Variance reduction for applications in computational statistical physics

Applied PDE seminar

Urbain Vaes
urbain.vaes@inria.fr

MATHERIALS – Inria Paris & CERMICS – École des Ponts ParisTech

27 October 2022

Outline

Part I: Mobility estimation for Langevin dynamics

Grigorios Pavliotis

Imperial College London

Department of Mathematics

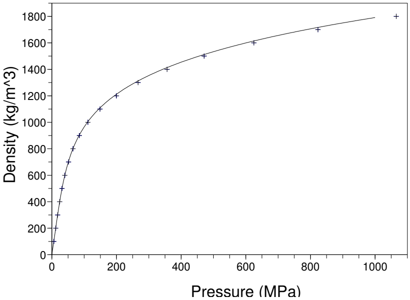
Gabriel Stoltz

École des Ponts ParisTech

CERMICS

Reference: G. A. PAVLIOTIS, G. STOLTZ, and U. VAES. Mobility estimation for Langevin dynamics using control variates. arXiv preprint, 2022

- Computation of macroscopic properties from Newtonians atomistic models:
  - Static properties, such as
    - the heat capacity and
    - the equations of state $P = P(\rho, T)$.
  - Dynamical properties, such as transport coefficients:
    - the viscosity;
    - the thermal conductivity;
    - the mobility of ions in solution.



Equation of state of argon at 300K.
- '+': molecular simulation;
- Solid line: experimental measurements[1].

- Numerical microscope: used in physics, biology, chemistry.

[1] `https://webbook.nist.gov/chemistry/fluid/`

Some background material on the Langevin equation

Consider the (one-particle) Langevin equation

$$\begin{cases} \mathrm{d}\mathbf{q}_t = \mathbf{p}_t \, \mathrm{d}t, \\ \mathrm{d}\mathbf{p}_t = -\nabla V(\mathbf{q}_t) \, \mathrm{d}t - \gamma \mathbf{p}_t \, \mathrm{d}t + \sqrt{2\gamma\beta^{-1}} \, \mathrm{d}\mathbf{W}_t, \end{cases} \qquad (\mathbf{q}_0, \mathbf{p}_0) \sim \mu,$$

where γ is the friction, V is a periodic potential, and $\beta = \frac{1}{k_{\mathrm{B}} T}$.

- The invariant probability measure is

$$\mu(\mathbf{q}, \mathbf{p}) = \frac{1}{Z} \, \mathrm{e}^{-\beta H(\mathbf{q}, \mathbf{p})} = \frac{1}{Z} \, \mathrm{e}^{-\beta \left(V(\mathbf{q}) + \frac{|\mathbf{p}|^2}{2} \right)}, \quad \text{on } \mathbf{T}^d \times \mathbf{R}^d.$$

- The generator of the associated Markov semigroup

$$\left(\mathrm{e}^{\mathcal{L}t} \varphi \right) (\mathbf{q}, \mathbf{p}) = \mathbf{E} \left(\varphi(\mathbf{q}_t, \mathbf{p}_t) \middle| (\mathbf{q}_0, \mathbf{p}_0) = (\mathbf{q}, \mathbf{p}) \right)$$

  is the following operator:

$$\mathcal{L} = (\mathbf{p} \cdot \nabla_{\mathbf{q}} - \nabla V(q) \cdot \nabla_{\mathbf{p}}) + \gamma \left(-\mathbf{p} \nabla_{\mathbf{p}} + \beta^{-1} \Delta_{\mathbf{p}} \right) =: \mathcal{L}_{\mathrm{ham}} + \gamma \, \mathcal{L}_{\mathrm{FD}}.$$

We denote by $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ the norm and inner product of $L^2(\mu)$, and

$$L^2_0(\mu) = \left\{ \varphi \in L^2(\mu) : \langle \varphi, 1 \rangle = \mathbf{E}_\mu \varphi = 0 \right\}.$$

Definition of the mobility

Consider Langevin dynamics with additional forcing in a direction $\mathbf{e}$:

$$\begin{cases} \mathrm{d}\mathbf{q}_t = \mathbf{p}_t \, \mathrm{d}t, \\ \mathrm{d}\mathbf{p}_t = -\nabla V(\mathbf{q}_t) \, \mathrm{d}t + \eta \mathbf{e} \, \mathrm{d}t - \gamma \mathbf{p}_t \, \mathrm{d}t + \sqrt{2\gamma\beta^{-1}} \, \mathrm{d}\mathbf{W}_t. \end{cases}$$

This dynamics admits a unique invariant probability distribution $\mu_\eta \in \mathcal{P}(\mathbf{T}^d \times \mathbf{R}^d)$.

Definition (Mobility)

The mobility in direction $\mathbf{e}$ is defined mathematically as

$$M_{\mathbf{e}} = \lim_{\eta \to 0} \frac{1}{\eta} \mathbf{E}_{\mu_\eta} [\mathbf{e}^\mathsf{T} \mathbf{p}]$$

$\approx$ factor relating the mean momentum to the strength of the inducing force.

- There is a symmetric mobility tensor $\mathbf{M}$ such that $M_{\mathbf{e}} = \mathbf{e}^\mathsf{T} \mathbf{M} \mathbf{e}$.
- **Einstein's relation:** $\mathbf{D} = \beta^{-1} \mathbf{M}$, with $\mathbf{D}$ the effective diffusion coefficient.

Effective diffusion

It is possible to show a functional central limit theorem for the Langevin dynamics[2]:

$$\varepsilon \mathbf{q}_{s/\varepsilon^2} \xrightarrow[\varepsilon\to 0]{} \sqrt{2\mathbf{D}}\,\mathbf{W}_s \qquad \text{weakly on } C([0,\infty)).$$

In particular, $\mathbf{q}_t/\sqrt{t} \xrightarrow[t\to\infty]{} \mathcal{N}(0, 2\mathbf{D})$ weakly.

