

Optimality vs Stability Trade-off in Ensemble Kalman Filters

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Bayeruth, Germany*

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Joint work with Prashant Mehta^{*} and Tryphon Georgiou⁺

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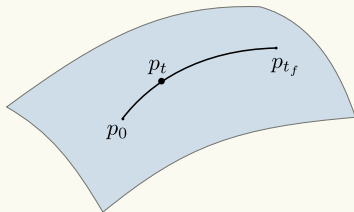
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Sep 15, 2022



Realizing probability flows with stochastic processes



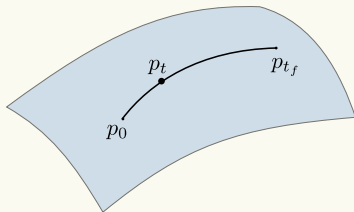
Problem: given a probability flow $\{p_t\}_{t \geq 0}$, construct a stochastic process $\{X_t\}_{t \geq 0}$ such that

$$\text{Law}(X_t) = p_t, \quad \forall t \geq 0.$$

Significance:

- interacting particle sampling algorithms (e.g. SVGD)
- simulating Wasserstein gradient flows
- diffusion-based generative models
- controlled particle filtering algorithms → this talk

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Realizing probability flows

Example

- Assume p_t is a one-dimensional Gaussian $N(0, \Sigma_t)$ where $\Sigma_t = 1 + 2t$.

- Assume X_t is of the form

$$dX_t = u_t dt + v_t dB_t, \quad X_0 \sim p_0.$$

- Design u_t and v_t such that $\text{Law}(X_t) = p_t$ for all $t \geq 0$.

- Solution:

$$dX_t = \sqrt{2}dB_t, \quad X_0 \sim N(0, 1)$$

- Why?

$$\text{mean: } \frac{d}{dt} \mathbb{E}[X_t] = 0 \quad \Rightarrow \quad \mathbb{E}[X_t] = \mathbb{E}[X_0] = 0 \quad \checkmark$$

$$\text{variance: } \frac{d}{dt} \text{Var}[X_t] = 2 \quad \Rightarrow \quad \text{Var}[X_t] = \text{Var}[X_0] + 2t = 1 + 2t \quad \checkmark$$

$$\text{distribution: } X_t \text{ is Gaussian} \quad \checkmark$$

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Question: Are there any other realizations?

■ Yes,

$$dX_t = \frac{X_t - \mathbb{E}[X_t]}{\text{Var}[X_t]} dt, \quad X_0 \sim N(0, 1).$$

■ Why?

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Question: How to simulate the two processes?

- Simulate N stochastic processes/particles $\{X_t^1, \dots, X_t^N\}$

stochastic: $dX_t^i = \mu(X_t^i)dt + \sigma(X_t^i)dW_t^i, \quad X_0^i = X(0, \omega)$

deterministic: $dX_t^i = \frac{1}{N} \sum_{j=1}^N \mu(X_t^j)dt, \quad X_0^i = X(0, \omega)$
 $\frac{dX_t^i}{dt} = \frac{1}{N} \sum_{j=1}^N \mu(X_t^j), \quad X_0^i = X(0, \omega)$

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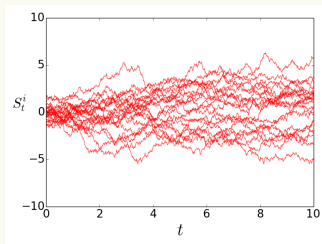
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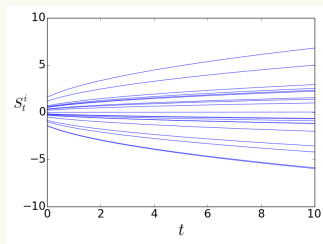
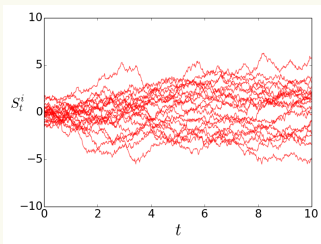


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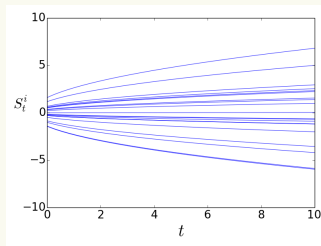
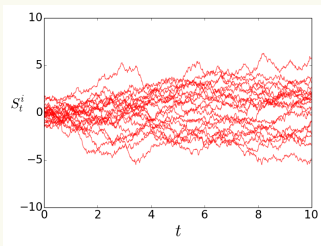
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Realizing probability flows

Questions

- Is there a principled approach to obtain these processes?
- In the mean-field limit, do they exhibit different (stability) properties?
- In finite- N setting, do they exhibit different approximation error?

