

Computationally tractable Bayesian inference for interacting particle system models

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A weakly interacting particle system

- For $W \in \dot{H}^{\alpha+1}(\mathbb{T}^d)$, $\alpha > 1 + d/2$, consider the system of SDEs

$$\begin{cases} dX_t^{n,i} = -\frac{1}{n} \sum_{j \neq i} \nabla W(X_t^{n,i} - X_t^{n,j}) dt + \sqrt{2} dB_t^i \\ X_0^{n,i} \sim \phi \end{cases}, \quad i = 1, \dots, n.$$

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- With $P_t^{n,k} := \text{Law}(X_t^{n,1}, \dots, X_t^{n,k})$, Lacker (Probab. Math. Phys., 2023) shows 'propagation of chaos', i.e. for any $t > 0$,

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- Goal:** infer W from measurements of $\rho = \rho_W$ (nonlinear inverse problem).

Data

Given some ‘ground truth’ $W_0 \in \dot{H}^{\alpha+1}$, observe regression data $Z_N = (Y_i, t_i, x_i)_{i=1}^N$ of the form

$$Y_i = \rho_{W_0}(t_i, x_i) + \varepsilon_i, \quad i = 1, \dots, N,$$

where $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$ and (t_i, x_i) are i.i.d. uniform on $[0, T] \times \mathbb{T}^d$.

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$$d\Pi(W | Z_N) \propto e^{\ell_N(W)} d\Pi(W),$$

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- Extract information about W from the posterior distribution, e.g. by computing the posterior mean $\bar{W}_N := \int W d\Pi(W | Z_N)$ or credible sets. This last step typically relies on **MCMC algorithms**.

Bayesian computations

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- Discretise the prior by projecting it onto \dot{E}_K , the space of mean-zero trigonometric polynomials of degree at most K , so that W is represented by the vector of dimension $D \simeq K^d \gg 1$ of its Fourier coefficients.

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Unadjusted Langevin Algorithm (ULA)

Choose a step size $\gamma > 0$ and an initialiser W_0 . For $\xi_k \stackrel{\text{iid}}{\sim} \mathcal{N}(0, I_D)$, do

$$W_{k+1} = W_k + \gamma \nabla \log(d\Pi(W_k | Z_N)) + \sqrt{2\gamma} \xi_{k+1},$$

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- Compute desired quantities, e.g. $\hat{W}_N = M^{-1} \sum_{k=1}^M W_k$

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- Computational hurdle: the map $\mathcal{G} : W \mapsto \rho_W$ is non-linear, meaning the posterior could be **non-log-concave** or even **multi-modal**. Because it is also **high-dimensional** ($D \gg 1$), sampling from this Gibbs measures is highly non-trivial.

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- Statistical hurdle: even if we can compute the posterior mean \bar{W}_N , we have no initial guarantees that \bar{W}_N will land close to the true W_0 (**consistency**).

Injectivity and stability

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- Assume that the initial condition $\phi \in H^\beta$ satisfies $\inf_x \phi(x) > \phi_{\min} > 0$ and is **ζ -deconvolvable**, i.e. its Fourier coefficients $\hat{\phi}_k$ do not decay too fast:

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Stability estimate

For any $W \in \dot{E}_K$ and $W_0 \in H^{\alpha+1}$, and for ϕ as above

$$\|W - P_{E_K} W_0\|_{L^2} \lesssim K^{3\zeta/2} \left(\|\rho_W - \rho_{W_0}\|_{L^2([0, T]; L^2)} + \|\rho_W - \rho_{W_0}\|_{H^1([0, T]; H^{-2})} \right)$$

Consistency

Using this stability estimate, we can use the framework of Nickl (EMS Press, 2023) for Gaussian priors to show a posterior contraction rate.

Theorem (Nickl, Pavliotis, Ray, AoS 2025)

For any $W_0 \in H^{\alpha+1}$, under the previous assumptions on ϕ , for some $\theta > 0$

$$\Pi(W \in E_{K_N} : \|W - W_0\|_{L^2} \lesssim N^{-\theta} \mid Z_N) \rightarrow 1 \text{ in } P_{W_0}^N\text{-probability}$$

In particular,

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Note: this solves the consistency problem! We now need to compute \bar{W}_N .

