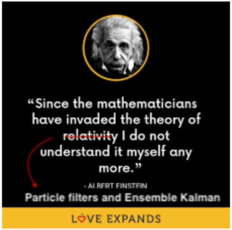
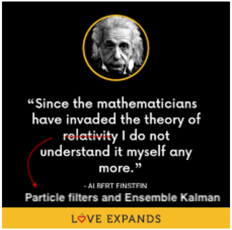
Some theoretical aspects of Particle Filters and Ensemble Kalman Filters

P. Del Moral

50th Annual meeting of the Statistical Society of Canada, Carleton University Ottawa, May 2023.



“Since the mathematicians have invaded the theory of relativity I do not understand it myself any more.”
- ALBERT EINSTEIN
Particle filters and Ensemble Kalman
LOVE EXPANDS



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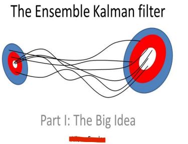

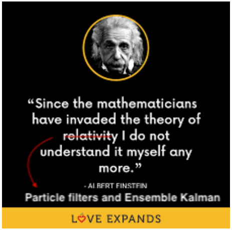

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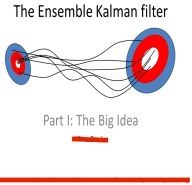

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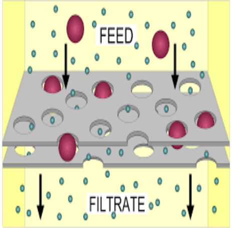

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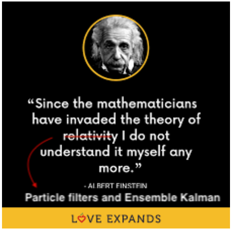

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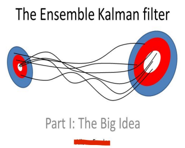

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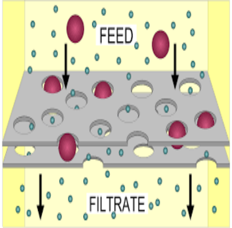

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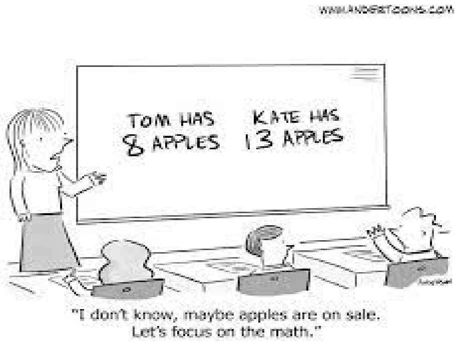

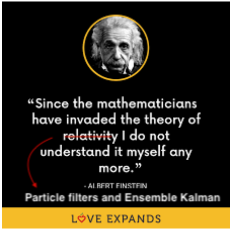

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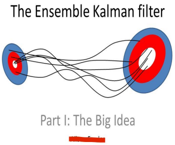

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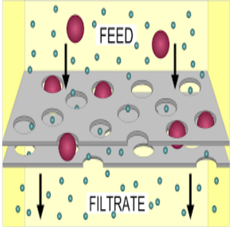

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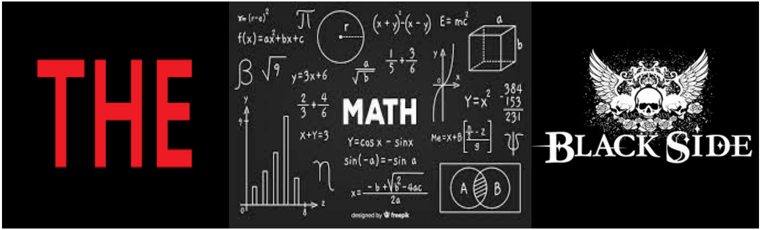

Brief review on filtering = X_t given observation Y_t

- **Linear+Gaussian world: Regression form., `Kalman filters`.**
- **Nonlinear/Non-Gaussian: Bayes rule, Nonlinear filtering eq.**
- **Application areas:**

  Data assimilation, forecasting, tracking, multiple objects tracking, machine learning...

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

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⇝ **stochastic perturbation formulation**

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A brief review on sampling X_1 given $X_0 \sim \eta_0(dx_0)$

Markov transition:

$$X_1 = A(X_0) + B(X_0)\ W_1 \quad \text{with} \quad W_1 \quad \text{i.i.d. } N(0,1)$$

when $x \mapsto (A(x), B(x))$ are **known**.