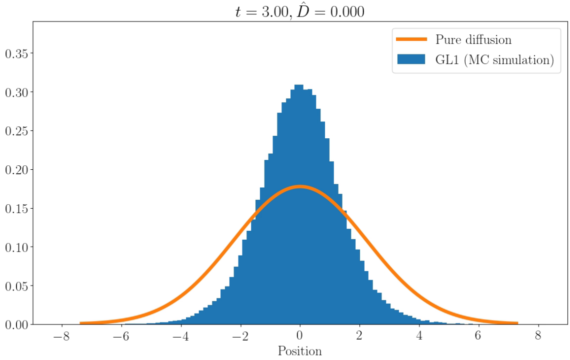


Figure: Histogram of $q_t/\sqrt{t}$. The potential $V(q) = -\cos(q)/2$ is illustrated in the background.

[2] R. N. Bhattacharya. On the functional central limit theorem and the law of the iterated logarithm

Mathematical expression for the effective diffusion (dimension 1)

Expression of D in terms of the solution to a Poisson equation

The effective diffusion coefficient is given by where $D = \langle \phi, p \rangle$ and ϕ is the solution to

$$-\mathcal{L}\phi = p, \qquad \phi \in L_0^2(\mu) := \left\{ u \in L^2(\mu) : \langle u, 1 \rangle = 0 \right\}.$$

Key idea of the proof: Apply Itô's formula to ϕ

$$\mathrm{d}\phi(q_s, p_s) = -p_s \, \mathrm{d}s + \sqrt{2\gamma\beta^{-1}} \, \frac{\partial \phi}{\partial p}(q_s, p_s) \, \mathrm{d}W_s$$

and then rearrange:

$$\begin{aligned} \varepsilon(q_{t/\varepsilon^2} - q_0) &= \varepsilon \int_0^{t/\varepsilon^2} p_s \, \mathrm{d}s \\ &= \underbrace{\varepsilon\Big(\phi(q_0, p_0) - \phi(q_{t/\varepsilon^2}, p_{t/\varepsilon^2})\Big)}_{\to 0} + \underbrace{\sqrt{2\gamma\beta^{-1}}\varepsilon \int_0^{t/\varepsilon^2} \frac{\partial \phi}{\partial p}(q_s, p_s) \, \mathrm{d}W_s}_{\to \sqrt{2D} W_t \text{ weakly by MCLT}} . \end{aligned}$$

In the multidimensional setting, $D_{\mathbf{e}} = \left\langle \phi_{\mathbf{e}}, \mathbf{e}^\mathsf{T} \mathbf{p} \right\rangle$ with $-\mathcal{L}\phi_{\mathbf{e}} = \mathbf{e}^\mathsf{T}\mathbf{p}$

Langevin dynamics: underdamped and overdamped regimes[3]

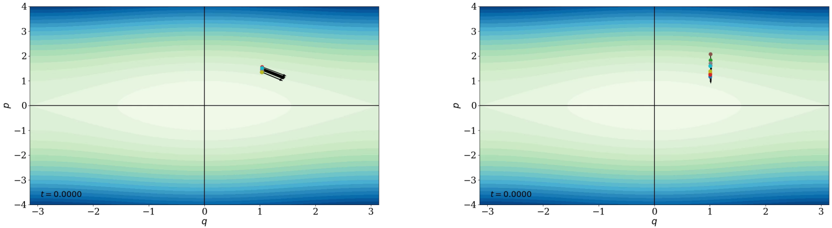


Figure: Langevin dynamics with friction $\gamma = 0.1$ (left) and $\gamma = 10$ (right)

- The underdamped limit as $\gamma \to 0$ is well understood in dimension 1 but not in the multi-dimensional setting. In dimension 1, it holds that

$$\phi = -\mathcal{L}^{-1} p = \gamma^{-1} \phi_{\mathrm{und}} + \mathcal{O}(\gamma^{-1/2}).$$

- Overdamped limit: as $\gamma \to \infty$, the rescaled process $t \mapsto q_{\gamma t}$ converges weakly to the solution of the overdamped Langevin equation:

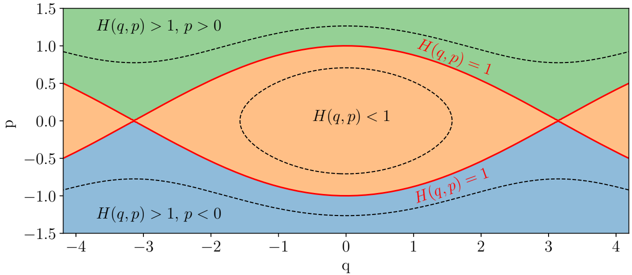
$$\dot{\mathbf{q}} = -\nabla V(q) + \sqrt{2\,\beta^{-1}}\,\dot{\mathbf{W}}.$$

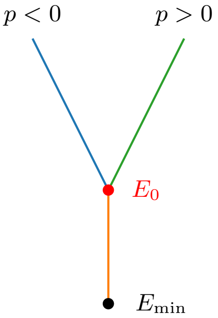
[3] M. Hairer and G. A. Pavliotis. From ballistic to diffusive behavior in periodic potentials. J. Stat. Phys., 2008.

As $\gamma \to 0$, the Hamiltonian of the rescaled process

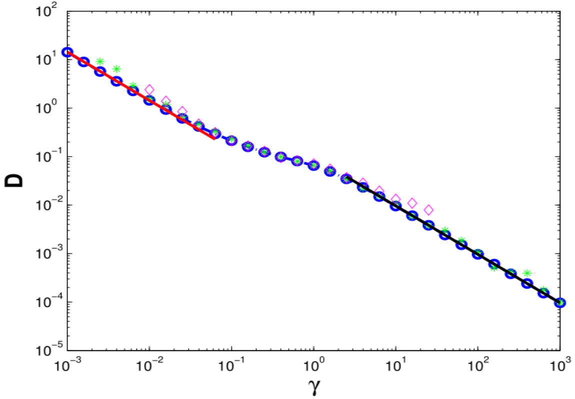
$$\begin{cases} q_\gamma(t) = q(t/\gamma), \\ p_\gamma(t) = p(t/\gamma), \end{cases}$$

converges weakly to a diffusion process on a graph.





In dimension 1, $\lim_{\gamma\to 0} \gamma D^\gamma = D_{\rm und} := \langle \phi_{\rm und}, p\rangle$ and $\lim_{\gamma\to\infty} \gamma D^\gamma = D_{\rm ovd}$.

