Nonlinear Assimilation via Score-based Sequential Langevin Sampling

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1 Introduction and Background

Score-based Sequential Langevin Sampling Prediction and Score Matching Update via Langevin Sampling Summary of Procedure

Convergence Analysis

Assumptions Convergence Analysis for Posterior Sampling Convergence Analysis for Assimilation

Output: Numerical Experiments Double-Well Potential Kolmogorov flow

G Conclusions

Numerical weather prediction (NWP) uses **physical models** of the atmosphere and oceans to predict the weather based on the **measurement data**.

Physical models

Governing equations of atmosphere:

- conservation of momentum
- conservation of mass
- conservation of energy
- the equation of state for ideal gases
- conservation equation for water mass

Measurement data



• • • •

Dynamics model: A discrete time unobserved stochastic process $(\mathbf{X}_k)_{k\geq 1}$ satisfying

$$\mathbf{X}_{k+1} = \mathcal{F}_k(\mathbf{X}_k, \mathbf{V}_k)$$

- \mathcal{F}_k is a known time-dependent model.
- V_k is a random variable with known distribution.

$$\rho_k(\mathbf{X}_{k+1}|\mathbf{X}_k) = p(\mathbf{X}_{k+1}|\mathbf{X}_k)$$

Dynamics model: A discrete time unobserved stochastic process $(X_k)_{k>1}$ satisfying

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Measurement model: A discrete time observed stochastic process $(\mathbf{Y}_k)_{k\geq 1}$ satisfying

 $\mathbf{Y}_k = \mathcal{G}_k(\mathbf{X}_k, \mathbf{W}_k)$

 $g_k(\mathbf{Y}_k|\mathbf{X}_k) = p(\mathbf{Y}_k|\mathbf{X}_k)$

 $\rho_k(\mathbf{X}_{k+1}|\mathbf{X}_k) = p(\mathbf{X}_{k+1}|\mathbf{X}_k)$

- \mathcal{G}_k is a known time-dependent measurement operator.
- ▶ **W**_k is a random measurement noise with known distribution.

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Data Assimilation

The goal of the data assimilation is to estimate the posterior distribution of the latent state \mathbf{X}_{k+1} given all available measurements $\mathbf{Y}_{[k+1]}$, that is, $\frac{\pi_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k+1]})}{\pi_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k+1]})}$ for each $k \ge 1$.

State-Space Model

Dynamics model	$\mathbf{X}_{k+1} = \mathcal{F}_k(\mathbf{X}_k, \mathbf{V}_k)$	\longleftrightarrow	State transition density	$\mathbf{\rho}_k(\mathbf{X}_{k+1} \mathbf{X}_k)$
Measurement model	$\mathbf{Y}_{k+1} = \mathcal{G}_{k+1}(\mathbf{X}_{k+1}, \mathbf{W}_k)$	\longleftrightarrow	Measurement likelihood	$\frac{g_{k+1}}{Y_{k+1}} (\mathbf{Y}_{k+1} \mathbf{X}_{k+1})$





Classical Methods for Data Assimilation



- How to estimate the prediction distribution $q_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k]})$?
- How to sample from the posterior distribution $\pi_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k+1]})$ given the prediction and likelihood?

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	$\pi_k(\mathbf{X}_k \mathbf{Y}_{[k]})$	$\rho_k(\mathbf{X}_{k+1} \mathbf{X}_k)$	$g_{k+1}(\mathbf{Y}_{k+1} \mathbf{X}_{k+1})$	Limitations
Kalman Filter	Gaussian approximation particle approximation	Gaussian	Gaussian	linear + Gaussian
Particle Filter		–	–	particle degeneracy

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How to estimate the score function $\nabla \log q_{k+1}(\cdot |\mathbf{Y}_{[k]})$ of the prediction distribution?

$$q_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k]}) = \int \rho_k(\mathbf{X}_{k+1}|\mathbf{X}_k) \pi_k(\mathbf{X}_k|\mathbf{Y}_{[k]}) \mathrm{d}\mathbf{X}_k$$

