Sticky Coupling as a Control Variate for Sensitivity Analysis

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Introduction

Motivation: Computing transport coefficients (mobility, thermal conductivity, shear viscosity) in statistical physics

Goal: Reduce the variance of the estimator of sensitivity/transport coefficient.

Dynamics

Consider the following family of SDEs with values in $\mathbb{R}^d$ and additive noise:

$$dX_t^\eta = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

where $b, F : \mathbb{R}^d \to \mathbb{R}^d$ are smooth, F bounded, $\beta > 0$, and $\eta \in \mathbb{R}$. We assume that for each η it admits a unique invariant measure ν_η.

Contractivity Assumption

We assume that there exists $m > 0$ and $M \geq 0$ such that

$$\langle x - y, b(x) - b(y)\rangle \leq -m\,|x-y|^2, \quad \text{if } |x-y| \geq M.$$

Transport coefficients

Estimator of linear response (observable R average 0 with respect to ν_0)

$$\widehat{\Phi}_{\eta,t} = \frac{1}{\eta t}\int_0^t R(X_t^\eta)\, ds \xrightarrow[t\to+\infty]{\text{a.s.}} \alpha_{R,\eta} := \frac{1}{\eta}\int_{\mathbb{R}^d} R\, d\nu_\eta = \alpha_R + \mathrm{O}(\eta)$$

Asymptotic variance $\lim_{t\to\infty} t\mathrm{Var}\left(\widehat{\Phi}_{\eta,t}\right) = \mathrm{O}(\eta^{-2})$

Coupling Based Estimator

Idea: Use the reference dynamics to reduce the variance and bias of the estimator:

$$\widehat{\Psi}_{\eta,t} = \frac{1}{\eta t}\int_0^t \left[R\left(X_s^\eta\right) - R\left(Y_s^0\right)\right] ds,$$

with $(X_t^\eta, Y_t^\eta)_{t\geq 0}$ the solution of following system with coupled driving noises $\left(W_t, \widetilde{W}_t\right)_{t\geq 0}$

$$dX_t^\eta = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

$$dY_t^0 = b\left(Y_t^0\right) dt + \sqrt{\frac{2}{\beta}} d\widetilde{W}_t.$$

Synchronous Coupling

Use the same Brownian motion to drive the two trajectories, i.e $W = \widetilde{W}$. In this case the difference process is C^1:

$$d\left(X_t^\eta - Y_t^0\right) = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right) - b\left(Y_t^0\right)\right) dt.$$

If the drift b is contractive everywhere, i.e. there exists $M = 0$, then

$$\left|X_t^\eta - Y_t^0\right| \leq \left(\left|X_0^\eta - Y_0^0\right| - \frac{\eta \|F\|_\infty}{2m}\right) \mathrm{e}^{-mt} + \frac{\eta\|F\|}{2m}.$$

Thus, if $X_0^\eta = Y_0^0$ then $\mathbb{E}\left[\left|\widehat{\Psi}_{\eta,t}^{\text{sync}}\right|^p\right]$ is uniformly bounded as $\eta \to 0$.

Sticky Coupling

If the drift is *not* contractive everywhere, synchronous coupling can fail spectacularly because the drift does not necessarily bring together the trajectories.

Idea: Use the noise to bring the trajectories together.

Constructed in [4], uses reflection coupling to bring the trajectories together and is stick in the sense that $\left|X_t^\eta - Y_t^0\right| \leq r_t^\eta$ a.s where $(r_t^\eta)_{t\geq 0}$ is diffusion on $[0,\infty)$ with a sticky boundary condition at zero

