

Some theoretical aspects of Particle Filters and Ensemble Kalman Filters

P. Del Moral

**Mathematical Foundations of Data Assimilation and Inverse
Problems - FoCM Paris June 2023.**

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- ▶ Law of large numbers, Ergodic theo, **Stoch. Perturbation theory.**

Analysis/Performance/Convergence/... Crude Monte Carlo

Sample mean $m_t := \frac{1}{N} \sum_{1 \leq i \leq N} X_t^i$ with **iid** copies X_t^i of X_t

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Key Observation:

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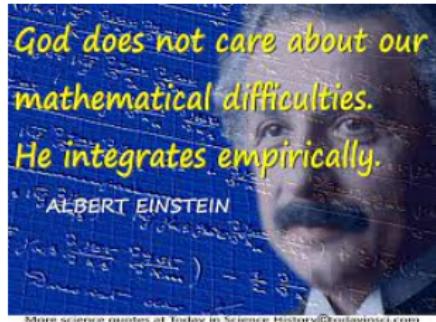
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$$\begin{aligned} X_1 &= \int a(X_0, x_0) \eta_0(dx_0) + W_1 = \mathbb{E}(a(X_0, \bar{X}_0) \mid X_0) + W_1 \\ &\stackrel{\text{ex}}{=} \int \sqrt{\log(1 + \|X_0 - x_0\|^2)} \eta_0(dx_0) + W_1 \end{aligned}$$

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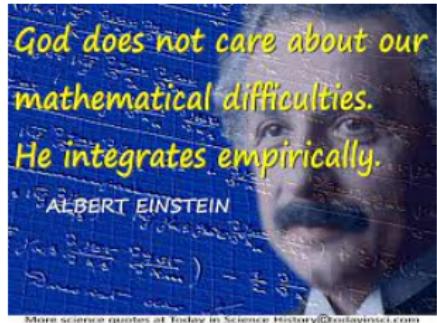


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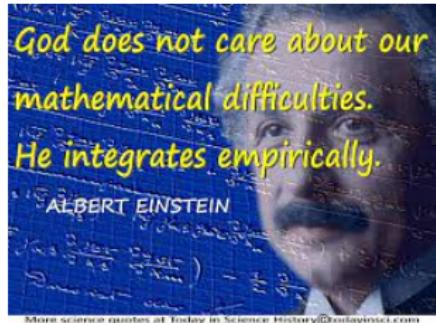


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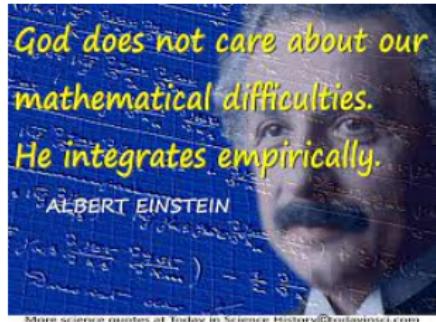
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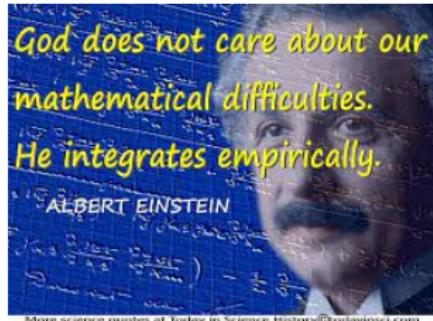
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but "almost iid" (propagation (initial) chaos) . . .

A brief review on sampling \bar{X}_{t+dt} given $\bar{X}_t \sim \eta_t(dx_t)$

Continuous time version = McKean-Vlasov/Interacting diffusions

$$d\bar{X}_t = \bar{X}_{t+dt} - \bar{X}_t = \left(\int b(\bar{X}_t, \textcolor{red}{x_t}) \eta_t(dx_t) \right) dt + \underbrace{\sqrt{dt} N(0, 1)}_{W_{t+dt} - W_t = dW_t}$$

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Continuous/Discrete time versions : Nonlinear/Interacting diffusions/jumps/accept-reject nonlinear Markov chains, . . .