Geometry of the likelihood function

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- Recall $d\Pi(W | Z_N) \propto e^{\ell_N(W)} d\Pi(W)$, $\ell_N(W) = -\frac{1}{2} \sum_{i=1}^N |Y_i - \rho_W(t_i, x_i)|^2$. We would like to show $-\ell(W) := -\ell_1(W)$ is convex. Assuming for the moment that $W \mapsto \rho_W$ is twice differentiable,

$$-\nabla^2 \ell(W) = \nabla \rho_W(t, x)^\top \nabla \rho_W(t, x) + (\rho_W(t, x) - Y) \nabla^2 \rho_W(t, x).$$

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- So the ‘average’ Hessian satisfies, for any h with $\|h\|_{\mathbb{R}^D} \leq 1$ (for some appropriate norm $\|\cdot\|_*$)

$$h^\top E_{W_0}[-\nabla^2 \ell(W)]h = \|h^\top \nabla \rho_W\|_{L_\lambda^2([0, T] \times \mathbb{T}^d)}^2 + O(\|\rho_W - \rho_{W_0}\|_*).$$

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- Nickl and Wang (JEMS, 2023) introduce **gradient stability**: $\|h^\top \nabla \rho_W\|_{L_T^2 L^2}^2 \gtrsim \|h\|_{\mathbb{R}^d}^2$, but no formula is available for $\nabla \rho_W$ since ρ_W is the solution to a non-linear PDE!

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- This formal derivation is made rigorous using the implicit function theorem in Banach spaces.

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- For given initial condition $\phi \in H^\beta$, regard $W \mapsto \rho_W$ as a map

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Theorem (C. and Nickl, 2026)

For any $W, H \in \dot{W}^{2,\infty}$, the Fréchet derivative $D\rho_W[H]$ is the unique $\mathbf{u} \in L^2([0, T]; H^{\beta+1}) \cap H^1([0, T]; H^{\beta-1})$ solving the linear parabolic PDE

$$\begin{cases} \partial_t \mathbf{u} - \Delta \mathbf{u} - \nabla \cdot (\mathbf{u} \nabla W * \rho_W) - \nabla \cdot (\rho_W \nabla W * \mathbf{u}) = \nabla \cdot (\rho_W \nabla H * \rho_W) \\ \mathbf{u}(0) = 0 \end{cases}$$

Moreover, the map $W \mapsto \rho_W$ is C^∞ in the Fréchet sense and higher order derivatives can be computed similarly.

The posterior is locally log-concave

Using that $D\rho_W[H]$ solves a PDE, we can now prove that gradient stability holds. For any $W, H \in \dot{E}_K$, provided ϕ is ζ -deconvolvable,

$$\|H^\top \nabla \rho_W\|_{L^2([0, T]; L^2)}^2 = \|D\rho_W[H]\|_{L^2([0, T]; L^2)}^2 \gtrsim K^{-6\zeta} \|H\|_{L^2}^2.$$

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Theorem (C. and Nickl, 2026)

For any $W_0 \in H^{\alpha+1}$ and any ζ -deconvolvable initial condition ϕ ,

$$\inf_{W \in \mathcal{B}} \lambda_{\min}(E_{W_0}[-\nabla^2 \ell(W)]) \gtrsim K^{-6\zeta} > 0$$

on a neighbourhood \mathcal{B} of $P_{E_K} W_0$ in \dot{E}_K of radius D^{-w} for appropriate $w > 0$.

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Combining the above with the consistency result, we can construct a **strongly globally log-concave** proxy posterior $\tilde{\Pi}(\cdot | Z_N)$ such that

$$\mathcal{W}_2^2(\tilde{\Pi}(\cdot | Z_N), \Pi(\cdot | Z_N)) = O_{P_{W_0}^N}(e^{-N^p}), \quad \text{for some } p > 0$$

Polynomial-time mixing of ULA

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Theorem (C. and Nickl, 2026)

Under regularity conditions and ζ -deconvolvability of ϕ , for any precision level $\varepsilon \geq N^{-P}$, $P > 0$, the warm-start ULA requires iterations growing as

$$O(N^{b_1} D^{b_2} \varepsilon^{-b_3}), b_1, b_2, b_3 > 0$$

to produce an output \hat{W}_ε that satisfies, with high $P_{W_0}^N$ -probability

$$\|\hat{W}_\varepsilon - \bar{W}_N\|_{L^2} \leq \varepsilon, \text{ as well as } \|\hat{W}_\varepsilon - W_0\|_{L^2} \leq \varepsilon$$

Thank you!

References

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- A regression step, e.g.

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Ideas for initialisation

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- A deterministic step, reminiscent of the **PINN** methodology,

$$\hat{W} \in \arg \min_W \|\mathcal{L}_W \hat{\rho}\|_{L^2([0, T]; L^2)}^2 + \text{pen}(W)$$