





Sticky Coupling as a Control Variate for Computing Transport Coefficients

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Outline

- Linear response for steady-state nonequilibrium dynamics
 - Perturbations of equilibrium dynamics
 - Definition of transport coefficients
 - Variance of NEMD estimator
- Couplings based estimators
 - Couplings based estimators
 - Synchronous coupling
 - Sticky coupling
- Numerical Illustrations
- Extensions and perspectives

Linear response for steady-state nonequilibrium dynamics

Nonequilibrium stochastic dynamics

Consider:

$$dX_{t}^{\eta} = \left(b\left(X_{t}^{\eta}\right) + \eta F\left(X_{t}^{\eta}\right)\right)dt + \sqrt{\frac{2}{\beta}}dW_{t},$$

where $b, F : \mathbb{R}^d \to \mathbb{R}^d$ Lipschitz, with F bounded, $\beta > 0$, and $\eta \in \mathbb{R}$.

Assumption

Contractivity at Infinity

There exists $M \ge 0$ and m > 0 such that

$$\langle x - y, b(x) - b(y) \rangle \leqslant -m |x - y|^2$$
, if $|x - y| \geqslant M$.

Example if $b(x) = -\nabla (V_1(x) + V_2(x))$, where V_1 is a confining potential and V_2 is a compactly supported.

Estimating transport coefficients

Observable R, s.t. $\nu_0(R)=0$, the transport coefficient α_R defined as:

$$\alpha_R = \lim_{\eta \to 0} \frac{\mathbb{E}_{\eta}(R)}{\eta} = \int_{\mathbb{R}^d} R \, \mathfrak{f} \, d\nu_0, \qquad \mathfrak{f} = -(\mathcal{L}_0^*)^{-1} \widetilde{\mathcal{L}}^* \mathbf{1},$$

Estimator of linear response:

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

Sources of error:

- ullet Statistical error with asymptotic variance $\mathrm{O}(\eta^{-2})$
- Bias from finite integration time
- Timestep discretization bias
- Bias $O(\eta)$ due to $\eta \neq 0$

Analysis of Variance

• Statistical error dictated by Central Limit Theorem:

$$\sqrt{t}\left(\widehat{\Phi}_{\eta,t} - \alpha_{\eta}\right) \xrightarrow[t \to +\infty]{\text{law}} \mathcal{N}\left(0, \frac{\sigma_{R,\eta}^2}{\eta^2}\right),$$

so $\hat{\Phi}_{\eta,t} = \alpha_{\eta} + O_P\left(\frac{1}{\eta\sqrt{t}}\right) \rightarrow \text{requires long simulation times } t \sim \eta^{-2}.$

Poisson equation $-\mathcal{L}_{\eta}\widetilde{R}_{\eta}=\Pi_{\eta}R$, the asymptotic variance given by

$$\begin{split} \sigma_{R,\eta}^2 &= \int_{\mathbb{R}^d} \Pi_{\eta} R \widetilde{R}_{\eta} \, d\nu_{\eta} = \int_{\mathbb{R}^d} R \widetilde{R}_0 \, d\nu_0 + \eta \int_{\mathbb{R}^d} R \left(\widetilde{R}_0 \mathfrak{f} + \widecheck{R} \right) \, d\nu_0 + \eta^2 \mathcal{R}_{\eta} \\ &= \sigma_{R,0}^2 + \eta \int_{\mathbb{R}^d} R \left(\widetilde{R}_0 \mathfrak{f} + \widecheck{R} \right) \, d\nu_0 + \eta^2 \mathcal{R}_{\eta}, \end{split}$$

where $\widetilde{R}_{\eta}=\widetilde{R}_{0}+\eta\widecheck{R}$; \widetilde{R}_{0} the solution of $-\mathcal{L}_{0}\widetilde{R}_{0}=R$ and \widecheck{R} nice.

Couplings Based Estimators

Couplings Based Estimator

Definition

A coupling of two random variables X and Y is a couple $\left(\widetilde{X},\widetilde{Y}\right)$ of random variables such that $\widetilde{X}\stackrel{\mathrm{Law}}{=} X$ and $\widetilde{Y}\stackrel{\mathrm{Law}}{=} Y$

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

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

with $(X_t^{\eta}, Y_t^{\eta})_{t \ge 0}$ the solution of

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

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

where the driving noises $\left(W_t,\widetilde{W}_t\right)_{t\geqslant 0}$ are cleverly coupled.