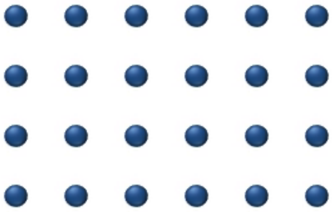


[4] G. A. Pavliotis and A. Vogiannou. Diffusive transport in periodic potentials: underdamped dynamics. Fluct. Noise Lett., 2008.

Open question: surface diffusion when $\gamma \ll 1$[5]

Applications:

- integrated circuits;
- catalysis.



In dimension > 1, it does not hold that $\gamma D_{\mathbf{e}}^{\gamma} \xrightarrow[\gamma \to 0]{} D_{\mathrm{und}}$ when V is non-separable, e.g.

$$V(\mathbf{q}) = -\frac{1}{2}\Big(\cos(q_1) + \cos(q_2)\Big) - \delta \cos(q_1)\cos(q_2)$$

Open question: behavior of the effective diffusion coefficient when $\gamma \ll 1$?

$$D_{\mathbf{e}}^{\gamma} = \lim_{t \to \infty} \frac{\mathbf{E}\left[\left|\mathbf{e}^{\mathsf{T}} \mathbf{q}_t\right|^2\right]}{2t} \sim \gamma^{-\sigma}, \qquad \sigma = ???$$

[5] Source of the video: `https://en.wikipedia.org/wiki/Surface_diffusion`

Brief literature review

Open question:

How does $D_{\mathbf{e}}^{\gamma}$ behave when $\gamma \ll 1$ and $d = 2$?

Various answers are given in the literature:

- $D_{\mathbf{e}}^{\gamma} \propto \gamma^{-1/2}$ for specific potentials[6];
- $D_{\mathbf{e}}^{\gamma} \propto \gamma^{-1/3}$ for specific potentials[7];
- $D_{\mathbf{e}}^{\gamma} \propto \gamma^{-\sigma}$ with σ depending on the potential[8].

Difficulty with $\gamma \ll 1$:

- Deterministic methods for the Poisson equation $-\mathcal{L}\phi_{\mathbf{e}} = \mathbf{e}^{\mathsf{T}}\mathbf{p}$ are ill-conditioned.
- Probabilistic methods are very slow to converge.

[6] L. Y. Chen, M. R. Baldan, and S. C. Ying. Surface diffusion in the low-friction limit: Occurrence of long jumps. Phys. Rev. B, 1996.

[7] O. M. Braun and R. Ferrando. Role of long jumps in surface diffusion. Phys. Rev. E, 2002.

[8] J. Roussel. Theoretical and Numerical Analysis of Non-Reversible Dynamics in Computational Statistical Physics. PhD thesis, Université Paris-Est, 2018.

Outline

Numerical approaches for calculating the effective diffusion coefficient

- Linear response approach:

$$D_{\mathbf{e}} = \lim_{\eta \to 0} \frac{1}{\beta \eta} \mathbf{E}_{\mu_\eta} \left(\mathbf{e}^\mathsf{T} \mathbf{p} \right).$$

where μ_η is the invariant distribution of the system with external forcing.

- Green–Kubo formula: Since $-\mathcal{L}^{-1} = \int_0^\infty \mathrm{e}^{t\mathcal{L}} \, \mathrm{d}t$,

$$\begin{aligned} D_{\mathbf{e}} &= \int -\mathcal{L}^{-1}(\mathbf{e}^\mathsf{T}\mathbf{p}) \, (\mathbf{e}^\mathsf{T}\mathbf{p}) \, \mathrm{d}\mu = \int_0^\infty \int \mathrm{e}^{t\mathcal{L}} (\mathbf{e}^\mathsf{T}\mathbf{p}) (\mathbf{e}^\mathsf{T}\mathbf{p}) \, \mathrm{d}\mu \, \mathrm{d}t \\ &= \int_0^\infty \mathbf{E}_\mu \big((\mathbf{e}^\mathsf{T}\mathbf{p}_0)(\mathbf{e}^\mathsf{T}\mathbf{p}_t) \big) \, \mathrm{d}t. \end{aligned}$$

- Einstein's relation:

$$D_{\mathbf{e}} = \lim_{t \to \infty} \frac{1}{2t} \mathbf{E}_\mu \left[\left| \mathbf{e}^\mathsf{T} (\mathbf{q}_t - \mathbf{q}_0) \right|^2 \right].$$

- Deterministic method, e.g. Fourier/Hermite Galerkin, for the Poisson equation

$$-\mathcal{L}\phi_{\mathbf{e}} = \mathbf{e}^\mathsf{T}\mathbf{p}, \qquad D_{\mathbf{e}} = \langle \phi_{\mathbf{e}}, p \rangle.$$

Consider the following estimator of the effective diffusion coefficient $D_{\mathbf{e}}$:

$$u(T) = \frac{\left|\mathbf{e}^\mathsf{T}(\mathbf{q}_T - \mathbf{q}_0)\right|^2}{2T}, \qquad (\mathbf{q}_0, \mathbf{p}_0) \sim \mu.$$

Bias of this estimator:

$$\mathbf{E}\big[u(T)\big] = D_{\mathbf{e}} - \int_0^\infty \left\langle \mathrm{e}^{t\mathcal{L}}(\mathbf{e}^\mathsf{T}\mathbf{p}), \mathbf{e}^\mathsf{T}\mathbf{p} \right\rangle \min\left\{1, \frac{t}{T}\right\} \mathrm{d}t.$$

Using the decay estimate for the semigroup[9]

$$\left\| \mathrm{e}^{t\mathcal{L}} \right\|_{\mathcal{B}\left(L_0^2(\mu)\right)} \leq L\,\mathrm{e}^{-\ell \min\{\gamma, \gamma^{-1}\} t},$$

we deduce

$$|\mathbf{E}[u(T)] - D_{\mathbf{e}}| \leq \frac{C \max\{\gamma^2, \gamma^{-2}\}}{T}.$$

[9] J. Roussel and G. Stoltz. Spectral methods for Langevin dynamics and associated error estimates. ESAIM: Math. Model. Numer. Anal., 2018.