- $\blacktriangleright \text{ Given: } \widehat{\mathbf{X}}_k^1, \dots, \widehat{\mathbf{X}}_k^n \sim^{\text{i.i.d.}} \widehat{\pi}_k(\mathbf{X}_k | \mathbf{Y}_{[k]}) \approx \pi_k(\mathbf{X}_k | \mathbf{Y}_{[k]}).$
- $\blacktriangleright \ \ \, \text{Prediction with dynamics model: } \underline{\mathbf{X}}_{k+1}^i = \mathcal{F}_k(\widehat{\mathbf{X}}_k^i, \mathbf{V}_k^i) \text{, for each } 1 \leq i \leq n.$

$$\underline{\mathbf{X}}_{k+1}^i \sim \widehat{q}_{k+1}(\underline{\mathbf{X}}_{k+1}|\underline{\mathbf{Y}}_{[k]}) := \int \rho_k(\underline{\mathbf{X}}_{k+1}|\underline{\mathbf{X}}_k) \widehat{\pi}_k(\underline{\mathbf{X}}_k|\underline{\mathbf{Y}}_{[k]}) \mathrm{d}\underline{\mathbf{X}}_k \approx q_{k+1}(\underline{\mathbf{X}}_{k+1}|\underline{\mathbf{Y}}_{[k]}).$$

Denoising score matching:

$$\widehat{\mathbf{s}}_{k+1}(\cdot|\mathbf{Y}_{[k]}) = \operatorname*{arg\,min}_{\mathbf{s}:\mathbb{R}\times\mathbb{R}^d\to\mathbb{R}^d} L_{k+1}(\mathbf{s}) = \mathbb{E}_{\underline{\mathbf{X}}_{k+1}\sim\widehat{q}_{k+1}(\cdot|\mathbf{Y}_{[k]})} \mathbb{E}_{\boldsymbol{\varepsilon}\sim N(0,\mathbf{I}_d)} \big[\|\sigma\mathbf{s}(\underline{\mathbf{X}}_{k+1} + \sigma\boldsymbol{\varepsilon}, \mathbf{Y}_{[k]}) + \boldsymbol{\varepsilon}\|_2^2 \big]$$

which is the score function of the Gaussian smoothed prediction distribution

$$\widehat{\mathbf{s}}_{k+1}(\cdot|\mathbf{Y}_{[k]}) := \nabla \log \Big(\int N(\cdot;\mathbf{X}_{k+1}, \sigma^2 \mathbf{I}_d) \widehat{q}_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k]}) \mathrm{d}\mathbf{X}_{k+1} \Big) \approx \nabla \log \widehat{q}_{k+1}(\cdot|\mathbf{Y}_{[k]})$$



How to sample from the posterior distribution $\pi_{k+1}(\cdot | \mathbf{Y}_{[k+1]})$ given the prediction and likelihood?

$\pi_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k+1]}) \propto \frac{g_{k+1}(\mathbf{Y}_{k+1}|\mathbf{X}_{k+1})q_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k]})}{g_{k+1}(\mathbf{X}_{k+1}|\mathbf{Y}_{[k]})}$

Langevin dynamics

$$\begin{aligned} \mathbf{d}\mathbf{Z}_t &= \nabla \log \pi_{k+1}(\mathbf{Z}_t | \mathbf{Y}_{[k+1]}) \mathbf{d}t + \sqrt{2} \mathbf{d}\mathbf{B}_t, \\ &= \left\{ \nabla \log g_{k+1}(\mathbf{Y}_{k+1} | \mathbf{Z}_t) + \nabla \log q_{k+1}(\mathbf{Z}_t | \mathbf{Y}_{[k]}) \right\} \mathbf{d}t + \sqrt{2} \mathbf{d}\mathbf{B}_t, \quad \mathbf{Z}_0 \sim \widehat{q}_{k+1}(\cdot | \mathbf{Y}_{[k]}). \end{aligned}$$

