

On Couplings for Kinetic Langevin Diffusions

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Sampling on $\mathbb{R}^d$ via diffusions

- ▶ **Target.** $\mu_{\text{target}}(dx) \propto e^{-U(x)} dx$ on $\mathbb{R}^d$, with $U \in C^1$.

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- ▶ Noise enters *only the velocity* $\Rightarrow$ **hypoelliptic**.

Diffusive-to-ballistic acceleration

- ▶ **Overdamped Langevin**¹: under a Poincaré inequality with constant m ,

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- ▶ A *square-root speedup* in ill-conditioned problems; the motivation for studying kinetic Langevin and its splitting discretizations.

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From SDE to MCMC: splitting schemes

- Decompose the generator into three solvable flows:

$$\underbrace{O_h}_{\text{OU step (exact)}}, \quad \underbrace{\theta_h^{(A)}}_{\text{kinematic}}, \quad \underbrace{\theta_h^{(B)}}_{\text{kick by } -\nabla U}.$$

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- **OBABO splitting:**

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- Second-order weakly accurate.
- One step is a deterministic map of two Gaussian increments $\xi_k = (\xi_k^{(1)}, \xi_k^{(2)}) \sim \mathcal{N}(0, \text{Id}_{2d})$:

$$Z_{k+1}^h = \Psi_{Z_k^h}(\xi_{k+1}), \quad Z_k^h = (X_k^h, V_k^h).$$

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Question

- ▶ (Z_n^h) on $\mathbb{R}^{2d}$: OBABO chain, step h , friction γ , invariant law $\mu = \mu_{\text{target}} \otimes \mathcal{N}(0, \text{Id}_d)$.

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For which initial laws ν does OBABO attain the
acceleration $t_{\text{mix}}(\nu, \varepsilon) \asymp \kappa^{1/2} \log(1/\varepsilon)$?

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1. Coupling characterisation of TV.

$$d_{\text{TV}}(\nu_1, \nu_2) = \inf_{(X, \tilde{X}): X \sim \nu_1, \tilde{X} \sim \nu_2} \mathbb{P}(X \neq \tilde{X}).$$

Construct a coupling of the two chains and bound $\mathbb{P}(\text{disagree})$.

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2. Wasserstein-to-TV regularisation.

$$d_{\text{TV}}(\delta_z P^n, \delta_{\tilde{z}} P^n) \leq C_n |z - \tilde{z}| \implies d_{\text{TV}}(\nu P^n, \tilde{\nu} P^n) \leq C_n W_1(\nu, \tilde{\nu}),$$

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High-acceptance localisation⁴ transfers these bounds to the Metropolis-adjusted chain.

⁴(B.-R. & Oberdörster (2024), EJP)

Markovian vs. non-Markovian couplings

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- ▶ **Now-equals-forever**: $Z_s^h = \tilde{Z}_s^h \Rightarrow Z_t^h = \tilde{Z}_t^h$ for $t \geq s$, a.s.
- ▶ **Non-Markovian**: the joint chain is not adapted as a Markov chain to $(\mathcal{F}_k)$; the driving noises $(\tilde{\xi}_k)$ may depend on the entire sequence (ξ_j) at once.

A brief history of couplings for *hypoelliptic* SDEs

- ▶ **Stochastic oscillator.**⁵

First hypoelliptic coupling: switching between synchronous and antithetic drivers.

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- ▶ **Wasserstein contraction for kinetic Langevin.**⁷

Hybrid sync/reflection in phase space, non-convex U .

- ▶ Discrete-time:⁸ step-size-restricted analogues for OBABO and variants.

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- ▶ **TV mixing via Wasserstein-to-TV regularisation.**⁹

Hypoelliptic smoothing transfers Wasserstein to TV control.

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⁹(Roberts & Rosenthal (2002); Madras & Sezer (2010); Monmarché (2021); Gouraud et al. (2025); Chak & Monmarché (2025))

Prior work: Chak & Monmarché (2025)

Theorem (Chak & Monmarché, 2025, Thm. 2.2)

Let $U \in C^2(\mathbb{R}^d)$ satisfy

- ▶ *bounded Hessian*: $|\nabla^2 U(x) v| \leq L |v|$ for all v, x ,
- ▶ *Hessian-Lipschitz (Frobenius)*: $\|\nabla^2 U(x) - \nabla^2 U(y)\|_F \leq L_H |x - y|$.