Variance of the estimator $u(T)$ for large T

For $T \gg 1$, it holds approximately that

$$\frac{\mathbf{e}^\mathsf{T}(\mathbf{q}_T - \mathbf{q}_0)}{\sqrt{2T}} \sim \mathcal{N}(0, D_\mathbf{e}) \qquad \rightsquigarrow \qquad \frac{u(T)}{D_\mathbf{e}} = \frac{\left|\mathbf{e}^\mathsf{T}(\mathbf{q}_T - \mathbf{q}_0)\right|^2}{2D_\mathbf{e}T} \sim \chi^2(1).$$

Therefore, we deduce

$$\lim_{T\to\infty} \mathbf{V}\big[u(T)\big] = 2D_\mathbf{e}^2.$$

The relative standard deviation (asymptotically as $T \to \infty$) is therefore

$$\lim_{T\to\infty} \frac{\sqrt{\mathbf{V}\big[u(T)\big]}}{\mathbf{E}\big[u(T)\big]} = \sqrt{2} \qquad \rightsquigarrow \text{independent of } \gamma.$$

Scaling of the mean square error when using J realizations

Assuming an asymptotic scaling as $\gamma^{-\sigma}$ of $D_\mathbf{e}$, we have

$$\forall \gamma \in (0,1), \qquad \frac{\mathrm{MSE}}{D_\mathbf{e}^2} \leq \frac{C}{\gamma^{4-2\sigma}T^2} + \frac{2}{J}$$

Variance reduction using control variates

Let $\phi_{\mathbf{e}}$ denote the solution to the Poisson equation

$$-\mathcal{L}\phi_{\mathbf{e}}(\mathbf{q},\mathbf{p}) = \mathbf{e}^{\mathsf{T}}\mathbf{p}, \qquad \phi_{\mathbf{e}} \in L^2_0(\mu)$$

and let $\psi_{\mathbf{e}}$ denote an approximation of $\phi_{\mathbf{e}}$. By Itô's formula, we obtain

$$\phi_{\mathbf{e}}(\mathbf{q}_T,\mathbf{p}_T) - \phi_{\mathbf{e}}(\mathbf{q}_0,\mathbf{p}_0) = -\int_0^T \mathbf{e}^{\mathsf{T}}\mathbf{p}_t \, \mathrm{d}t + \sqrt{2\gamma\beta^{-1}} \int_0^T \nabla_{\mathbf{p}}\phi_{\mathbf{e}}(\mathbf{q}_t,\mathbf{p}_t)\cdot \mathrm{d}\mathbf{W}_t.$$

Therefore

$$\begin{aligned}\mathbf{e}^{\mathsf{T}}(\mathbf{q}_T - \mathbf{q}_0) &= \int_0^T \mathbf{e}^{\mathsf{T}}\mathbf{p}_t \, \mathrm{d}t \\ &\approx -\psi_{\mathbf{e}}(\mathbf{q}_T,\mathbf{p}_T) + \psi_{\mathbf{e}}(\mathbf{q}_0,\mathbf{p}_0) + \sqrt{2\gamma\beta^{-1}} \int_0^T \nabla_{\mathbf{p}}\psi_{\mathbf{e}}(\mathbf{q}_t,\mathbf{p}_t)\cdot \mathrm{d}\mathbf{W}_t =: \xi_T.\end{aligned}$$

which suggests the improved estimator

$$v(T) = \frac{\left|\mathbf{e}^{\mathsf{T}}(\mathbf{q}_T - \mathbf{q}_0)\right|^2}{2T} - \left(\frac{|\xi_T|^2}{2T} - \lim_{T\to\infty} \mathbf{E}\left[\frac{|\xi_T|^2}{2T}\right]\right).$$

Smaller bias if $-\mathcal{L}\psi_{\mathbf{e}} \approx \mathbf{e}^{\mathsf{T}}\mathbf{p}$:

$$\left|\mathbf{E}\left[v(T)\right] - D_{\mathbf{e}}^{\gamma}\right| \leq \frac{L\max\{\gamma^2, \gamma^{-2}\}}{T\ell^2} \left\|\mathbf{e}^{\mathsf{T}}\mathbf{p} + \mathcal{L}\psi_{\mathbf{e}}\right\| \left(\beta^{-1/2} + \|\mathcal{L}\psi_{\mathbf{e}}\|\right).$$

Smaller variance:

$$\mathbf{V}\left[v(T)\right] \leq C\left(T^{-1}{\|\phi_{\mathbf{e}} - \psi_{\mathbf{e}}\|_{L^4(\mu)}}^2 + \gamma{\|\nabla_{\mathbf{p}}\phi_{\mathbf{e}} - \nabla_{\mathbf{p}}\psi_{\mathbf{e}}\|_{L^4(\mu)}}^2\right) \times \left(T^{-1}\|\phi_{\mathbf{e}} + \psi_{\mathbf{e}}\|_{L^4(\mu)}^2 + \gamma\|\nabla_{\mathbf{p}}\phi_{\mathbf{e}} + \nabla_{\mathbf{p}}\psi_{\mathbf{e}}\|_{L^4(\mu)}^2\right).$$

Construction of $\psi_{\mathbf{e}}$ in the one-dimensional setting. We consider two approaches:

- Approximate the solution to the Poisson equation by a Galerkin method.
- Use asymptotic result for the Poisson equation:

$$\gamma\phi \xrightarrow[\gamma\to 0]{L^2(\mu)} \phi_{\mathrm{und}},$$

which suggests letting $\psi = \phi_{\mathrm{und}}/\gamma$.