- Prediction score estimation
- Euler-Maruyama discretization
- Score-based Langevin Monte Carlo

$$\widehat{\mathbf{Z}}_{(k+1)h} = \widehat{\mathbf{Z}}_{kh} + h\left\{\nabla \log g_{k+1}(\mathbf{Y}_{k+1}|\widehat{\mathbf{Z}}_{kh}) + \widehat{\mathbf{s}}_{k+1}(\widehat{\mathbf{Z}}_{kh},\mathbf{Y}_{[k]})\right\} + \sqrt{2h}\xi_k, \quad \widehat{\mathbf{Z}}_0 \sim \widehat{q}_{k+1}(\cdot|\mathbf{Y}_{[k]}).$$

Interpolations between the prediction and posterior distribution:

 $\pi_{k+1}^m(\cdot|\mathbf{Y}_{[k+1]}) \propto \pi_{k+1}(\cdot|\mathbf{Y}_{[k+1]})^{\beta_m}q_{k+1}(\cdot|\mathbf{Y}_{[k]})^{1-\beta_m}, \quad 0 \leq m \leq M$

• Annealing schedule:
$$0 \equiv \beta_0 < \beta_1 < \cdots < \beta_M \equiv 1$$
.



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Score-based Sequential Langevin Sampling

Summary of Procedure



Algorithm 1: Score-based Sequential Langevin Sampling for data assimilation.

Input: The observations $(\mathbf{Y}_k)_{k \in \mathbb{N}}$, the dynamics model $(\mathcal{F}_k)_{k \in \mathbb{N}}$, the likelihood $\{g_k(\mathbf{Y}_k|\cdot)\}_{k \in \mathbb{N}}$. **Output:** A particle approximation $\widehat{\mathbf{X}}_{k+1}^1, \ldots, \widehat{\mathbf{X}}_{k+1}^n$ to the distribution $\pi_{k+1}(\cdot|\mathbf{Y}_{k+1}|)$.

- 1 # Initial posterior sampling.
- ² Sample from the gauss of the initial prior distribution $\underline{X}_1^1, \dots, \underline{X}_1^n \sim^{i.i.d.} \widehat{q}_1$.
- ³ Estimate the score from $\{\underline{X}_{i}^{i}\}_{i=1}^{n}$ by score matching $\widehat{\mathbf{s}}_{1}$.
- 4 Sample from the posterior $\widehat{\pi}_1(\cdot|\mathbf{y}_1)$ by Langevin sampling: $\widehat{\mathbf{X}}_1^1, \dots, \widehat{\mathbf{X}}_1^n \leftarrow \text{ALMC}(\underline{\mathbf{X}}_1^1, \dots, \underline{\mathbf{X}}_1^n, \widehat{\mathbf{s}}_1, g_1(\mathbf{Y}_1|\cdot)).$
- 5 # Recursive posterior sampling.
- $\mathbf{6} \; \mathsf{for}\, \underline{k=1,2,\dots}\, \mathsf{do}$
- 7 # Prediction step.
- 8 Run the dynamics model: $\underline{\mathbf{X}}_{k+1}^i \leftarrow \mathcal{F}_k(\widehat{\mathbf{X}}_k^i, \mathbf{V}_k^i)$ with $\mathbf{V}_k^i \sim p_{\mathbf{V}}$ for $1 \le i \le n$.
- Solution Score from $\{\underline{\mathbf{X}}_{k+1}^i\}_{i=1}^n$ by score matching $\widehat{\mathbf{s}}_{k+1}(\cdot, \mathbf{Y}_{[k]})$.
- 10 # Update step.
- Sample from the posterior $\pi_{k+1}(\cdot|\mathbf{Y}_{[k+1]})$ by Langevin sampling:

$$\widehat{\mathbf{X}}_{k+1}^{1}, \dots, \widehat{\mathbf{X}}_{k+1}^{n} \leftarrow \text{ALMC}(\underline{\mathbf{X}}_{k+1}^{1}, \dots, \underline{\mathbf{X}}_{k+1}^{n}, \widehat{\mathbf{s}}_{k+1}(\cdot, \mathbf{Y}_{[k]}), g_{k+1}(\mathbf{Y}_{k+1}|\cdot))$$