There exist $\beta, h_0 > 0$ depending on L, L_H such that for all $h \leq h_0$, $n \geq 2$ with $hn \leq 1$:

$$d_{\text{TV}}(\pi_n(\delta_z), \pi_n(\delta_{\tilde{z}})) \leq \beta \left[\frac{1}{(hn)^{3/2}} + \frac{1}{(hn)^{1/2}} + (hn)^{1/2} \right] |\tilde{z} - z|.$$

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- ▶ **Mechanism.** An explicit *coalescence map* $\Psi_{z, \tilde{z}}^n$ built from an ansatz, with bound $d_{\text{TV}}(\pi_n(\delta_z), \pi_n(\delta_{\tilde{z}})) \leq d_{\text{TV}}(\text{Law}(\xi), \text{Law}(\Psi_{z, \tilde{z}}^n(\xi)))$ closed by ¹.

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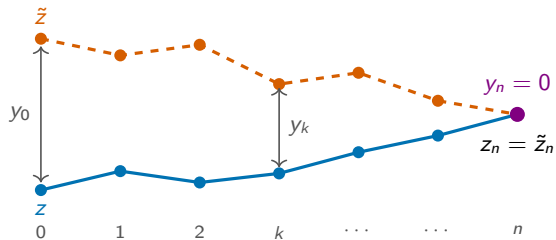
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- ▶ **Our take.** Read $\Psi_{z, \tilde{z}}^n$ as the *noise transport* of a non-Markovian coupling; *optimise* the trajectory and *realise* the coupling.

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Coalescence map

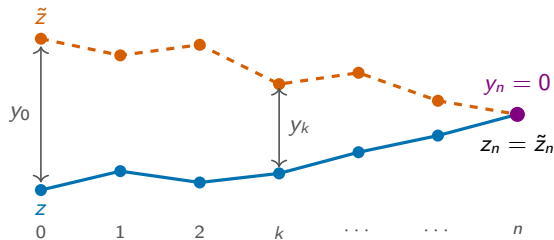


Chain map. OBABO from z driven by noise

$\xi = (\xi_1, \dots, \xi_n)$:

$$z = z_0 \rightarrow z_1 \rightarrow \dots \rightarrow z_n =: \Psi_z^n(\xi).$$

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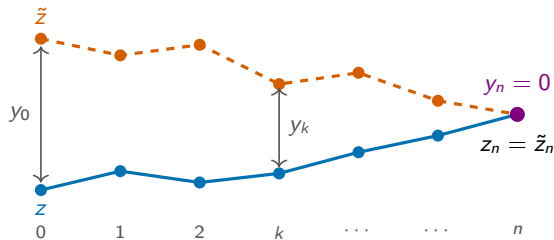
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with $y_0 = \tilde{z} - z$ and $y_n = 0$.

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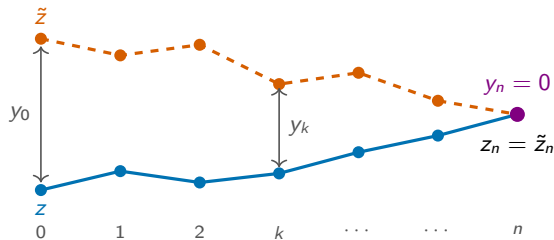
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Coalescence map. Given the noise ξ for the z -chain, $\tilde{\xi} := \Psi_{z, \tilde{z}}^n(\xi)$ is the noise that drives the $\tilde{z}$ -chain s.t.:

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Optimization. The interior $y_1, \dots, y_{n-1}$ is free, and later picked by LQ optimization.

General lemma: TV bound between a reference and a perturbed Gaussian

Lemma (B.-R. & Eberle, 2023, Lem. 15)

Let $\xi \sim \mathcal{N}(0, \text{Id}_d)$ and $\Phi: \mathbb{R}^d \rightarrow \mathbb{R}^d$ be a C^1 diffeomorphism. Then

$$d_{\text{TV}}(\text{Law}(\xi), \text{Law}(\Phi(\xi))) \leq \sqrt{2 \text{KL}},$$

where $\text{KL} = \mathbb{E}\left[\frac{1}{2}|\Phi(\xi) - \xi|^2 + \text{tr}(D\Phi(\xi) - \text{Id}) - \log|\det D\Phi(\xi)|\right]$.

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Sketch.

- ▶ Pinsker gives the first inequality;
- ▶ Change of variables yields $\text{KL} = \mathbb{E}\left[\frac{1}{2}|\Phi(\xi) - \xi|^2 + (\Phi(\xi) - \xi) \cdot \xi - \log |\det D\Phi(\xi)|\right]$;
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□

Remark (OBABO). For the OBABO coalescence map (next slide), $D\Psi_{z,\bar{z}}^n$ is block lower-triangular with identity diagonal: $\text{tr}(D\Psi - \text{Id}) \equiv 0$, $\det D\Psi \equiv 1$, and $d_{\text{TV}} \leq \mathbb{E}[|\Psi_{z,\bar{z}}^n(\xi) - \xi|^2]^{1/2}$.