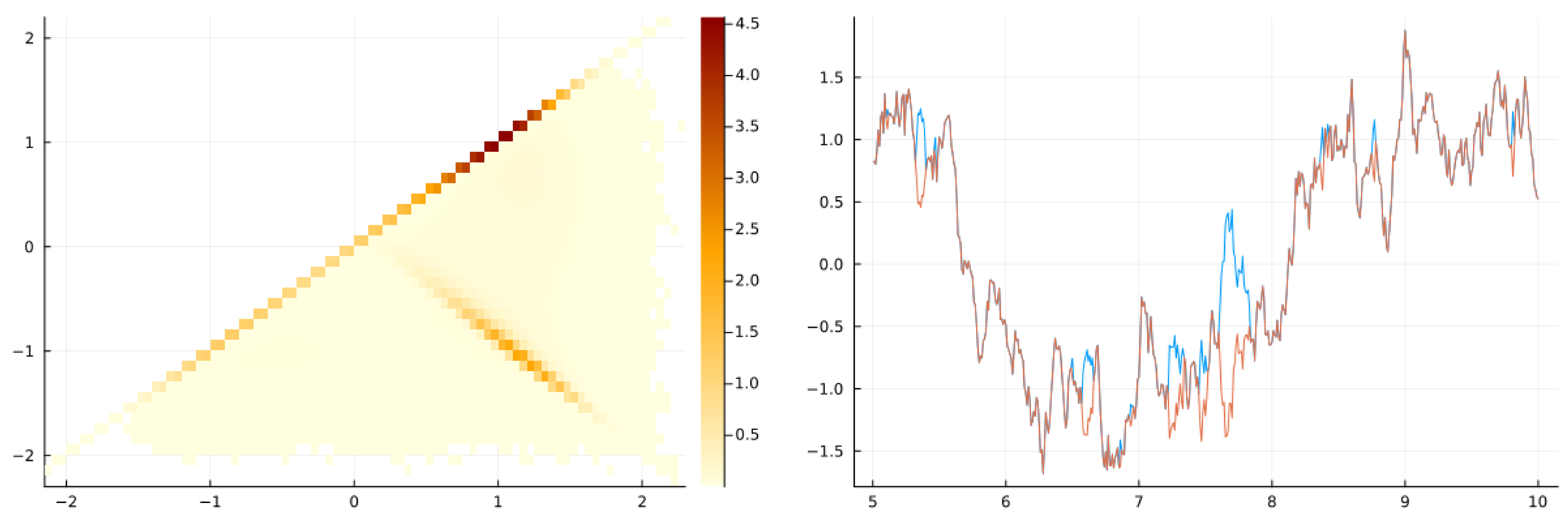


Figure: Sticky coupling of a 1D particle in a double well potential perturbed by a constant force to the right, i.e. $b(x) = -4x\left(x^2-1\right)$ and $\eta F(x) = 1$. **Left:** histogram of coupled process; **Right:** segment of trajectory of coupled process

Problem: Sticky coupled process is highly degenerate. Zero set of r^η is a fat random Cantor set. Existence of invariant measure and its ergodic properties are unclear.