- 12 end
- 13 return $\underline{\widehat{X}}_{k+1}^1, \dots, \widehat{X}_{k+1}^n$

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A1. Lipschitz score. For each $k \in \mathbb{N}$, the posterior score is λ -Lipschitz on \mathbb{R}^d , that is, for each $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^d$,

 $\|\nabla \log \pi_{k+1}(\mathbf{x}_1 | \mathbf{Y}_{[k+1]}) - \nabla_{\mathbf{x}} \log \pi_{k+1}(\mathbf{x}_2 | \mathbf{Y}_{[k+1]})\|_2 \le \lambda \|\mathbf{x}_1 - \mathbf{x}_2\|_2.$

A2. Log-Sobolev inequality. For each $k \in \mathbb{N}$, the posterior distribution satisfies a log-Sobolev inequality with constant C_{LSI} , that is, for each function $f \in C_0^{\infty}(\mathbb{R}^d)$,

 $\operatorname{Ent}(f^2) \leq 2C_{\mathrm{LSI}} \mathbb{E}\left[\|\nabla f\|_2^2 \right],$

where the entropy is defined as $\operatorname{Ent}(g) = \mathbb{E}[g \log g] - \mathbb{E}[g] \log \mathbb{E}[g]$, and the expectation is taken with respect to the posterior distribution $\pi_{k+1}(\cdot |\mathbf{Y}_{[k+1]})$.

A3. Boundedness and condition number. For each $k \in \mathbb{N}$,

- there exists $B \ge 1$ such that $\rho_k(\mathbf{x}|\mathbf{X}_k), \|\nabla \rho_k(\mathbf{x}|\mathbf{X}_k)\|_{\infty} \le B$ for $\mathbf{x} \in \mathbb{R}^d$,
- there exists $D \ge 1$ such that $q_{k+1}(\mathbf{x}|\mathbf{Y}_{[k]}) \ge D^{-1}$ for $\mathbf{x} \in \Omega_{k+1} := \operatorname{supp}(q_{k+1}(\cdot|\mathbf{Y}_{[k]}))$,
- $q_1(\mathbf{x}), \|\nabla q_1(\mathbf{x})\|_{\infty} \leq B$ and $q_1(\mathbf{x}) \geq D^{-1}$ for $\mathbf{x} \in \Omega_1 := \operatorname{supp}(q_1)$, and
- there exists $\kappa > 0$ such that

$$\frac{\sup_{\mathbf{x}} g_1(\mathbf{Y}_1|\mathbf{x})}{\int g_1(\mathbf{Y}_1|\mathbf{x}) q_1(\mathbf{x}) d\mathbf{x}'} \frac{\sup_{\mathbf{x}} g_{k+1}(\mathbf{Y}_{k+1}|\mathbf{x})}{\int g_{k+1}(\mathbf{Y}_{k+1}|\mathbf{x}) q_{k+1}(\mathbf{x}|\mathbf{Y}_{[k]}) d\mathbf{x}} \leq \kappa$$

A4. Error of score matching. There exists a score matching tolerance $\Delta \in (0, 1)$ such that

$$\begin{split} \mathbb{E}_{\underline{\mathbf{X}}_{1}} \left[\| \nabla_{\mathbf{x}} \log \widehat{q}_{1}(\underline{\mathbf{X}}_{1}) - \widehat{\mathbf{s}}_{1}(\underline{\mathbf{X}}_{1}) \|_{2}^{2} \right] &\leq \Delta^{2}, \\ \mathbb{E}_{\underline{\mathbf{X}}_{k+1}} \left[\| \nabla_{\mathbf{x}} \log \widehat{q}_{k+1}(\underline{\mathbf{X}}_{k+1} | \mathbf{Y}_{[k]}) - \widehat{\mathbf{s}}_{k+1}(\underline{\mathbf{X}}_{k+1}, \mathbf{Y}_{[k]}) \|_{2}^{2} \right] &\leq \Delta^{2}, \end{split}$$