Why OBABO has a lower-triangular coalescence Jacobian

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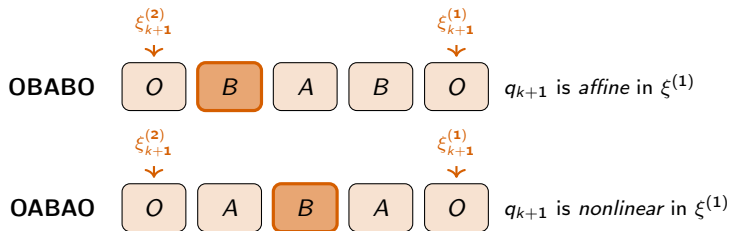
Why? Inductively, $\tilde{\xi}_i = \xi_i + g_i(\xi_1, \dots, \xi_{i-1})$. Hence $\frac{\partial \tilde{\xi}_i}{\partial \xi_j} = \begin{cases} I, & j = i, \\ *, & j < i, \\ 0, & j > i, \end{cases}$

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Quantitative TV bound for OBABO

Theorem (B.-R.-Cox-Schieven)

Let $\gamma, h > 0$, $n \in \mathbb{N}$, and $U \in C^2(\mathbb{R}^d)$ with ∇U L -Lipschitz. Then for all $z, \tilde{z} \in \mathbb{R}^{2d}$:

$$d_{\text{TV}}(\pi_n(\delta_z), \pi_n(\delta_{\tilde{z}})) \leq \frac{1}{\gamma^{1/2}} \left[\frac{5}{(hn)^{3/2}} + \frac{12 + 5\gamma}{(hn)^{1/2}} + \frac{L(\gamma h)^{1/2}}{(1 - e^{-\gamma h})^{1/2}} \left(1 + \frac{hn}{1 + \gamma hn} \right) (hn)^{1/2} \right] |\tilde{z} - z|.$$

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- ▶ **Realized by an explicit non-Markovian coupling.**

The optimal noise-transport trajectory (force-free)

Force-free bound. For $\nabla U \equiv 0$, Lemma 15 reduces to a controlled L^2 cost on the gap trajectory y_k :

$$d_{\text{TV}} \leq \frac{1}{2} \left(\sum_{k=1}^n |E_k|^2 \right)^{1/2}, \quad E_{k+1} = -L_h^{-1}(y_{k+1} - A_h y_k).$$

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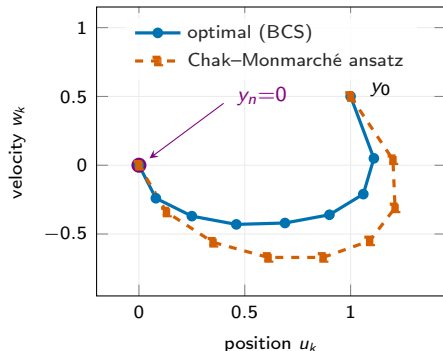
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LQ-optimal trajectory. Minimum-energy control $\min_E \|E\|^2$ s.t. $y_0 = \Delta z$, $y_n = 0$. Closed form via controllability Gramian:

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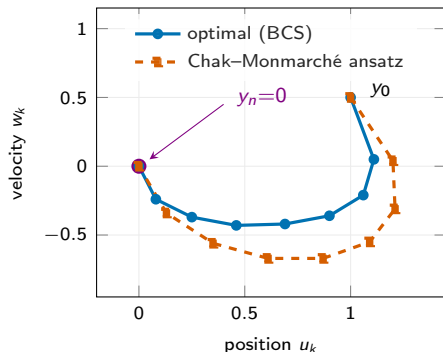
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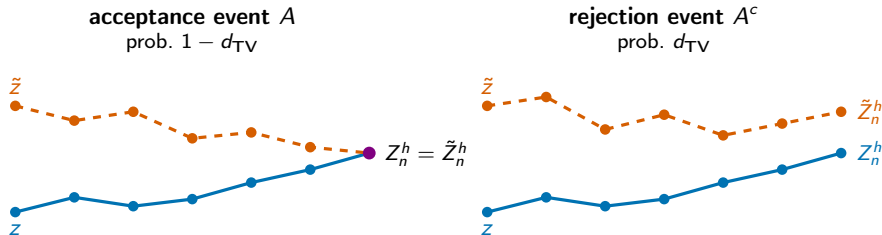
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Design principle (EGZ & BCS). Construct for $\nabla U \equiv 0$, then treat ∇U as a Lipschitz perturbation.