Variance of Coupling Based Estimator

 μ_{η} invariant measure of the coupled process. The asymptotic variance is given by

$$\widetilde{\sigma}_{R,\eta}^{2} = \frac{2}{\eta^{2}} \int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \left(\widetilde{R}_{\eta}(x) - \widetilde{R}_{0}(y) \right) \left(\Pi_{\eta} R(x) - \Pi_{0} R(y) \right) \mu_{\eta} \left(dx \, dy \right)$$

$$\leq \frac{2}{\eta^{2}} \left(\int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \left(\widetilde{R}_{\eta}(x) - \widetilde{R}_{0}(y) \right)^{2} \mu_{\eta} \left(dx \, dy \right) \right)^{1/2}$$

$$\times \left(\int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \left(\Pi_{\eta} R(x) - \Pi_{0} R(y) \right)^{2} \mu_{\eta} \left(dx \, dy \right) \right)^{1/2}$$

$$\int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \left(\widetilde{R}_{\eta}(x) - \widetilde{R}_{0}(y) \right)^{2} \mu_{\eta} (dx \, dy)$$

$$\leq 2 \int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \left[\left(\widetilde{R}_{\eta}(x) - \widetilde{R}_{0}(x) \right)^{2} + \left(\widetilde{R}_{0}(x) - \widetilde{R}_{0}(y) \right)^{2} \right] \mu_{\eta} (dx \, dy)$$

Synchronous Coupling

By choosing $W=\widetilde{W}$, we can *synchronously* couple the X^{η} and Y^0 , giving

$$d\left(X_{t}^{\eta}-Y_{t}^{0}\right)=\left(b\left(X_{t}^{\eta}\right)-b\left(Y_{t}^{0}\right)+\eta F\left(X_{t}^{\eta}\right)\right)dt.$$

If the drift is strongly contractive everywhere, i.e.

$$\langle x - y, b(x) - b(y) \rangle \leqslant -m |x - y|^2, \quad \forall x, y \in \mathbb{R}^d,$$
 (2)

then we have pointwise control over the distance between the coupled trajectories:

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

As a consequence,

$$\mathbb{E}\left[\left|\widehat{\Psi}_{\eta,t}^{\mathrm{sync}}\right|^{p}\right] \leqslant C\left(\frac{\left|X_{0}^{\eta}-Y_{0}^{0}\right|^{p}}{\eta^{p}}\mathrm{e}^{-pmt}+\left(1-e^{-p\lambda t}\right)^{p}\left(\frac{\eta\left\|F\right\|}{2m}\right)^{p}\right),$$

and a fortiori bounded variance and bias as $\eta\downarrow 0$ if $\left|X_0^{\eta}-Y_0^0\right|^p=O\left(\eta^p\right)$.

Synchronous Coupling

In fact long as we have sufficient contractivity, say due to sufficiently high temperature¹ or in the underdamped case², we can control the moments of the estimator as

$$\mathbb{E}\left[\left|\widehat{\Psi}_{\eta,t}^{\mathrm{sync}}\right|^{p}\right] \leqslant C\left(\frac{\left|X_{0}^{\eta}-Y_{0}^{0}\right|^{p}}{\eta^{p}}\mathrm{e}^{-pmt}+\left(1-e^{-p\lambda t}\right)^{p}\left(\frac{\eta\left\|F\right\|}{2m}\right)^{p}\right),$$

Moral: When there is enough strong contractivity, synchronous coupling is hard to beat.

What to do when we do not have enough strong contractivity?

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¹P. Monmarché (2022) Wasserstein contraction and Poincaré inequalities for elliptic diffusions at high temperature

 $^{^2}$ P. Monmarché (2023) Almost sure contraction for diffusions on \mathbb{R}^d . Applications to generalized Langevin diffusions.