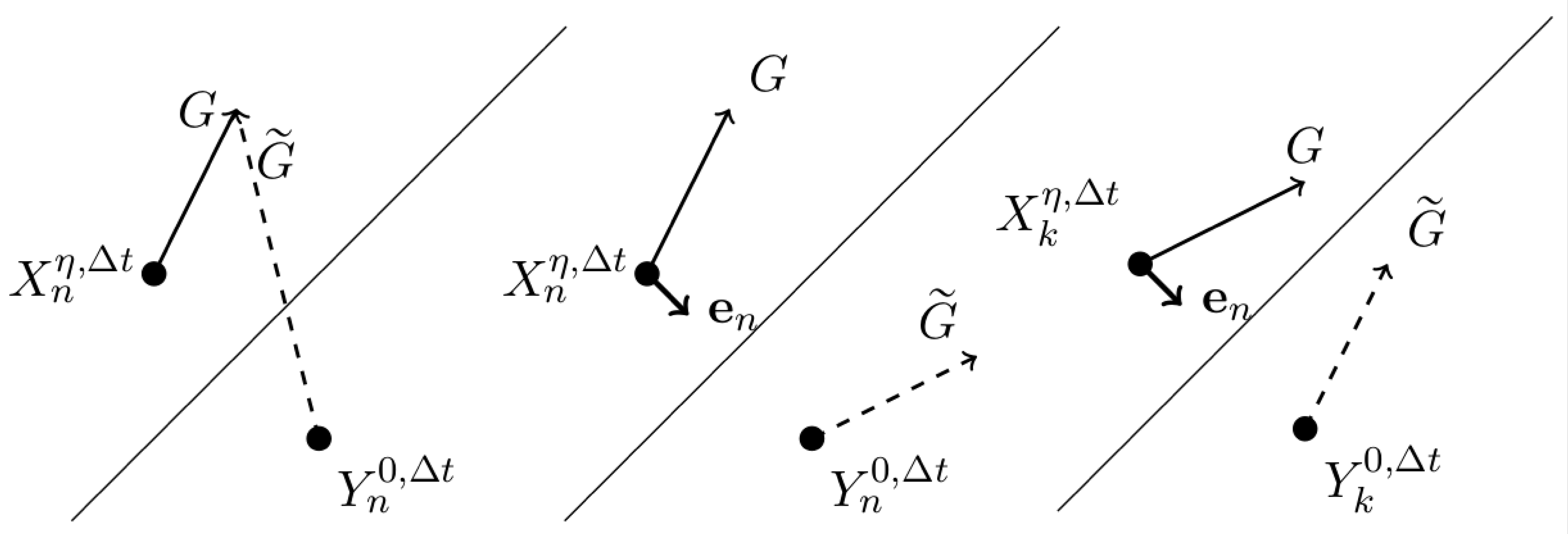
Discrete Sticky Coupling

Work around: Use discrete-time sticky coupling [2]: $G_{n+1} \sim \mathcal{N}(0, \mathrm{Id})$ and $U_{n+1} \sim \mathrm{Unif}([0,1])$

$$X_{n+1}^{\eta,\Delta t} = X_n^{\eta,\Delta t} + \Delta t\left[b\left(X_n^{\eta,\Delta t}\right) + \eta F\left(X_n^{\eta,\Delta t}\right)\right] + \sqrt{\frac{2\Delta t}{\beta}} G_{n+1},$$

$$Y_{n+1}^{0,\Delta t} = \begin{cases} X_{n+1}^{\eta,\Delta t}, & \text{if } U_{n+1} \leq p_{\Delta t,\beta}\left(X_n^{\eta,\Delta t}, Y_n^{0,\Delta t}, G_{n+1}\right), \\ Y_n^{0,\Delta t} + \Delta t b\left(Y_n^{0,\Delta t}\right) + \sqrt{\frac{2\Delta t}{\beta}}\left[\mathrm{Id} - 2\mathbf{e}_n\mathbf{e}_n^T\right] G_{n+1} & \text{otherwise,} \end{cases}$$

with $p_{\Delta t,\beta}(x,y,g)$ being the overlap of the two trajectories marginal transition densities at the n-th step.



(a) Collision (b) Reflection resulting in separation (c) Reflection resulting in contraction

The discrete-time sticky coupled process admits a unique invariant probability measure, $\mu_{\eta,\Delta t}$ and is geometrically ergodic with respect to this measure. Furthermore, we can control the mass $\mu_{\eta,\Delta t}$ puts off the diagonal:

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} \mathbf{1}_{\{x\neq y\}} \mathrm{e}^{-c\left(|x|^2+|y|^2\right)} \mu_{\eta,\Delta t}(dx\,dy) \leq C\eta\left(\nu_{\eta,\Delta t}\left(\mathrm{e}^{-c|x|^2}\right) + \nu_{0,\Delta t}\left(\mathrm{e}^{-c|x|^2}\right)\right).$$

Discrete-time Estimator

We introduce the following discrete-time estimator of $\alpha_{R,\eta}$

$$\widehat{\Psi}_{\eta,N}^{\text{sticky},\Delta t} = \frac{1}{\eta N}\sum_{n=0}^{N-1}\left[R\left(X_n^{\eta,\Delta t}\right) - R\left(Y_n^{0,\Delta t}\right)\right]$$