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Nonlinear evol. = Discrete McKean-Vlasov + Standard Markov

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Standard MCMC tools cannot be applied on the fly

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[$\subset$ Mean field particle sampler]

Note: Running cost N^2

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Continuous time version = McKean-Vlasov/Interacting diffusions

$$dX_t = X_{t+dt} - X_t = \left(\int b(X_t, x_t)\ \eta_t(dx_t) \right)\ dt + \underbrace{\sqrt{dt}\ N(0,1)}_{W_{t+dt} - W_t = dW_t}$$

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$\rightsquigarrow$ particle filters, GA, SMC, DMC,. . .

Say N = precision (nb of samples/particles, time steps $\Delta t = 1/N, \ldots$)

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

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

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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 $t \leqslant 6 \Longrightarrow$ **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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- 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)
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- $\supset$ **New approach: stochastic perturbation $\sim$ stability limiting process**

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(first time-uniform estimates for mean field particle systems)

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$\rightsquigarrow$ **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.
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$\rightsquigarrow$ **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/likelihoods... stabilizing effects !!

Uniform estimates for EnKF continuous time models

For stable signals

- AAP-18 (Unif. EnKBF)+ Tugaut.
- SIAM-17 (Unif. En-Extended KBF)+ Kurtzmann, Tugaut.
- EJP-18 (Stability Extended KBF)+ Kurtzmann, 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.
- $\rightsquigarrow$ MCSS-23 Review article (+ Bishop, Arxiv 20)

Continuous time **Linear+Gaussian filtering problem**

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

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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

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

Reformulation $\rightsquigarrow$ Nonlinear Kalman-Bucy diffusion

$\Longleftrightarrow$ **McKean-Vlasov type diffusions $\overline{X}_t$ such that (given $\mathcal{Y}_t$)**

$$\eta_t := \mathrm{Law}(\overline{X}_t) \; = \; \mathcal{N}\left[\widehat{X}_t, P_t\right]$$

$\rightsquigarrow$ **Interacting with their conditional mean and covariance matrices**

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

2 classes of McKean-Vlasov type diffusions

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

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

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BUT <u>NOT</u> CONSISTENT WITH THE OPTIMAL FILTER

The Ensemble Kalman-Bucy filter

(Case 1) Mean field interpretation $\rightsquigarrow$ $N+1$ interacting diffusions

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

with the rescaled particle covariance matrices

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

and the sample mean

$$m_t := \frac{1}{N+1} \sum_{1\leqslant i\leqslant N+1} \xi_t^i.$$

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

Th1: The EnKF equations

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\begin{aligned}
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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Key observations:

- Orthogonal martingales $(M_t, \overline{M}_t)$ and $m_0 \perp p_0$ (well known iid).

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- *In one dimension* [`AAP19 + Bishop-Kamatani-Rémillard`]:
  Vanilla EnKF p_t **heavy tailed invariant measure**.
  Deterministic EnKF p_t **Gaussian tailed invariant measure**.

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

- `1d-discrete time/EnKF (+ Horton, Arxiv 21, AAP 23)`
- $\rightsquigarrow$ `EnKF Review article (+ Bishop, Arxiv 20, MCSS 23)`

Linear+Gaussian+discrete 1*d*-filtering problem

$$\left\{\begin{array}{rcl} X_{n+1} & = & A\,X_n + B\,W_{n+1} \qquad X_0 \sim \mathcal{N}(\widehat{X}_0^-, P_0) \\ Y_n & = & C\,X_n + D\,V_n \qquad\qquad n \in \mathbb{N} := \{0,1,2\ldots\} \end{array}\right.$$

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

One-step predictor & Optimal filter = Gaussian

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

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$\rightsquigarrow$ **Kalman filter (1960s') = Gauss-Legendre regression (1800s')**

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

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

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

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Selection/ **Mutation**:

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

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Sample means $\simeq$ Conditional expectations:

$$\forall n \in \mathbb{N} \qquad \widehat{X}_n^{\text{PF}} := \frac{1}{N}\sum_{1\leqslant i\leqslant N} \xi_n^i \simeq_{N\to\infty} \widehat{X}_n$$

