{e}^{-\beta V}\right)^{-1} := Z^{-1}$, and

$$\boxed{\Lambda^{\star}_{\mathrm{Hom}} = 4\pi^2 Z^{-1}}$$

Numerical results - 3



$(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^\star_{\rm Hom}$



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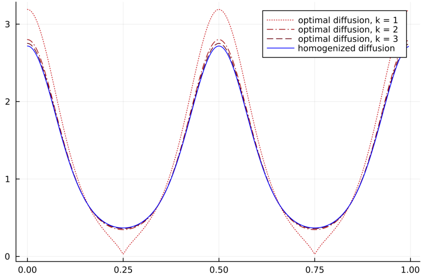
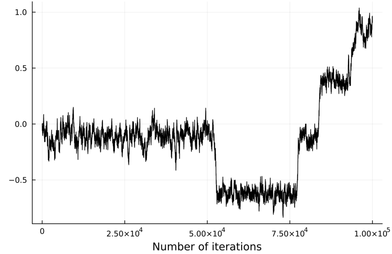


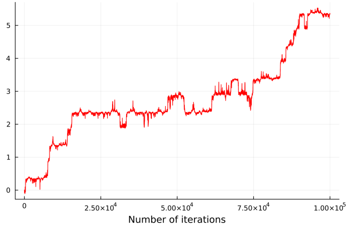
$(\mathcal{D}^{k,\star})_{k\geqslant 1}$ and $\mathcal{D}^\star_{\rm Hom}$ (rescaled with $1/k$ unit cell)

Numerical results - Application to sampling experiments - 1

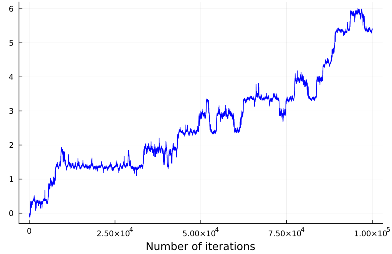
$$V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$$



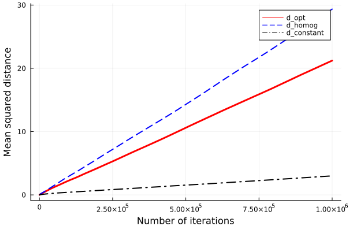
Constant diffusion coefficient



Optimal diffusion coefficient



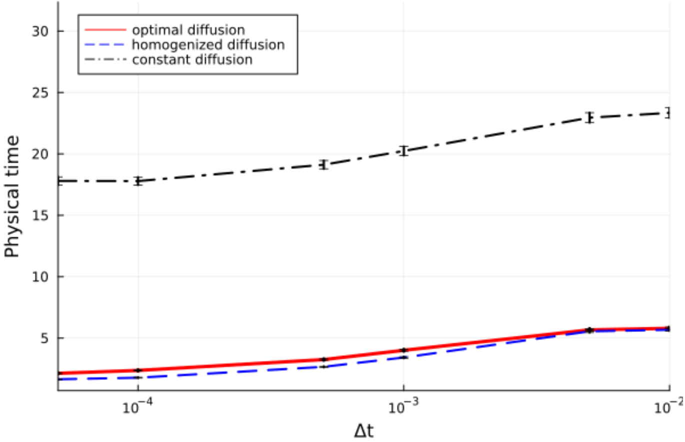
Homogenized diffusion coefficient



Mean square distance (averaged)

Numerical results - Application to sampling experiments - 2

Diffusion coefficient	Constant	Homogenized	Optimal
Spectral gap	2.16	10.57	11.23



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

Conclusion

• Using a position-dependant diffusion coefficient can help **sample rare events, cross energy barriers**, etc.

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$$\mathcal{D}(q) \propto \mathrm{e}^{\beta F(\xi(q))}$$

Conclusion

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• In high-dimension, use free energy F and coordinate reaction ξ:

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• Spectral gap is only one criterion: sampling issues when $\mathcal{D}^\star(q) \approx 0$

• Normalization constraint on $\mathcal{D}$: which one to choose ?