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~> Particle filters, GA, SMC, DMC, ..., EnKF, ...

1. Find some possibly nonlinear process

$$\bar{X}_t \sim \text{Law}(X_t \mid Y_0, \dots, Y_t)$$

2. Then apply mean field particle methodology

Say $N = \text{precision}$ (nb of samples/particles, time steps $\Delta t = 1/N, \dots$)

Maths literature abounds with fancy bounds/theo of the type:

"Theorem": Mean error/bias/variance/estimate at time $t \leq e^{7t}/N$

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Impossible to run such particle algorithm

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or $\Rightarrow e^{c_1 t}/N, c_2(t)$ with $0 < c_i, c_j(t) < \infty$.

BUT $t \leq 6 \implies$ Eventually use all sand grains on earth



Particle Filters discrete time models

Personal "crude" $c_1 e^{c_2 t} / \sqrt{N}$ mean error style estimates

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(unbiasedness properties + first rigorous, MPRF 96)
- ▶ General particle methodology, AAP 98, LPD+CLT+...SPA 98,...

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Time uniform estimates-stable signals (first time unif. mean field particle)

- ▶ Stab Particle filters/GA (+ Guionnet CRAS 99, IHP 98/01)
- ▶ Feynman-Kac/particle filters (+ Miclo, Sem Proba 00)+.....
- ▶ ⇒ New approach: stochastic perturbation \sim stability limiting process

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~~> Stability Markov & Positive/Feynman-Kac semigroups

- ▶ Lyapunov sg. & illustrations + Arnaudon, Ouhabaz SAA 23
- ▶ Stability positive sg. + Horton AAP23



Stochastic perturbation \sim stability limiting process

Applications to Measure-valued processes & diffusion flows

- Interacting jumps + Arnaudon EJP-20.
- Interacting diffusions + Arnaudon AAP-20.
- Interpolation diffusion flows + Singh SPA-22 (CRAS-20).

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~ Linear-Gaussian world - possibly unstable/transient "signals"

- Stability Kalman-Bucy filters + Bishop SIAM-17.
- Inflation/localisation + Bishop, S. Pathiraja SPA-17.
- Harmonic Oscillator ($Y = 0$) + Horton CIMP-23/Arxiv21.

KEY OBS:

Innovation/Weights/Penalties/likenesses... stabilizing effects !!

Uniform estimates for EnKF continuous time models

For stable signals

- ▶ AAP-18/Arxiv-16 (Unif. EnKBF)+ Tugaut.
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Ensemble KB filters for possibly unstable/transient signals

- ▶ AAP-19 (1d-case)+ Bishop, Kamatani, Rémillard.
- ▶ IHP-19 (Perturbation Stoch. Riccati)+ Bishop, A. Niclas.
- ▶ EJP-19 (Stability Stoch. Riccati)+ Bishop.
- ▶ ↗ MCSS-23 Review article (+ Bishop, Arxiv 20)

Continuous time **Linear+Gaussian filtering problem**

$$\begin{cases} dX_t &= A X_t \, dt + R^{1/2} \, dW_t \in \mathbb{R}^r \\ dY_t &= C X_t \, dt + \Sigma^{1/2} \, dV_t \quad \rightsquigarrow \mathcal{Y}_t := \sigma(Y_s, s \leq t). \end{cases}$$

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Optimal \mathbb{L}_2 -estimate = Kalman-Bucy filter

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with **the gain given by the matrix Riccati equation**

$$\partial_t P_t = \text{Ricc}(P_t) := AP_t + P_tA' - P_t S P_t + R \quad \text{with} \quad S := C' \Sigma^{-1} C$$

Reformulation \rightsquigarrow Nonlinear Kalman-Bucy diffusion

\iff McKean-Vlasov type diffusions \bar{X}_t such that (given \mathcal{Y}_t)

$$\eta_t := \text{Law}(\bar{X}_{\textcolor{red}{t}}) = \mathcal{N}\left[\hat{X}_t, P_t\right]$$