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BUT for any $A > 1$

$$\xi_0^{i-} = x_0^i > \frac{B}{A-1}\sqrt{2\log N} \Longrightarrow \lim_{n\to\infty} \mathbb{E}\left[\left|\widehat{X}_n^{\mathrm{PF}} - \widehat{X}_n\right|\right] = +\infty$$

Mean equations

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

Offline Riccati equations

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

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

Reminder:

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

Conditional-Nonlinear Markov chain ($\mathfrak{Perfect\ Sampler}$)

$$\left\{\begin{array}{rcl}\widehat{\mathfrak{X}}_n & = & \mathfrak{X}_n + \mathfrak{gain}_n \left(Y_n - (C\,\mathfrak{X}_n + D\,\mathfrak{V}_n)\right) \quad \text{with} \quad \mathfrak{gain}_n := C\mathfrak{P}_n/(C^2\mathfrak{P}_n + D^2) \\ \mathfrak{X}_{n+1} & = & A\,\widehat{\mathfrak{X}}_n + B\,\mathfrak{W}_{n+1}.\end{array}\right.$$

$(\mathfrak{V}_n, \mathfrak{W}_n)$ copies of (V_n, W_n) and $\mathfrak{P}_n$ variance of the state $\mathfrak{X}_n$.

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$$\Downarrow$$

Consistency property:

$$\mathfrak{X}_n \sim \mathcal{N}\left(\widehat{X}_n^-, P_n = \mathfrak{P}_n\right) \quad \text{and} \quad \widehat{\mathfrak{X}}_n \sim \mathcal{N}\left(\widehat{X}_n, \widehat{P}_n\right).$$

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

EnKF = Mean field interacting particle sampler

$$\begin{cases} \widehat{\xi}^i_n &= \xi^i_n + g_n \left(Y_n - (C\xi^i_n + D\mathcal{V}^i_n)\right) \quad \text{with} \quad g_n := Cp_n/(C^2p_n + D^2) \\ \xi^i_{n+1} &= A\,\widehat{\xi}^i_n + B\,\mathcal{W}^i_{n+1} \qquad i \in \{1, \ldots, N+1\} \end{cases}$$

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

$$p_n := \frac{1}{N} \sum_{1 \leqslant i \leqslant N+1} (\xi_n^i - m_n)^2$$

with the sample mean

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

$$\left\{\begin{array}{rcl}\widehat{m}_n & = & m_n + g_n\,(Y_n - Cm_n) + \frac{1}{\sqrt{N+1}}\,\widehat{\upsilon}_n \\ \widehat{p}_n & = & (1-g_nC)\,p_n + \frac{1}{\sqrt{N}}\,\widehat{\nu}_n \end{array}\right. \quad \left\{\begin{array}{rcl} m_{n+1} & = & A\,\widehat{m}_n + \frac{1}{\sqrt{N+1}}\,\upsilon_{n+1} \\ p_{n+1} & = & A^2\,\widehat{p}_n + R + \frac{1}{\sqrt{N}}\,\nu_{n+1}. \end{array}\right.$$

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local perturbations υ_n, ν_n and $\widehat{\nu}_n, \widehat{\upsilon}_n$ in terms of non central χ^2

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local perturbations υ_n, ν_n and $\widehat{\nu}_n, \widehat{\upsilon}_n$ in terms of non central χ^2

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

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

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

Theo 1: $\exists ! \pi = \pi \mathcal{K}$ & $\exists\, \mathcal{U}(p) = 1 + u(p + 1/p)$ s.t. $\beta_{\mathcal{U}}(\mathcal{K}) < 1$

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$$\|\mu_1 \mathcal{K}^n - \mu_2 \mathcal{K}^n\|_{\mathcal{U}} \leqslant \beta_{\mathcal{U}}(\mathcal{K})^n \|\mu_1 - \mu_2\|_{\mathcal{U}}.$$

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

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

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

Time uniform estimates for any A

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

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

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

& Uniform control of the bias

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

Time uniform estimates for any A

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

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

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

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"Running" projects:

1- Multivariate version with B. Nasri & B. Rémillard.
2- Ensemble Extended Kalman Filters:
($\rightsquigarrow$ `Continuous time +Kurtzmann, Tugaut, EJP-18`)
3- Nonlinear/non-consistent EnKF $\in$ high. dim. data assimilation.
4-...