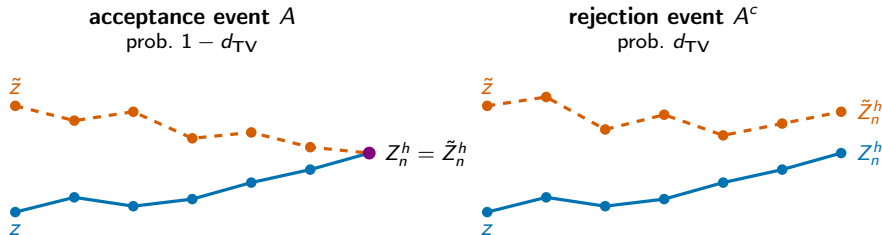
The non-Markovian coupling

- ▶ Sample $\xi \sim \mathcal{N}(0, \text{Id}_{2dn})$; proposal $\tilde{\xi}_* := \Psi_{z, \tilde{z}}^n(\xi)$; maximally couple ξ to $\tilde{\xi}_*$.
- ▶ On accept: $\tilde{\xi} = \tilde{\xi}_*$ — chains meet at time n . On reject: $\tilde{\xi}$ drawn independently — chains evolve independently.
- ▶ $\mathbb{P}(Z_n^h \neq \tilde{Z}_n^h) = d_{\text{TV}}(\text{Law}(\xi), \text{Law}(\Psi_{z, \tilde{z}}^n(\xi)))$.



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- ▶ **Non-Markovian**, designed for horizon n : $\tilde{\xi}$ depends on the whole ξ at once; intermediate chains generally disagree.

Are Markovian couplings enough?

- ▶ Test problem: **quadratic potential** $U(x) = \alpha|x|^2$, $\alpha \geq 0$, overdamped regime $\gamma^2 > 4\alpha$.

$$dX_t = V_t dt, \quad dV_t = -\alpha X_t dt - \gamma V_t dt + \sqrt{2\gamma} dW_t.$$

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- ▶ Question: can a *Markovian* coupling match this rate?

No Markovian coupling matches the TV decay

Theorem (B.-R.-Cox-Schieven, continuous time)

Under $\gamma^2 > 4\alpha \geq 0$: (upper) if $\lambda_- \Delta x = \Delta v$, $\Delta x \neq 0$, then $d_{TV} \leq Ce^{\lambda_- t} |\Delta z|$; (lower) for every Markovian coupling μ and every Δz , $\mu(Z_t \neq \tilde{Z}_t) \geq c_\mu \min(t^{-1/2}, e^{\lambda_+ t})$ for $t \geq t_\mu$.

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- Extends (Banerjee & Kendall (2016)) (Kolmogorov diffusion) to kinetic Langevin.

The canonical Markovian candidate: iterated one-shot

- ▶ For linear Markov chains $Z_{k+1} = A_k Z_k + B_k \xi_{k+1}$:
 - ▶ Greedy: maximize the meeting probability *at the next step* by reflection coupling.
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- ▶ For kinetic Langevin: necessarily suboptimal (by Theorem above). By how much?

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Exact meeting probability for iterated one-shot

Theorem (B.-R.-Cox-Schieven)

Let $(Z_k, \tilde{Z}_k)$ be the iterated one-shot coupling of the linear chain

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- ▶ Free kinetic Langevin ($\alpha=0$, $\Delta z=(\Delta x, -\gamma\Delta x)$): $\mathbb{P}(Z_k^h \neq \tilde{Z}_k^h) \geq c h^{-1} e^{\lambda - hk}$ — saturates the $h^{-1} e^{\lambda - hk}$ term in the impossibility bound.

Summary and outlook

- ▶ Sharp TV bound for OBABO via an LQ-optimal coalescence map; realised by an explicit non-Markovian rejection sampler. Drops Hessian-Lipschitz and $hn \leq 1$ of (Chak & Monmarché (2025)).
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Open.

- ★ **Acceleration** at rate $\kappa^{-1/2}$: *reduced* to proving W_1 contraction at this rate.
- ▶ Underdamped regime $\gamma^2 < 4\alpha$ (rigidity uses real eigenvalues).

Related directions.

- ▶ KL / Rényi divergences¹; other splittings²; Metropolis adjustment³.

¹(B.-R., Mitra & Wibisono (2026))

²(Schuh & Whalley (2025))

³(B.-R. & Oberdörster (2024))

Thank you!

On Couplings for Kinetic Langevin Diffusions

joint work with **Sonja Cox** and **Roy Schieven**

Questions?

Thanks to **Pierre Monmarché**, **Andreas Eberle**, and **Stefan Oberdörster**
for fruitful discussions.