\rightsquigarrow Interacting with their conditional mean and covariance matrices

$$\mathcal{P}_{\eta_t} = \eta_t \left[(\mathbf{e} - \eta_t(\mathbf{e})) (\mathbf{e} - \eta_t(\mathbf{e}))' \right] \quad \text{with} \quad \mathbf{e}(x) := x.$$

2 classes of McKean-Vlasov type diffusions

1) "Vanilla EnKF" (\rightsquigarrow (corrected) discrete time - Evensen 94)

$$d\bar{X}_t = A \bar{X}_t dt + R^{1/2} d\bar{W}_t + \mathcal{P}_{\eta_t} C' \Sigma^{-1} \left[dY_t - \left(C \bar{X}_t dt + \Sigma^{1/2} d\bar{V}_t \right) \right]$$

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Tempting to replace "A x" and "C x" by $A(x)$, $C(x)$ (often done)

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Tempting to replace "A x" and "C x" by $A(x)$, $C(x)$ (often done)

BUT NOT CONSISTENT WITH THE OPTIMAL FILTER

Example: Extended Kalman-Bucy Ensemble filter ($A(x)$)

$$\begin{cases} d\hat{X}_t &= A(\hat{X}_t) dt + P_t C' \Sigma^{-1} (dY_t - C\hat{X}_t dt) \\ \partial_t P_t &= \partial A(\hat{X}_t) P_t + P_t \partial A(\hat{X}_t)' - P_t S P_t + R \end{cases}$$

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Nonlinear/McKean-Vlasov-type diffusion

$$d\bar{X}_t = \mathcal{A}(\bar{X}_t, \eta_t(e)) dt + R^{1/2} d\bar{W}_t$$

$$+ \mathcal{P}_{\eta_t} C' \Sigma^{-1} (dY_t - (C\bar{X}_t dt + \Sigma^{1/2} d\bar{V}_t))$$

$$\mathcal{A}(x, m) := A(m) + \partial A(m) (x - m)$$

Example: Extended Kalman-Bucy Ensemble filter ($A(x)$)

$$\begin{cases} d\hat{X}_t &= A(\hat{X}_t) dt + P_t C' \Sigma^{-1} (dY_t - C\hat{X}_t dt) \\ \partial_t P_t &= \partial A(\hat{X}_t) P_t + P_t \partial A(\hat{X}_t)' - P_t S P_t + R \end{cases}$$

Nonlinear/McKean-Vlasov-type diffusion

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Refs:

- ▶ SIAM-17/Arxiv-16(Extended EnKBF)+ Kurtzmann, Tugaut.
- ▶ EJP-18 (Stability Extended KBF)+ Kurtzmann, Tugaut.

The Ensemble Kalman-Bucy filter

(Ex. Case 1) Mean field sampler $\rightsquigarrow N + 1$ interacting diffusions

$$d\xi_t^i = A \xi_t^i dt + R^{1/2} d\bar{W}_t^i + p_t C' \Sigma^{-1} \left[dY_t - \left(C \xi_t^i dt + \Sigma^{1/2} d\bar{V}_t^i \right) \right]$$

with the rescaled particle covariance matrices

$$p_t := \frac{1}{N} \sum_{1 \leq i \leq N+1} (\xi_t^i - m_t) (\xi_t^i - m_t)'$$

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where are the Kalman-Bucy filter and the Riccati equations ?

Perturbation theorem(s):

$$dm_t = A m_t dt + p_t C' \Sigma^{-1} (dY_t - Cm_t dt) + \frac{1}{\sqrt{N+1}} dM_t$$

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This talk = answer these 2 questions for 1D linear/Gaussian

- ▶ 1d-discrete time/EnKF (+ Horton, Arxiv 21, AAP 23)
- ▶ ~ EnKF Review article (+ Bishop, Arxiv 20, MCSS 23)