Sticky Coupling

One can constructed a coupling such that $\left(X_t^{\eta}-Y_t^0\right)_{t\geqslant 0}$ is sticky at 0 in the sense that they the difference is controlled by a one-dimensional process $(r_t^{\eta})_{t\geqslant 0}$ that spends a positive amount of time at 0

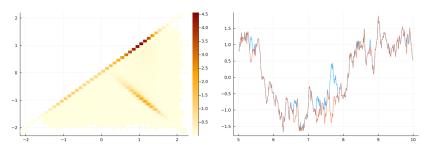


Figure: Sticky coupling of a 1D particle in a double well potential perturbed by a constant force to the right. **Left:** histogram of coupled process; **Right:** segment of trajectory of coupled process

³A. Eberle, R. Zimmer (2019) Sticky couplings of multidimensional diffusions with different drifts

Difficulties with Continuous-Time Sticky Coupling

- Non-explicit construction—constructed as the limit point of a tight family of processes
- Long-time properties of sticky coupled process are unclear. Unknown if it is ergodic, admits a unique invariant measure, etc.
- Convergence of discrete approximations also unclear

These difficulties arise because the limit object is highly degenerate. If it satisfied an SDE, the equation would have discontinuous coefficients and likely could not admit a strong solution.

The problem is that we have a "sticky" diffusion in \mathbb{R}^d

Work instead with discrete version of sticky coupling ⁴. Consider the estimator

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

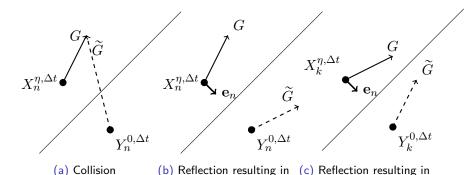
with $\left\{X_n^{\eta,\Delta t},Y_n^{0,\Delta t}\right\}_{k\in\mathbb{N}}$ the discrete sticky coupling of the Euler-Maruyama discretizations of $(X_t^\eta)_{t\geqslant 0}$ and $(Y^0)_{t\geqslant 0}$. Let $\{G_k\}_{k\geqslant 1}$ and $\{U_k\}_{k\geqslant 1}$ be i.i.d sequences of Gaussian and uniform random variables respectively. Evolution given by

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

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⁴A. Durmus, A. Eberle, A. Enfroy, A. Guillin, P. Monmarché (2021) *Discrete sticky couplings of functional autoregressive processes*

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



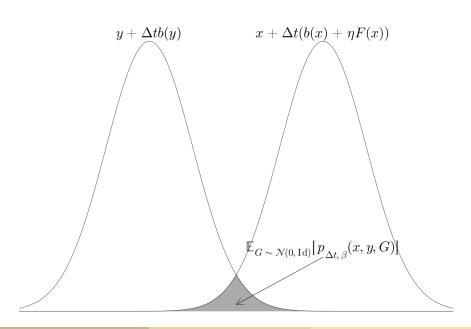
separation

contraction

$$\mathbf{E}\left(x,y\right) = y - x + \Delta t \left[b(y) - b(x) - \eta F(x)\right],$$

$$\mathbf{e}\left(x,y\right) = \begin{cases} \frac{\mathbf{E}\left(x,y\right)}{|\mathbf{E}\left(x,y\right)|} & \text{if } \mathbf{E}\left(x,y\right) \neq 0\\ \mathbf{e}_{0} & \text{otherwise,} \end{cases}$$

$$p_{\Delta t,\beta}\left(x,y,z\right) = \min \left\{1, \frac{\varphi\left(\sqrt{\frac{\beta}{2\Delta t}}\left|\mathbf{E}\left(x,y\right)\right| - \left\langle\mathbf{e}\left(x,y\right),z\right\rangle\right)}{\varphi\left(\left\langle\mathbf{e}\left(x,y\right),z\right\rangle\right)} \right\},$$



Proposition

For Δt sufficiently small, the discrete-time sticky coupled process $\left\{X_k^{\eta},Y_k^0\right\}_{k\in\mathbb{N}}$ admits a unique invariant measure, $\mu_{\eta,\Delta t}$. Furthermore it is geometrically ergodic wrt to this measure.