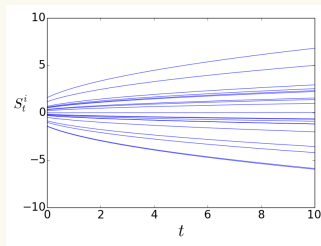
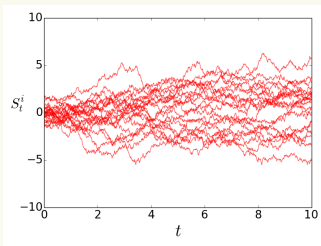


This paper: study these questions for controlled particle filtering algorithms

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This paper: study these questions for controlled particle filtering algorithms

Filtering problem

Model:

state process : $\{X_t\}_{t \geq 0}$

observation process : $\{Z_t\}_{t \geq 0}$

posterior dist. : $\pi_t := \mathbb{P}(X_t | \mathcal{Z}_t)$ where $\mathcal{Z}_t := \sigma(Z_s; s \in [0, t])$

Objective: compute the posterior distribution π_t .

Approach:

- realize $\{\pi_t\}_{t \geq 0}$ with a stochastic process $\{\bar{X}_t\}_{t \geq 0}$ s.t.

$$\text{Law}(\bar{X}_t) = \pi_t, \quad \forall t \geq 0.$$

- simulate \bar{X}_t as a system of N interacting particles $\{\bar{X}_t^1, \dots, \bar{X}_t^N\}$,

$$\frac{1}{N} \sum_{i=1}^N \delta_{\bar{X}_t^i} \approx \text{Law}(\bar{X}_t) = \pi_t.$$

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Filtering problem

Linear-Gaussian setting

Model:

state process : $dX_t = AX_t dt + \sigma_B dB_t$

observation process : $dZ_t = HX_t dt + \sigma_W dW_t$

posterior dist. : $\pi_t := \mathbb{P}(X_t | \mathcal{Z}_t)$ where $\mathcal{Z}_t := \sigma(Z_s; s \in [0, t])$

Kalman filter: posterior dist. π_t is Gaussian $N(m_t, \Sigma_t)$ where

$$dm_t = Am_t + K_t(dZ_t - Hm_t dt) =: \mathcal{T}_t(m_t, \Sigma_t)$$

$$\frac{d\Sigma_t}{dt} = 2A\Sigma_t + \sigma_B^2 - H^2\Sigma_t^2 =: \text{Ricc}(\Sigma_t)$$

Ensemble Kalman filter:

- Realize π_t with a stochastic process \bar{X}_t .
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Ensemble Kalman filter

Construction of \bar{X}_t

- Let $\pi_t = N(m_t, \Sigma_t)$ where $dm_t = \mathcal{T}_t(m_t, \Sigma_t)$ and $\dot{\Sigma}_t = \text{Ricc}(\Sigma_t)$.

- Assume \bar{X}_t is of the form

$$d\bar{X}_t = u_t dt + v_t dZ_t + r_t d\bar{B}_t + q_t d\bar{W}_t, \quad \bar{X}_0 \sim \bar{\pi}_0$$

- Find u_t, v_t, r_t, q_t such that

$$\text{Law}(\bar{X}_t) = \pi_t, \quad \forall t \geq 0$$

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where $\bar{m}_t = \mathbb{E}[\bar{X}_t | \mathcal{Z}_t]$, $\bar{\Sigma}_t = \text{Var}[\bar{X}_t | \mathcal{Z}_t]$, and (G, r, q) satisfy

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Ensemble Kalman filter

Three established forms

- EnKF with perturbed observation [Reich 2011]

$$\textbf{P-EnKF:} \quad d\bar{X}_t = A\bar{X}_t dt + \sigma_B d\bar{B}_t + \bar{K}_t(dZ_t - H\bar{X}_t dt - d\bar{W}_t)$$

- Square-root EnKF [Bergemann & Reich 2012]

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- Deterministic EnKF [Taghvaei & Mehta 2016]

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Ensemble Kalman filter

Three established forms

- EnKF with perturbed observation [Reich 2011]

P-EnKF:
$$d\bar{X}_t = A\bar{X}_t dt + \sigma_B d\bar{B}_t + \bar{K}_t(dZ_t - H\bar{X}_t dt - d\bar{W}_t)$$

- Square-root EnKF [Bergemann & Reich 2012]

S-EnKF:
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Ensemble Kalman filter

Stability with respect to error in initial condition

- By construction

$$\text{Law}(\bar{X}_t) = \pi_t, \quad \forall t \geq 0, \quad \text{if } \underline{\text{Law}(\bar{X}_0) = \pi_0}.$$

- What if $\text{Law}(\bar{X}_0) \neq \pi_0$? Does $\text{Law}(\bar{X}_t) \rightarrow \pi_t$ as $t \rightarrow \infty$?