Linear + Gaussian + discrete 1d-filtering problem

$$\begin{cases} X_{n+1} = A X_n + B W_{n+1} & X_0 \sim \mathcal{N}(\hat{X}_0^-, P_0) \\ Y_n = C X_n + D V_n & n \in \mathbb{N} := \{0, 1, 2, \dots\} \end{cases}$$

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$$\Downarrow \quad \mathcal{Y}_n := (Y_0, \dots, Y_n)$$

One-step predictor & Optimal filter = Gaussian

$$\text{Law}(X_n \mid \mathcal{Y}_{n-1}) = \mathcal{N}(\hat{X}_n^-, P_n) \quad \& \quad \text{Law}(X_n \mid \mathcal{Y}_n) = \mathcal{N}(\hat{X}_n, \hat{P}_n)$$

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~~> Kalman filter (1960s') = Gauss-Legendre regression (1800s')

$$(\hat{X}_n^-, P_n) \xrightarrow{\text{updating}} (\hat{X}_n, \hat{P}_n) \xrightarrow{\text{prediction}} (\hat{X}_{n+1}^-, P_{n+1})$$

Particle filters = GA = SMC = DMC = ...

$$\left(\xi_n^{i-} \right)_{1 \leq i \leq N} \in \mathbb{R}^N \xrightarrow{\text{Selection}} \left(\xi_n^j \right)_{1 \leq j \leq N} \xrightarrow{\text{Mutation}} \left(\xi_{n+1}^{i-} \right)_{1 \leq i \leq N}$$

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$$\xi_n^j \sim \sum_{1 \leq i \leq N} \frac{e^{-(Y_n - C\xi_n^{i-})^2/(2D^2)}}{\sum_{1 \leq j \leq N} e^{-(Y_n - C\xi_n^{j-})^2/(2D^2)}} \delta_{\xi_n^{i-}} \quad \text{and set} \quad \xi_{n+1}^{j-} := A \xi_n^j + B W_{n+1}^j$$

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and for $|A| < 1$? \rightsquigarrow Time-uniform estimates (new coming article)
 \rightsquigarrow find stable twisted guiding mutations (up to change of weights/probab)

(Conditional) Mean equations

$$\begin{cases} \hat{X}_n^- = \hat{X}_n^- + \text{Gain}_n \left(Y_n - C\hat{X}_n^- \right) & \text{with } \text{Gain}_n := CP_n/(C^2P_n + D^2) \\ \hat{X}_{n+1}^- = A\hat{X}_n^- \end{cases}$$

Offline Riccati equations

$$\begin{cases} \hat{P}_n = (1 - G_n C)P_n = P_n/(1 + SP_n) & \text{with } S := (C/D)^2 \\ P_{n+1} = A^2\hat{P}_n + R & \text{with } R = B^2 \end{cases}$$

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$$\rightsquigarrow P_{n+1} = \phi(P_n) := \frac{aP_n + b}{cP_n + d} \quad \text{with } (a, b, c, d) := (A^2 + RS, R, S, 1)$$

Reminder:

P_n and $(\hat{X}_n - X_n)$ are stable for any A (Kalman/Bucy-Stab Theory) !

Conditional-Nonlinear Markov chain (Perfect Sampler)

$$\begin{cases} \hat{\mathfrak{x}}_n &= \mathfrak{x}_n + \text{gain}_n (Y_n - (C\mathfrak{x}_n + D\mathcal{Y}_n)) \quad \text{with} \quad \text{gain}_n := C\mathfrak{p}_n / (C^2\mathfrak{p}_n + D^2) \\ \mathfrak{x}_{n+1} &= A\hat{\mathfrak{x}}_n + B\mathcal{W}_{n+1}. \end{cases}$$

$(\mathcal{Y}_n, \mathcal{W}_n)$ copies of (V_n, W_n) and \mathfrak{p}_n variance of the state \mathfrak{x}_n .

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Consistency property:

$$\mathbf{x}_n \sim \mathcal{N}\left(\hat{\mathbf{X}}_n^-, P_n = \mathbf{p}_n\right) \quad \text{and} \quad \hat{\mathbf{x}}_n \sim \mathcal{N}\left(\hat{\mathbf{X}}_n, \hat{P}_n\right).$$

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Nb: The Sakov & Oke (a.k.a. deterministic EnKF) discrete time versions are **NOT consistent**.

