

# 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).

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

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



# Bayesian computations

- 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

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

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



# Challenges

- 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**).



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## Stability estimate

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

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



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  $\phi$ , 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,

$$\|\bar{W}_N - W_0\|_{L^2} = O_{P_{W_0}^N}(N^{-\theta})$$

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

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- Recall  $d\Pi(W \mid Z_N) \propto e^{\ell_N(W)} d\Pi(W)$ ,  $\ell_N(W) = -\frac{1}{2} \sum_{i=1}^N |Y_i - \rho_W(t_i, x_i)|^2$ . 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  $\|\cdot\|_*$ )

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

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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  $\rho_W$  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  $C^\infty$  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  $\phi$  is  $\zeta$ -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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For any  $W_0 \in H^{\alpha+1}$  and any  $\zeta$ -deconvolvable initial condition  $\phi$ ,

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

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

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

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- We study ‘warm-start’ ULA and assume we are given a feasible initialiser  $W_{\text{init}}$  into  $\mathcal{B}$ . Ideas for initialisation can be found in Wang (2026).

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- We start from  $W_{\text{init}}$  and run ULA on the proxy  $\tilde{\Pi}(\cdot \mid Z_N)$ .

## Theorem (C. and Nickl, 2026)

Under regularity conditions and  $\zeta$ -deconvolvability of  $\phi$ , 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  $\hat{W}_\varepsilon$  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!**



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# Ideas for initialisation

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

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