Stability

Assume the pair (A, σ_B) is controllable and the pair (A, H) is observable. Then,

$$\mathbb{E}[\mathcal{W}_2(\bar{\pi}_t, \pi_t)] \leq C e^{-\lambda_0 t} \mathcal{W}_2(N(\bar{m}_0, \bar{\Sigma}_0), N(m_0, \Sigma_0)) + e^{\int_0^t G_s ds} \mathcal{W}_2(N(\bar{m}_0, \bar{\Sigma}_0), \bar{\pi}_0)$$

- 1st term: error in the initial mean and variance
- Converges exponentially to zero with rate $\lambda_0 > 0$ for all forms of EKF.
- 2nd term: how “non-Gaussian” is the initial distribution
- Its asymptotic behavior depends on the choices for G_s

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- The error depends on the initial condition and on the initial distribution
- Converges exponentially to zero with rate λ_0 for all forms of EKF
- And converges to the initial condition for the initial distribution
- The convergence behavior depends on the way the process is perturbed

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Ensemble Kalman filter

Stability for the three forms of EnKF

- Assuming correct initial mean and variance (so that the first term is zero):

$$\text{P-EnKF: } \mathbb{E}[\mathcal{W}_2(\bar{\pi}_t, \pi_t)] \leq (\text{const.})e^{-\lambda_0 t}$$

$$\text{S-EnKF: } \mathbb{E}[\mathcal{W}_2(\bar{\pi}_t, \pi_t)] \leq (\text{const.})e^{-\lambda_1 t} \quad 0 < \lambda_1 < \lambda_0$$

$$\text{D-EnKF: } \mathbb{E}[\mathcal{W}_2(\bar{\pi}_t, \pi_t)] \geq (\text{const.})$$

- P-EnKF and S-EnKF are exponentially stable.
- convergence rate of P-EnKF is strictly larger than S-EnKF.
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Finite- N error analysis

- system of interacting particles:

$$dX_t^i = \mathcal{T}_t(m_t^{(N)}, \Sigma_t^{(N)}) + G_t(X_t^i - m_t^{(N)})dt + r_t dB_t^i + q_t dW_t^i$$

- objective: analyze the empirical approximation error

$$\bar{\pi}_t \approx \pi_t^{(N)} := \frac{1}{N} \sum_{i=1}^N \delta_{X_t^i}$$

Error analysis for empirical variance

Assume $\sup_{t \geq 0} \mathbb{E}[(r_t^2 + q_t^2) \bar{\Sigma}_t] = M < \infty$. Then, the error in empirical variance

$$\lim_{t \rightarrow \infty} \mathbb{E}[(\Sigma_t^{(N)} - \Sigma_t)^2] \leq (\text{const.}) \frac{M}{N}$$

- Error is due to stochastic terms in the dynamics

$$\text{P-EnKF: } M \propto \sigma_B^2 + H^2, \quad \text{S-EnKF: } M \propto \sigma_B^2, \quad \text{D-EnKF: } M = 0$$

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Summary and conclusions

- General form of EnKF:

$$d\bar{X}_t = \mathcal{T}_t(\bar{m}_t, \bar{\Sigma}_t) + G_t(\bar{X}_t - \bar{m}_t)dt + r_t d\bar{B}_t + q_t d\bar{W}_t$$

$$\text{s.t. } 2G_t\bar{\Sigma}_t + r_t^2 + q - t^2 = \text{Ricc}(\bar{\Sigma}_t)$$

- Analysis for three established forms:

Algorithm	G_t	r_t	q_t	Stability rate	finite- N error
P-EnKF	$A - \bar{\Sigma}_t H^2$	σ_B	$\Sigma_t H$	λ_0	$\propto N^{-1}(\sigma_B^2 + H^2)$
S-EnKF	$A - \frac{1}{2}\bar{\Sigma}_t H^2$	σ_B	0	$\frac{\lambda_0 - A}{2}$	$\propto N^{-1}\sigma_B^2$
D-EnKF	$A - \bar{\Sigma}_t H^2 + \frac{\sigma_B^2}{2\bar{\Sigma}_t}$	0	0	0	0

- a trade-off between stability and finite- N error
- Is this fundamental? Are there design principles that take this into consideration?

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