Theorem 1 *Let $\eta_* > 0$ and R such that $\nu_0(R) = 0$. Assume that $X^{\eta,\Delta t}$ and $Y^{0,\Delta t}$ have the same initial value. Under the contractivity assumption and some technical assumptions, there exists $K_1, K_2 > 0$ such that*

$$\forall \eta \in [-\eta_*, \eta_*], \quad \lim_{N\to\infty} N\mathrm{Var}\left(\widehat{\Psi}_{\eta,N}^{\text{sticky},\Delta t}\right) \leq \frac{K_1}{\eta},$$

and

$$\left|\mathbb{E}\left[\widehat{\Psi}_{\eta,N}^{\Delta t}\right] - \alpha_{R,\eta}\right| \leq K_2\left(\frac{1}{\Delta t N} + \Delta t\right).$$

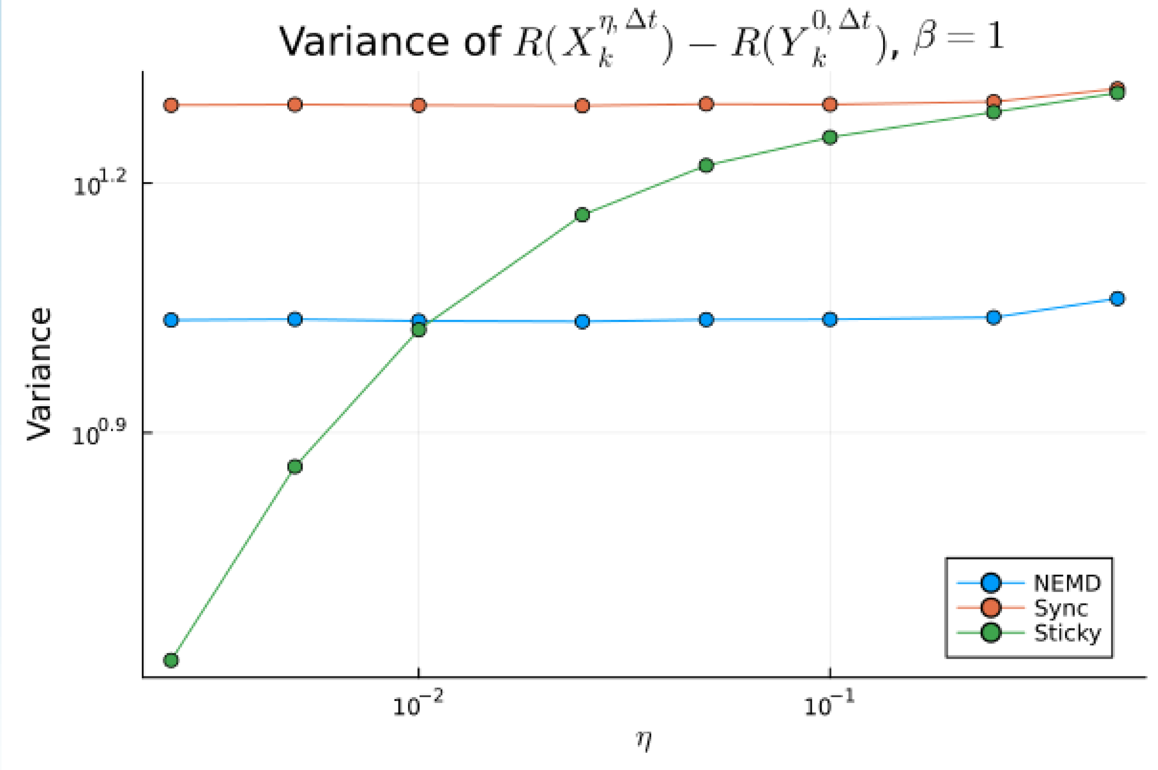
Numerical Illustration

Example: Lennard-Jones Cluster in 2D:

The drift is given by $b(x) = -\nabla(U_1 + U_2)$ with interaction part U_1

$$U_1(x) = \sum_{i\geq j}\left[\left(\frac{1}{|r_{ij}|}\right)^{12} - 2\left(\frac{1}{|r_{ij}|}\right)^6\right],$$

with $r_{ij} = |x^i - x^j|$ if $i < j$ and $r_{ii} = |x^i|$. And U_2 a confinig potential For F we use sine shear on each particle.



Code available: github.com/shiva-darshan/sticky_coupling

References

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