Construction of the approximate solution $\psi_{\mathbf{e}}$ in dimension 2

We consider the potential

$$V(\mathbf{q}) = -\frac{1}{2}\Big(\cos(q_1) + \cos(q_2)\Big) - \delta \cos(q_1)\cos(q_2).$$

- For this potential, $\mathbf{D}$ is isotropic $\rightsquigarrow$ sufficient to consider $\mathbf{e} = (1,0)$,

$$D_{(1,0)} = \left\langle \phi_{(1,0)}, p_1 \right\rangle, \qquad -\mathcal{L}\phi_{(1,0)}(\mathbf{q},\mathbf{p}) = p_1.$$

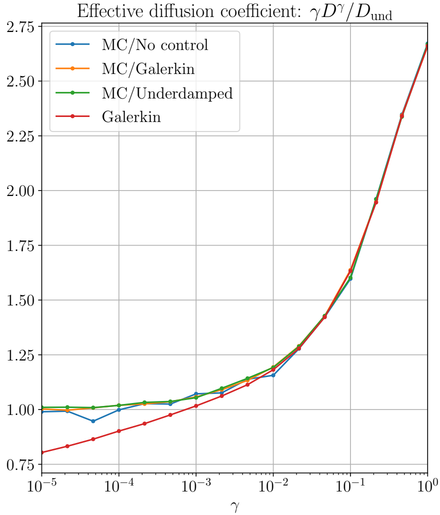
- If $\delta = 0$, then the solution is $\phi_{(1,0)}(\mathbf{q},\mathbf{p}) = \phi_{1\mathrm{D}}(q_1, p_1)$, where $\phi_{1\mathrm{D}}$ solves

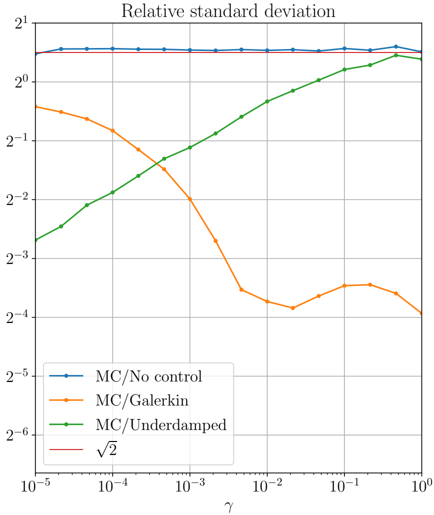
$$-\mathcal{L}_{1\mathrm{D}}\phi_{1\mathrm{D}}(q,p) = p, \qquad V_{1\mathrm{D}}(q) = \frac{1}{2}\cos(q).$$

- We take $\psi_{(1,0)}(\mathbf{q},\mathbf{p}) = \psi_{1\mathrm{D}}(q_1, p_1)$, where $\psi_{1\mathrm{D}} \approx \phi_{1\mathrm{D}}$.

Outline

Numerical experiments for the one-dimensional case (1/2)





Numerical experiments for the one-dimensional case (2/2)

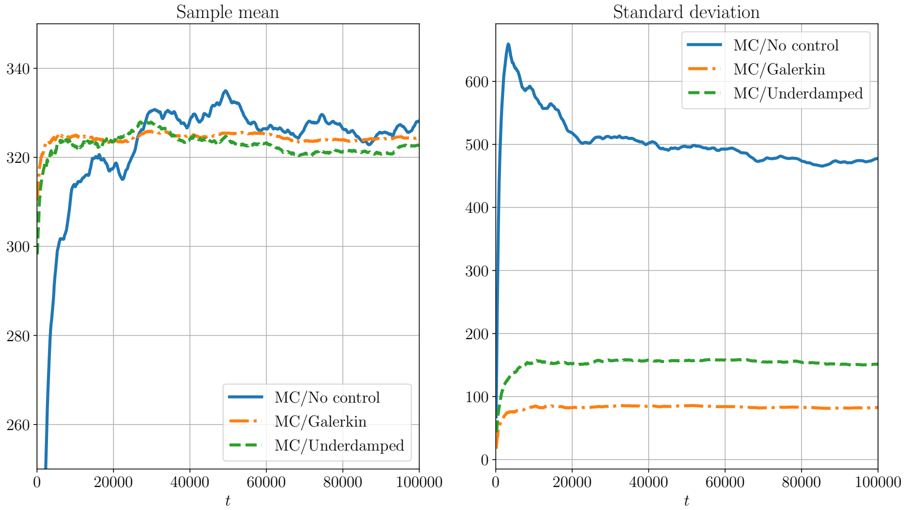
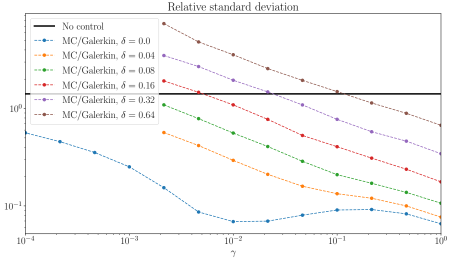
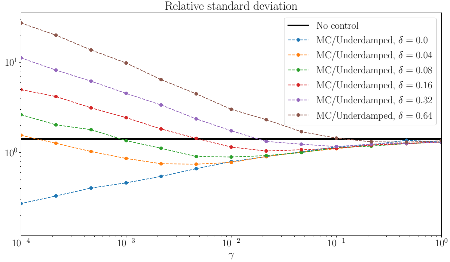


Figure: Evolution of the sample mean and standard deviation, estimated from $J = 5000$ realizations for $\gamma = 10^{-3}$.

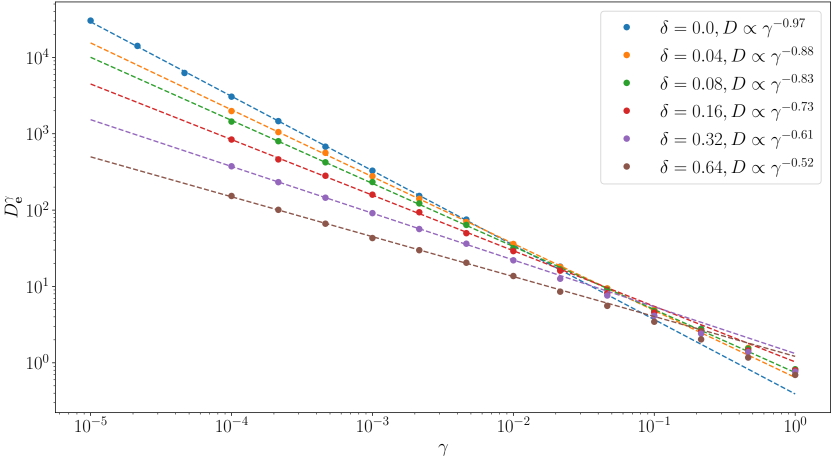
Performance of the control variates approach in dimension 2





- Variance reduction is possible if $|\delta| / \gamma \ll 1$;
- Control variates are not very useful as $\gamma \to 0$ and δ is fixed. . .