Proof: Use Hairer & Mattingly strategy⁵

Denote by $T^{\eta,\Delta t}$ the Markov kernel of the coupled process

Contractivity implies $e^{c|x|^2} + e^{c|y|^2}$ is a Lyapunov function.

 $p_{\Delta t,\beta}(x,y,z)>0 \implies$ always strictly positive probability of returning to the diagonal

 $\forall K > 0$ there exists $\rho_{K,\Delta t} \in (0,1)$ such that

$$\inf_{\max\{|x|,|y|\}\leqslant K}T^{\eta,\Delta t}\left(\left(x,y\right),\cdot\right)\geqslant\rho_{K,\Delta t}\xi_{K}\left(\cdot\right)$$

with ξ_K the uniform probability on $\{x = y\} \cap \{\max\{|x|, |y|\} \le K\}$

⁵M. Hairer and J. Mattingly Yet another look at Harris's ergodic theorem for Markov chains

Performance of the Sticky Coupling Based Estimator

The coupling based estimator improves by η^{-1} factor of :

Theorem

Let $\eta_*>0$ and $R\in \mathscr{S}$ such that $\nu_0(R)=0$. Assume that X^η and Y^0 have the same initial value. If the two previously stated assumptions hold and Δt small enough, then $\left\{X_k^{\eta,\Delta t},Y_k^{0,\Delta t}\right\}_{k\in\mathbb{N}}$ satisfies a CLT and there exists K_1,K_2 such that

$$\forall \eta \in [-\eta_*, \eta_*], \quad \lim_{N \to \infty} N \operatorname{Var}\left(\widehat{\Psi}_{\eta, N}^{\Delta t}\right) \leqslant \frac{K_1}{\eta},$$
 (3)

and

$$\left| \mathbb{E} \left[\widehat{\Psi}_{\eta,N}^{\Delta t} \right] - \alpha_{R,\eta} \right| \leqslant K_2 \left(\frac{1}{N} + \Delta t \right). \tag{4}$$

Key Idea of Proof

Proposition

Under the same hypothesis as the theorem, there exists c > 0 such that

Heuristic "proof" of proposition

$$\int_{\mathbb{R}^{d}} \left(e^{c|x|} + e^{c|y|} \right) \mathbf{1}_{\{x \neq y\}} d\mu_{\eta, \Delta t} (dx dy)$$

$$\leq \mu_{\eta, \Delta t} (\{x \neq y\}) \int_{\mathbb{R}^{d}} \left(e^{c|x|} + e^{c|y|} \right) d\mu_{\eta, \Delta t} (dx dy), \tag{5}$$

The sticky coupled process spends an $O(\eta)$ proportion of time off the diagonal. Furthermore $\mu_{\eta,\Delta t}$ is clearly a coupling of $\nu_{\eta,\Delta t}$ and $\nu_{0,\Delta t}$.

Numerical Illustrations

Numerical Illustrations: Strongly Convex Potential

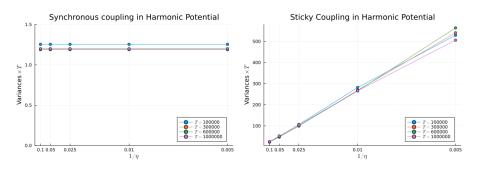
Consider a 2-dimensional Ornstein-Uhlenbeck process

$$dX_t^{\eta} = -\begin{bmatrix} 1 & -\eta \\ 0 & 1 \end{bmatrix} X_t^{\eta} dt + \sqrt{\frac{2}{\beta}} dW_t;$$

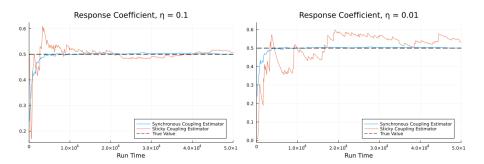
here $b(x) = -\nabla U = -x$ and $F(x) = [x_2 \ 0]^T$. We choose as response function the covariance between the components. In this case α_R is explicitly calculable.