EnKF = Mean field interacting particle sampler

$$\begin{cases} \widehat{\xi}_n^i &= \xi_n^i + \textcolor{blue}{g}_n (Y_n - (C\xi_n^i + D\mathcal{V}_n^i)) \quad \text{with} \quad \textcolor{blue}{g}_n := C\textcolor{blue}{p}_n / (C^2 \textcolor{blue}{p}_n + D^2) \\ \xi_{n+1}^i &= A\widehat{\xi}_n^i + B\mathcal{W}_{n+1}^i \quad i \in \{1, \dots, N+1\} \end{cases}$$

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$(\mathcal{V}_n^i, \mathcal{W}_n^i)$ copies of (V_n, W_n) and re-scaled sample variance

$$\textcolor{blue}{p}_n := \frac{1}{N} \sum_{1 \leq i \leq N+1} (\xi_n^i - \textcolor{red}{m}_n)^2$$

with the sample mean

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Perturbation theo. (*Up to a change of probability space*)

$$\left\{ \begin{array}{lcl} \hat{m}_n & = & m_n + g_n (Y_n - Cm_n) + \frac{1}{\sqrt{N+1}} \hat{v}_n \\ \hat{p}_n & = & (1 - g_n C) p_n + \frac{1}{\sqrt{N}} \hat{\nu}_n \end{array} \right. \quad \left\{ \begin{array}{lcl} m_{n+1} & = & A \hat{m}_n + \frac{1}{\sqrt{N+1}} v_{n+1} \\ p_{n+1} & = & A^2 \hat{p}_n + R + \frac{1}{\sqrt{N}} \nu_{n+1}. \end{array} \right.$$

Perturbation theo. (*Up to a change of probability space*)

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Corollary: p_n Markov chain $\mathcal{K}(p, dq) =$ Stochastic Riccati eq.

$$p_{n+1} = \phi(p_n) + \frac{1}{\sqrt{N}} \delta_{n+1} \quad \text{with} \quad \delta_{n+1} := A^2 \hat{v}_n + \nu_{n+1}.$$

Stab. theo. (cf. 10 pages section 2 in (+Arnaudon, Ouhabaz SAA 23))

Theo 1: \exists Lyapunov fct. $\mathcal{U}(p) = 1 + u(p + 1/p)$ s.t. $\beta_{\mathcal{U}}(\mathcal{K}) < 1$

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Key/difficulty: Estimates/Expo. decays $\forall A$ of random products

$$\mathcal{E}_{I,n} := \prod_{I \leq k \leq n} \frac{A}{1 + Sp_k}$$

OK for $|A| < 1$ but also for $|A| \geq 1$ unstable/effective dimension/...

Time uniform estimates for any A

Theo 1 [(Under) Bias]: $\forall k \geq 1 \exists \iota_k < \infty$ s.t. $\forall N \geq 1 \forall n \geq 0$

$$0 \leq P_n - \mathbb{E}(p_n) \leq \iota_1 / N$$

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& Uniform control of the bias ($N \geq N_k$)

$$\mathbb{E} \left(|\mathbb{E}(\hat{m}_n \mid \mathcal{Y}_n) - \hat{X}_n|^k \right)^{1/k} \leq \iota_k/N$$

Time uniform estimates for any A

Theo 2 [\mathbb{L}_k -mean errors]: $\forall k \geq 1 \exists \iota_k < \infty$ s.t. $\forall N \geq 1 \forall n \geq 0$

$$\mathbb{E} \left(|\hat{m}_n - \hat{X}_n|^k \right)^{1/k} \vee \mathbb{E} \left(|p_n - P_n|^k \right)^{1/k} \leq \iota_k / \sqrt{N}.$$

(state estimates for $N \geq N_k$)

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Many other results/fairly complete analysis: multivariate central limit theorems, exponential decays random products, . . .