Scaling of the mobility in dimension 2



Summary of part I and perspectives for future work

In this part, we presented

- a variance reduction approach for efficiently estimating the mobility;
- numerical results showing that the scaling of the mobility is not universal.

Perspectives for future work:

- Use alternative methods (PINNs, Gaussian processes) to solve the Poisson equation;
- Study and improve variance reduction approaches for other transport coefficients.

Part II: importance sampling for overdamped Langevin dynamics

Martin Chak

Sorbonne Université

Tony Lelièvre

École des Ponts ParisTech

CERMICS & Inria

Gabriel Stoltz

École des Ponts ParisTech

CERMICS & Inria

Outline

Objective of the sampling problem

Calculate averages with respect to

$$\mu = \frac{e^{-V}}{Z}, \qquad Z = \int_{\mathbf{T}^d} e^{-V}.$$

Often in applications:

- The dimension d is large;
- The normalization constant Z is unknown;
- We cannot generate i.i.d. samples from μ.

Markov chain Monte Carlo (MCMC) approach:

$$I := \mu(f) \approx \mu^T(f) := \frac{1}{T}\int_0^T f(Y_t)\,\mathrm{d}t$$

for a Markov process $(Y_t)_{t\geq 0}$ that is ergodic with respect to μ.

Example: overdamped Langevin dynamics

$$\mathrm{d}Y_t = -\nabla V(Y_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t, \qquad Y_0 = y_0.$$

Importance sampling in the MCMC context

If $(X_t)_{t\geq 0}$ is a Markov process ergodic with respect to

$$\mu_U = \frac{\mathrm{e}^{-V-U}}{Z_U}, \qquad Z_U = \int_{\mathbf{T}^d} \mathrm{e}^{-V-U},$$

then $I = \mu(f)$ may be approximated by

$$\mu_U^T(f) := \frac{\displaystyle \frac{1}{T}\int_0^T (f\,\mathrm{e}^U)(X_t)\,\mathrm{d}t}{\displaystyle \frac{1}{T}\int_0^T (\mathrm{e}^U)(X_t)\,\mathrm{d}t}.$$

Markov process: overdamped Langevin dynamics

$$\mathrm{d}X_t = -\nabla(V+U)(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t, \qquad X_0 = x_0.$$

Asymptotic variance: Under appropriate conditions, it holds that

$$\sqrt{T}\big(\mu_U^T(f) - I\big) \xrightarrow[T\to\infty]{\text{Law}} \mathcal{N}\big(0, \sigma_f^2[U]\big).$$

Objective

Find U such that the asymptotic variance $\sigma_f^2[U]$ is minimized.

Background: importance sampling in the i.i.d. setting (1/2)

Given i.i.d. samples $\{X^1, X^2, \dots\}$ from μ_U, we define

$$\mu_U^N(f) := \frac{\sum_{n=1}^N (f\,\mathrm{e}^U)(X^n)}{\sum_{n=1}^N (\mathrm{e}^U)(X^n)} = I + \frac{\frac{1}{N}\sum_{n=1}^N \left((f-I)\,\mathrm{e}^U\right)(X^n)}{\frac{1}{N}\sum_{n=1}^N (\mathrm{e}^U)(X^n)},$$

Numerator: by the central limit theorem,

$$\frac{1}{\sqrt{N}}\sum_{n=1}^N \left((f-I)\,\mathrm{e}^U\right)(X^n) \xrightarrow[N\to\infty]{\text{Law}} \mathcal{N}\left(0, \int_{\mathbf{T}^d} \left|(f-I)\,\mathrm{e}^U\right|^2 \mathrm{d}\mu_U\right)$$

Denominator: by the strong law of large numbers,

$$\frac{1}{N}\sum_{n=1}^N \left(\mathrm{e}^U\right)(X^n) \xrightarrow[N\to\infty]{\text{a.s.}} \frac{Z}{Z_U}.$$

Therefore, by Slutsky's theorem,

$$\sqrt{N}\left(\mu_U^N(f) - I\right) \xrightarrow[T\to\infty]{\text{Law}} \mathcal{N}\left(0, s_f^2[U]\right), \qquad s_f^2[U] := \frac{Z_U^2}{Z^2}\int_{\mathbf{T}^n} \left|(f-I)\,\mathrm{e}^U\right|^2 \mathrm{d}\mu_U.$$

Background: importance sampling in the i.i.d. setting (2/2)

By the Cauchy–Schwarz inequality, it holds that

$$s_f^2[U] \geq \frac{Z_U^2}{Z^2} \left(\int_{\mathbf{T}^d} |f - I| \, \mathrm{e}^U \, \mathrm{d}\mu_U \right)^2 = \frac{1}{Z^2} \left(\int_{\mathbf{T}^d} |f - I| \, \mathrm{e}^{-V} \right)^2,$$

with equality when $|f - I| \, \mathrm{e}^U$ is constant.

Optimal importance distribution

The optimal μ_U in the i.i.d. setting is

$$\mu_U \propto |f - I| \, \mathrm{e}^{-V}$$

Objectives:

- Is there a counterpart of this formula in the MCMC setting?
- If not, can we approximate the optimal distribution numerically?

Outline

Formula for the asymptotic variance

Let $\mathcal{L}_U$ denote the generator of the Markov semigroup associated to the modified potential;

$$\mathcal{L}_U = -\nabla(V+U)\cdot\nabla + \Delta.$$

Limit theorem

Under appropriate conditions, it holds that

$$\sqrt{T}\big(\mu_U^T(f) - I\big) \xrightarrow[T\to\infty]{\text{Law}} \mathcal{N}\big(0, \sigma_f^2[U]\big).$$

The asymptotic variance is given by

$$\sigma_f^2[U] = \frac{2Z_U^2}{Z^2}\int_{\mathbf{T}^d} \phi_U (f-I)\, \mathrm{e}^U \, \mathrm{d}\mu_U,$$

where ϕ_U is the unique solution in $H^1(\mu_U)\cap L_0^2(\mu_U)$ to

$$-\mathcal{L}_U\phi_U = (f-I)\,\mathrm{e}^U\,.$$

Main ideas of the proof: central limit theorem for martingales, Slutsky's theorem.