$$R(x) = x_1 x_2, \qquad \alpha_R = \frac{1}{2\beta}$$

Numerical Illustrations: Strongly Convex Potential



Numerical Illustrations: Strongly Convex Potential



Numerical Illustrations: Lennard-Jones Fluid

For less trivial example, we consider an 18 particles 2-D Lennard-Jones fluid. For $x=\left(x_1^1,x_2^1,x_1^2,x_2^2,\ldots,x_1^{18},x_2^{18}\right)$, the interaction is given by

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

with $r_{ij} = |x^i - x^j|$ if i < j and $r_{ii} = |x^i|$. The confinement is give by

$$U_2(x) = \sum_{i=1}^{18} \left[\max \left\{ |x_1^i| - 5, 0 \right\}^2 + \max \left\{ |x_2^i| - 5, 0 \right\}^2 \right].$$

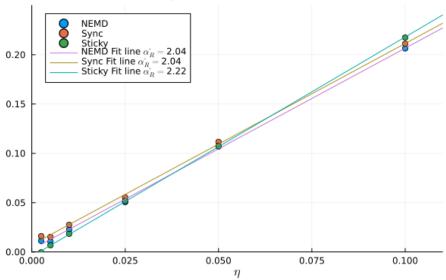
Thus $b(x) = -\nabla U = -\nabla (U_1 + U_2)$. For F we use sine shear

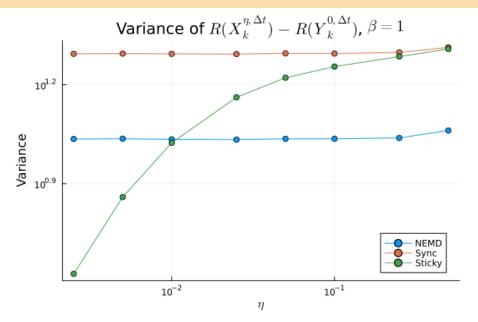
$$(F(x))_i = \begin{cases} \sin(\pi x_2^k/5) & \text{if } i = 2k - 1\\ 0 & \text{otherwise} \end{cases}$$

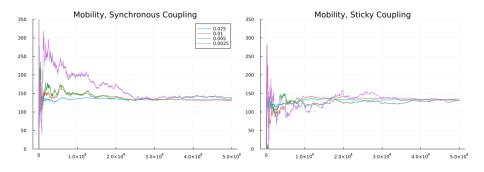
and we measure the mobility response

$$R(x) = F(x)^T \nabla U(x)$$









Some Extensions and Perspectives

- Componentwise and particle system coupling: Prefactors likely behave badly as $d \to \infty$. Idea: For particle clusters, couple each particle to either its same number particle or nearest particle in the other cluster⁶
- Hybrid coupling: Reflective part gives sticky coupling a long tail, while synchronous is unbeatable when there's contractivity. This suggests a hybrid approach of mixing sticky and synchronous couplings.
- Extension to Riemann manifolds: adapt reflection coupling part to geometry of the manifold via Kendall-Cranston coupling ⁷
- Extension to kinetic Langevin dynamics 8 9

Je vous remercie de votre attention!

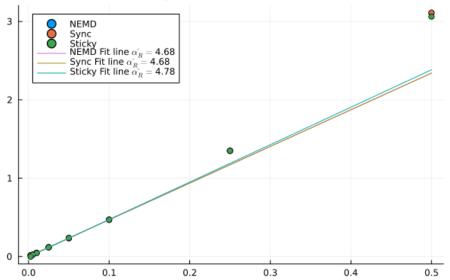
⁶see works by A. Eberle, K. Schuh, R. Zimmer

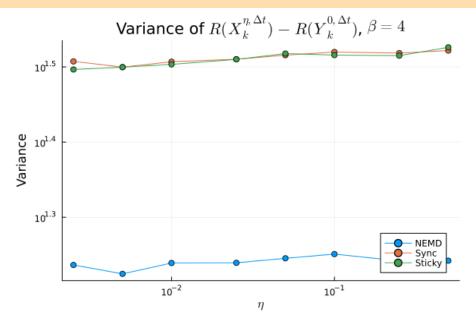
⁷A. Eberle (2016) Reflection couplings and contraction rates for diffusions

 $^{^8}$ A. Eberle, A. Guillin, R. Zimmer (2019) Couplings and quantitative contraction rates for Langevin dynamics