Perspectives - 1

• Adapt to nonequilibrium dynamics: non-gradient force F, use biasing scalar function $\mathcal{E} > 0$

$$\mathrm{d}q_t^\eta = \mathcal{E}(q_t^\eta)\left(-\nabla V(q_t^\eta) + \eta F(q_t^\eta)\right)\mathrm{d}t + \sqrt{2\mathcal{E}(q_t^\eta)}\mathrm{d}W_t.$$

• $\mathcal{L}_{\mathcal{E}}^\eta$ is not self-adjoint: optimize real part of the spectral gap

• Antisymmetric part in the gen. eigen. problem, complex eigenvalues

$$(A - \eta M)\, u_{\mathcal{E}} = \Lambda(\mathcal{E}) B(\mathcal{E}) u_{\mathcal{E}}$$

$A \in \mathcal{S}_d$, $M \in \mathcal{A}_d$, $B \in \mathcal{S}_d^{++}$

Perspectives - 2

- Adapt to QSD: from a metastable state A, if $\nu^{\mathcal{D}}$ is a QSD *i.e.*

$$\begin{cases} \mathcal{L}_{\mathcal{D}}^{*}\nu_{\mathcal{D}} = \lambda(\mathcal{D})\nu_{\mathcal{D}} & \text{on } A \\ \nu_{\mathcal{D}} = 0 & \text{on } \partial A \end{cases}$$

- Then to accelerate convergence, we maximize $\lambda_2 - \lambda_1$ which amounts to

$$\max_{\mathcal{D}+\text{ proper normalization}} \lambda_2(\mathcal{D})$$

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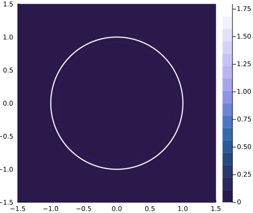
Thank you !

Which diffusion coefficient? Anisotropic case

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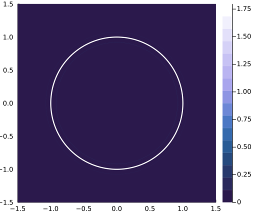
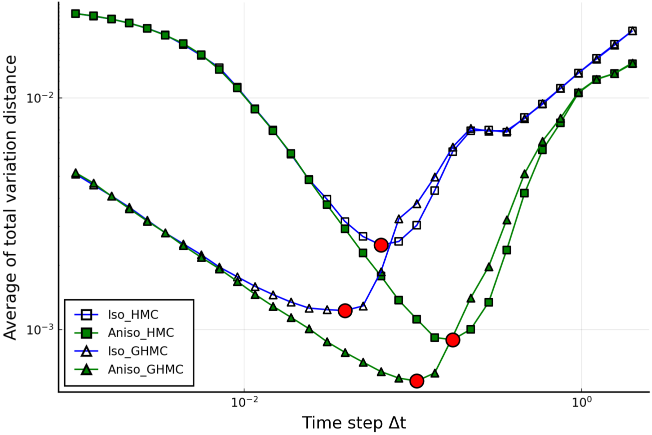
Computing: after fixed number of iterations, distance to the invariant measure of the angle distribution (uniform on $[0, 2\pi]$)





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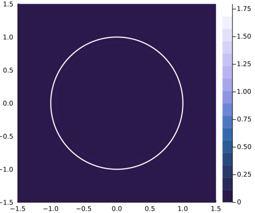

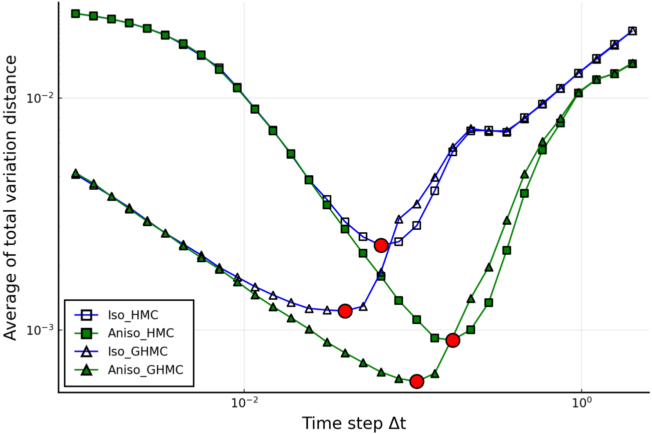

⇒ Compromise: small/large time steps (exploration vs rejection)

H-convergence

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 $\xi \in \mathbb{R}^d$,

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