Explicit optimal U in dimension 1

In dimension one, it holds that

$$\sigma_f^2[U] \geq \frac{2}{Z^2} \inf_{A \in \mathbf{R}} \left(\int_{\mathbf{T}} \left| F(x) + A \right| \mathrm{d}x \right)^2. \qquad (1)$$

where

$$F(x) := \int_0^x \left(f(\xi) - I \right) \mathrm{e}^{-V(\xi)} \, \mathrm{d}\xi.$$

This inequality (1) is an equality for

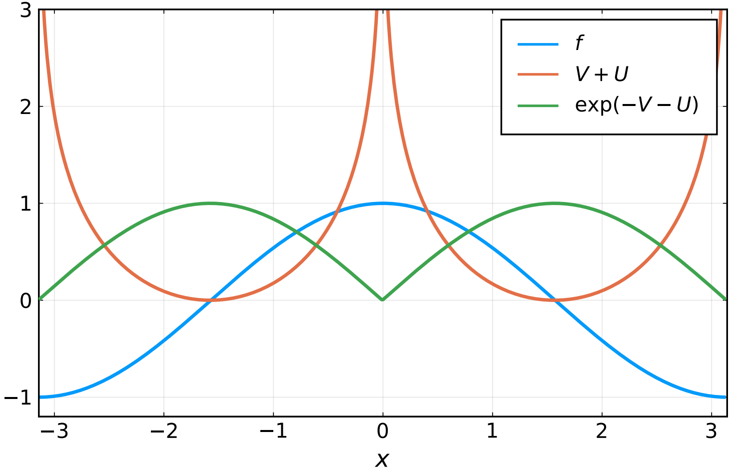
$$U(x) = U_*(x) = -V(x) - \ln |F(x) + A_*|,$$

where A_* is the constant achieving the infimum in (1).

- The potential U_* is generally singular: impractical for numerics...
- The lower bound in (1) can be approached by a smooth U.

Example (1/2)

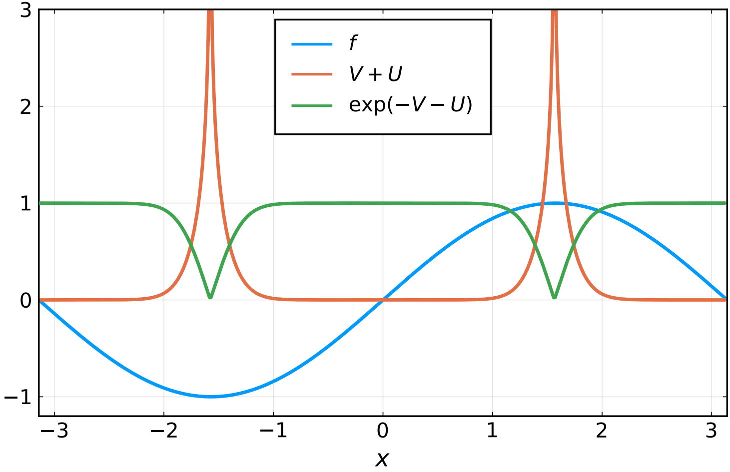
Assume that $V = 0$ and $f(x) = \cos(x)$.



$\rightsquigarrow$ The optimal potential "divides" the domain into two parts.

Example (2/2)

Assume that $V(x) = 5\cos(2x)$ and $f(x) = \sin(x)$. The target measure is multimodal.



Variance reduction by a factor > 1000!

Finding the optimal U in the multidimensional setting

Proposition (Functional derivative of the asymptotic variance)

Let ϕ_U denote the solution to

$$-\mathcal{L}_U \phi_U = (f - I)\, \mathrm{e}^U \,. \tag{2}$$

Under appropriate conditions, it holds for all $\delta U \in C^\infty(\mathbf{T}^d)$ that

$$\begin{aligned} \frac{1}{2} \mathrm{d}\sigma_f^2[U] \cdot \delta U &:= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left(\sigma_f^2[U + \varepsilon \delta U] - \sigma_f^2[U] \right) \\ &= \frac{Z_U^2}{Z^2} \int_{\mathbf{T}^d} \delta U \left(|\nabla \phi_U|^2 - \int_{\mathbf{T}^d} |\nabla \phi_U|^2 \, \mathrm{d}\mu_U \right) \mathrm{d}\mu_U \,. \end{aligned} \tag{3}$$

Steepest descent approach:

- Solve the Poisson equation (2) numerically;
- Construct an ascent direction G for σ_f^2 using (3), e.g. $\delta U = |\nabla \phi_U|^2$;
- Perform a step in this direction: $U \leftarrow U - \eta G$;
- Repeat until convergence.

No smooth minimizers

Corollary (No smooth minimizer)

Unless f is constant, there is no perturbation potential $U \in C^\infty(\mathbf{T}^n)$ that is a critical point of $\sigma_f^2[U]$.

Proof. Assume by contradiction that U_* is smooth critical point. Then

$$0 = \frac{1}{2} \mathrm{d}\sigma_f^2[U_*] \cdot \delta U = \frac{Z_U^2}{Z^2} \int_{\mathbf{T}^d} \delta U \left(|\nabla \phi_{U_*}|^2 - \int_{\mathbf{T}^d} |\nabla \phi_{U_*}|^2 \, \mathrm{d}\mu_{U_*} \right) \mathrm{d}\mu_{U_*},$$

for all $\delta U \in C^\infty(\mathbf{T}^d)$.

- Therefore, it must hold that $|\nabla \phi_{U_*}|^2 = C$ is constant.
- Since ϕ_{U_*} is a smooth function, there is $x \in \mathbf{T}^d$ such that $\nabla \phi_{U_*}(x) = 0$.
- Consequently $C = 0$ and so $\nabla \phi_{U_*} = 0$: contradiction because then $\mathcal{L}_{U_*} \phi_{U_*} = 0$.

$\rightsquigarrow$ The optimal perturbation potential is not convenient in practice...

Example (1/2)

Assume that $V = 0$ and $f(x) = \sin(x_1) + \sin(x_2)$.