⁹N. Bou-Rabee, A. Eberle, R. Zimmer (2020) *Coupling and Convergence for Hamiltonian Monte Carlo*







Analysis of Variance/Finite-Time Bias of Standard Estimator

• **Statistical error** dictated by Central Limit Theorem:

$$\sqrt{t} \left(\widehat{\Phi}_{\eta,t} - \alpha_{\eta} \right) \xrightarrow[t \to +\infty]{\text{law}} \mathcal{N} \left(0, \frac{\sigma_{R,\eta}^2}{\eta^2} \right), \qquad \sigma_{R,\eta}^2 = \sigma_{R,0}^2 + \mathcal{O}(\eta)$$

so
$$\hat{\Phi}_{\eta,t} = \alpha_{\eta} + O_P\left(\frac{1}{n\sqrt{t}}\right) \rightarrow \text{requires long simulation times } t \sim \eta^{-2}$$

• Finite time integration bias: $\left|\mathbb{E}\left(\widehat{\Phi}_{\eta,t}\right) - \alpha_{\eta}\right| \leqslant \frac{K}{nt}$

Bias due to $t < +\infty$ is $O\left(\frac{1}{nt}\right) \to \text{typically smaller than statistical error}$

ullet Key equality for the proofs: introduce $-\mathcal{L}_{\eta}\widehat{R}_{\eta}=R-\int_{\mathbb{R}^d}\!\!R\,d
u_{\eta}$

$$\widehat{\Phi}_{\eta,t} - \frac{1}{\eta} \int_{\mathbb{R}^d} \!\! R \, d\nu_{\eta} = \frac{\widehat{R}_{\eta}(X_0^{\eta}) - \widehat{R}_{\eta}(X_t^{\eta})}{\eta t} + \frac{\sqrt{2}}{\eta t \sqrt{\beta}} \int_0^t \!\! \nabla \widehat{R}_{\eta}(X_s^{\eta}) \cdot dW_s$$
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More Ideas of Proof of Theorem

Denote by $\nu_{\eta,\Delta t}$, and $\nu_{0,\Delta t}$ the invariant measures of the respective discrete marginal processes and let $\Pi_{\eta,\Delta t}$ and $\Pi_{0,\Delta t}$ be the operators that center function with respect to these measures. Denote by $P^{\eta,\Delta t}$ and $P^{0,\Delta}$ their Markov kernels.

The CLT follows ergodicity, constructing an explicit solution to the discrete Poisson equation

$$\Delta t^{-1} \left(\operatorname{Id} - T^{\eta, \Delta t} \right) u(x, y) = \Pi_{\eta, \Delta t} R(x) - \Pi_{0, \Delta t} R(y),$$

and a CLT for Markov chains 10 . This further gives an expression for the asymptotic variance, $\sigma^2_{R,\eta,\Delta t}$ in terms of the

$$\widehat{R}_{\eta,\Delta t} = \Delta t \left(\operatorname{Id} - P^{\eta,\Delta t} \right)^{-1} \Pi_{\eta,\Delta t} R,$$

and

$$\widehat{R}_{0,\Delta t} = \Delta t \left(\operatorname{Id} - P^{0,\Delta t} \right)^{-1} \Pi_{0,\Delta t} R.$$

¹⁰R. Douc et. al (2018) Markov Chains

More Ideas of Proof of Theorem

A long computation adapting the strategies of Leimkuhler, et. al $(2015)^{11}$ and Plechac, et. al $(2021)^{12}$ lets us bound the bias and variance with terms of the form

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{K}_n(x) + \mathcal{K}_n(y)) \, \mathbf{1}_{\{x \neq y\}} \, d\mu_{\eta, \Delta t} \, (dx \, dy) \,,$$

and higher order terms. (Recall $K_n = 1 + |x|^n$). It only remains to control this integral.

 $^{^{11}}$ B. Leimkuhler, C. Matthews, and G. Stoltz *The computation of averages from equilibrium and non-equilibrium Langevin molecular dynamics*

¹²P. Plechac, G. Stoltz, and T. Wang Convergence of the likelihood ratio method for linear response of non-equilibrium stationary states