for each $k \in \mathbb{N}$. Here the expectation $\mathbb{E}_{\underline{\mathbf{X}}_1}[\cdot]$ is taken with respect to $\underline{\mathbf{X}}_1 \sim \widehat{q}_1$, and the expectation $\mathbb{E}_{\underline{\mathbf{X}}_{k+1}}[\cdot]$ is taken with respect to $\underline{\mathbf{X}}_{k+1} \sim \widehat{q}_{k+1}(\cdot |\mathbf{Y}_{[k]})$.





- Early-stopping: Trade-off between the convergence of Langevin dynamics and score estimation error.
- <u>Condition number</u>: How the score matching error Δ effects the posterior error.

C. Duan (WHU)

Score-based Sequential Langevin Sampling

Under Assumptions A1 to A4. Suppose that the initial prior error satisfy

$$\varepsilon_{\text{init}} := \|\nabla_{\mathbf{x}} \log q_1 - \nabla_{\mathbf{x}} \log \widehat{q}_1\|_{L^{\infty}(\mathbb{R}^d)}.$$

Then for each time step $k \in \mathbb{N}$ and error tolerance $\varepsilon \in (0, 1)$,

$$\|\pi_{k+1}(\cdot|\mathbf{Y}_{[k+1]}) - \widehat{\pi}_{k+1}(\cdot|\mathbf{Y}_{[k+1]})\|_{\mathrm{TV}} \leq \widetilde{\mathcal{O}}(\varepsilon_{\mathrm{init}} + \varepsilon),$$

where the $\widetilde{\mathcal{O}}$ notation omits logarithmic factors of $\varepsilon_{\text{init}}$ and ε , and the constant behind the $\widetilde{\mathcal{O}}$ notation is independent of $\varepsilon_{\text{init}}$ and ε . Moreover, the step size h, the number of the Langevin iterations K and the score matching error Δ satisfy:

$$\begin{split} h &= \Theta\Big(\frac{\varepsilon^2}{dC_{\rm LSI}\lambda^2}\Big), \quad K = \Theta\Big(\frac{d\lambda^2 C_{\rm LSI}^2}{\varepsilon^2}\log\Big(\frac{\eta_{\chi}^2}{\varepsilon^2}\Big)\Big), \\ \Delta &= \Theta\Big(\frac{\varepsilon^2}{\sqrt{\kappa B^3 D^3 C_{\rm LSI}}}\frac{1}{\log(\varepsilon^{-2}\eta_{\chi}^2) + \eta_{\chi}}\Big). \end{split}$$

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Double-Well Potential

Dynamics model:

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \beta \mathrm{d}B_t$$

- Double-well potential: $U(x) = x^4 2x^2$. Measurement model:
 - Linear measurement model:
 - $Y_k = X_k + \sigma W_k$
 - Nonlinear measurement model:

$$Y_k = \exp(X_k - \gamma_k) + \sigma W_k$$



Kolmogorov flow

Dynamics model:

$$\begin{cases} \partial_t \mathbf{u} = -(\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} - \frac{1}{\rho} \nabla p + \mathbf{F}, \\ 0 = \nabla \cdot \mathbf{u}. \end{cases}$$

Measurement model:

- Low-resolution observation
- Sparse observation
- Partial observation



Ablation study: influence of the prediction score

- Score-based Langevin sampling
- Langevin sampling without prediction score
- Ensemble maximum likelihood estimation





Uncertainty quantification



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- Improvement of the computational efficiency.
- Provable non-log-concave posterior sampling.
- Refined error bounds for long-time assimilation.
- Applications in the real data.

<u>Reference:</u> Zhao Ding, Chenguang Duan, Yuling Jiao, Jerry Zhijian Yang, Cheng Yuan, and Pingwen Zhang. Nonlinear Assimilation via Score-based Sequential Langevin Sampling. arXiv:2411.13443.

Thanks for your attention!

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