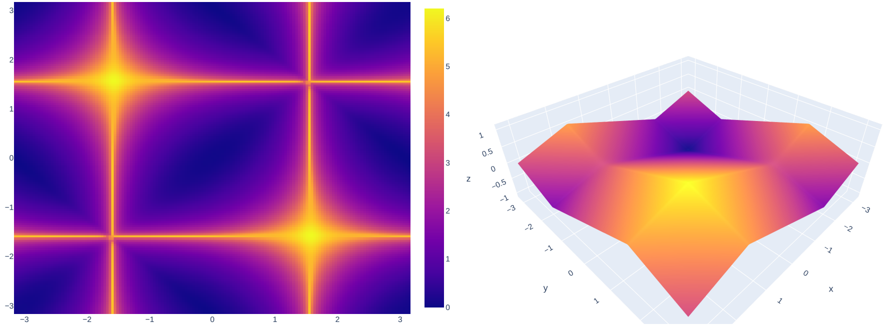
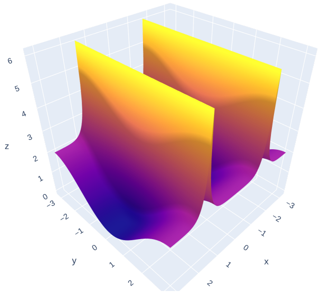


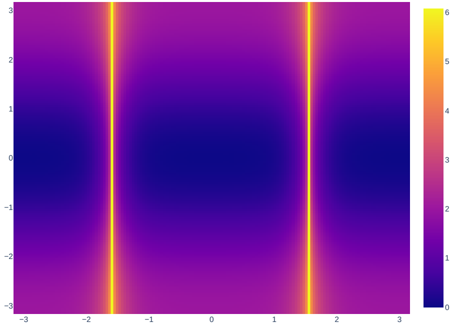
Figure: Optimal total potential (left) together with the solution to the associated Poisson equation (right).

$\rightsquigarrow$ The domain is again divided into subdomains that suffice for estimating I.

Example (2/2): multimodal target e^{-V}

Assume that $V(x) = 2\cos(x_1) - \cos(x_2)$ and $f(x) = \sin(x_1)$.





Variance reduction by a factor ≈ 6!

Outline

Alternative: minimizing the expected variance over a class of observables

Assume that the observables are well described by a Gaussian random field

$$f = \sum_{j=1}^{J} \sqrt{\lambda_j} u_j f_j, \qquad u_j \sim \mathcal{N}(0,1), \qquad \lambda_j \in (0,\infty).$$

Question: can we find U such that $\sigma^2[U] := \mathbf{E}\big(\sigma_f^2[U]\big)$ is minimized?

- It holds that
$$\sigma^2[U] = \sum_{j=1}^{J} \lambda_j \sigma_{f_j}^2.$$
- The functional derivative of $\sigma^2[U]$ is given by
$$\frac{1}{2} \mathrm{d}\sigma^2[U] \cdot \delta U = \frac{Z_U^2}{Z^2} \int_{\mathbf{T}^d} \left(\delta U - \int_{\mathbf{T}^d} \delta U \, \mathrm{d}\mu_U \right) \left(\sum_{j=1}^{J} \lambda_j |\nabla \phi_j|^2 \right) \mathrm{d}\mu_U .$$
- The steepest descent approach can be employed in this case too!

Here $V(x) = 2\cos(2x_1) - \cos(x_2)$ and $f \sim \mathcal{N}\big(0, (\Delta + \mathcal{I})^{-1}\big)$.

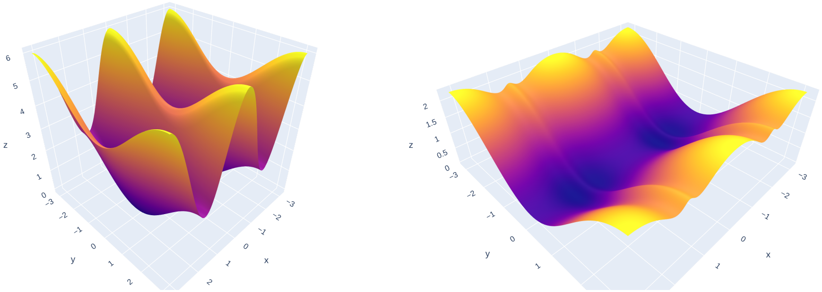


Figure: Potential V (left) and optimal potential $V + U$ (right).

Summary of part II and perspectives for future work

In this part,

- We studied an importance sampling approach for the overdamped Langevin dynamics.
- We proposed an approach for calculating the optimal perturbation potential.

Perspectives:

- Solving the Poisson equation accurately is not possible in high dimension.
- Application to high-dimensional systems:

$$U(x) = U\big(\xi(x)\big), \qquad \xi \text{ reaction coordinate.}$$

Thank you for your attention!

Connection with the asymptotic variance of MCMC estimators

Ergodic theorem[10]: for an observable $\varphi \in L^1(\mu)$,

$$\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(\mathbf{q}_s, \mathbf{p}_s)\,\mathrm{d}s \xrightarrow[t\to\infty]{a.s.} \mathbf{E}_\mu \varphi.$$

Central limit theorem[11]: If the following Poisson equation has a solution $\phi \in L^2(\mu)$,

$$-\mathcal{L}\phi = \varphi - \mathbf{E}_\mu \varphi,$$

then a central limit theorem holds:

$$\sqrt{t}\big(\widehat{\varphi}_t - \mathbf{E}_\mu \varphi\big) \xrightarrow[t\to\infty]{\text{Law}} \mathcal{N}(0, \sigma_\varphi^2), \qquad \sigma_\varphi^2 = \langle \phi, \varphi - \mathbf{E}_\mu \varphi \rangle\,.$$

Connection with effective diffusion: Apply this result with $\varphi(\mathbf{q},\mathbf{p}) = \mathbf{e}^\mathsf{T}\mathbf{p}$.

[10] W. Kliemann. Recurrence and invariant measures for degenerate diffusions. Ann. Probab., 1987.
[11] R. N. Bhattacharya. On the functional central limit theorem and the law of the iterated logarithm for Markov processes. Z. Wahrsch. Verw. Gebiete, 1982.