Ensemble Kalman filter in high dimensions

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Joint work with Andrew J. Majda

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Content

- The Ensemble Kalman filter (EnKF)
  - Problem setup,
  - Origin,
  - Formulation,
  - Impact.
- High dimensional challenges for EnKF.
- Main theorem with effective dimension:
  - A variant of EnKF,
  - with a low effective dimension p,
  - reaches its proclaimed performance,

  if the ensemble size $K > Cp$ for a constant C.
- Main theorem with localization:
  - A local EnKF,
  - with a stable local covariance structure,
  - reaches its proclaimed performance,

  if the ensemble size $K > C_L \log d$ for a constant C_L.

- Signal-observation system with random coefficients

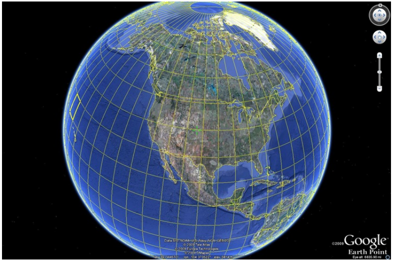
$$\text{Signal:}\quad X_{n+1} = A_n X_n + B_n + \xi_{n+1}, \quad \xi_{n+1} \sim \mathcal{N}(0, \Sigma_n)$$
$$\text{Observation:}\quad Y_{n+1} = H_n X_{n+1} + \zeta_{n+1}, \quad \zeta_{n+1} \sim \mathcal{N}(0, I_q)$$

  Goal: estimate X_n based on $Y_1, \ldots, Y_n$
- A_n, B_n, H_n (stationary) sequence of random matrices and vectors.
- A_n can be unstable sometimes. H_n can be on and off.
- Nonlinear settings:

$$X_{n+1} = \Psi_n(X_n) + \xi_{n+1}, \quad Y_{n+1} = H_n(X_{n+1}) + \zeta_{n+1}.$$

Weather forecast

- Signal: $X_{n+1} = \Psi_n(X_n) + \xi_{n+1}$,
  Observation: $Y_{n+1} = H_n X_{n+1} + \zeta_{n+1}$.
- Weather forecast:
  Signal: atmosphere and ocean, "follows" a PDE.
  Obs: weather station, satellite, sensors.....
- Main challenge: high dimension, $d \sim 10^6 - 10^8$.



Kalman filter: derivation

- Question: $x_0 \sim \mathcal{N}(m_0, R_0)$,
  $x_1 = Ax_0 + B + \xi, y_1 = Hx_1 + \zeta$, how to find y_1?
- Forecast: $x_1 \sim \mathcal{N}(Am_0 + B, AR_0A^T + \Sigma) = \mathcal{N}(\hat{m}, \widehat{R})$.
- Assimilation: $p(x_1|y_1)$: apply Bayes' formula
  Log of the unormalized likelihood:

$$
\begin{aligned}
&-\frac{1}{2}(x_1 - \hat{m})\widehat{R}^{-1}(x_1 - \hat{m}) - \frac{1}{2}(Hx_1 - y_1)^2 \\
&= -\frac{1}{2}(x_1 - m_1)(\widehat{R}^{-1} + H^T H)(x_1 - m_1) + r(y_1).
\end{aligned}
$$

  New mean and covariance

$$
\begin{aligned}
m_1 &= \hat{m} + \widehat{R}H^T(I + H\widehat{R}H^T)^{-1}(y_1 - H\hat{m}) \\
R_1 &= (\widehat{R}^{-1} + H^T H)^{-1} = \widehat{R} - \widehat{R}H^T(I + H\widehat{R}H^T)^{-1}H\widehat{R}.
\end{aligned}
$$

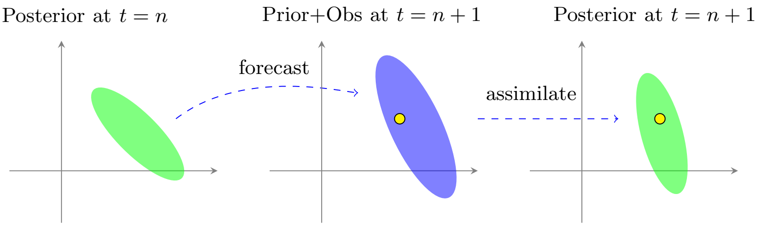
Kalman filter

- Use Gaussian: $X_n|_{Y_{1\dots n}} \sim \mathcal{N}(m_n, R_n)$
- Forecast step: $\hat{m}_{n+1} = A_n m_n + B_n$, $\widehat{R}_{n+1} = A_n R_n A_n^T + \Sigma_n$.
- Assimilation step: apply the Kalman update rule

$$m_{n+1} = \hat{m}_{n+1} + \mathcal{G}(\widehat{R}_{n+1})(Y_{n+1} - H_n \hat{m}_{n+1}), \quad R_{n+1} = \mathcal{K}(\widehat{R}_{n+1})$$

$$\mathcal{G}(C) = CH_n^T(I_q + H_n C H_n^T)^{-1}, \quad \mathcal{K}(C) = C - \mathcal{G}(C) H_n C$$

- Complexity: $O(d^3)$.



A brief history: Kalman filter

1958: designed by Rudolf Kalman (1930-2016)

- Discovered on a late night halted train ride.
- First paper was in published in mechanical engineering, not electrical engineering.
- Second paper was rejected at first.
- 1960: Stanley Schmidt at NASA invited Kalman.
- Extended Kalman filter: used in the Apollo project.
- Most core theories were developed by Kalman.
- Easy to teach in an engineering undergrad course.
- Implemented by digital computers.

EnKF (G. Evensen 1994)

- Monte Carlo: use samples to represent a distribution:

$$X^{(1)}, \dots, X^{(K)} \sim p, \quad \frac{1}{K}\sum_{k=1}^{K} \delta_{X^{(k)}} \approx p.$$

- Ensemble $\{X_n^{(k)}\}_{k=1}^K$ to represent $\mathcal{N}(\overline{X}_n, C_n)$

$$\overline{X}_n = \frac{\sum X_n^{(k)}}{K}, \quad S_n = [\Delta X_n^{(1)}, \cdots, \Delta X_n^{(K)}], \quad C_n = \frac{S_n S_n^T}{K-1}.$$

Ensemble Kalman filter (EnKF)

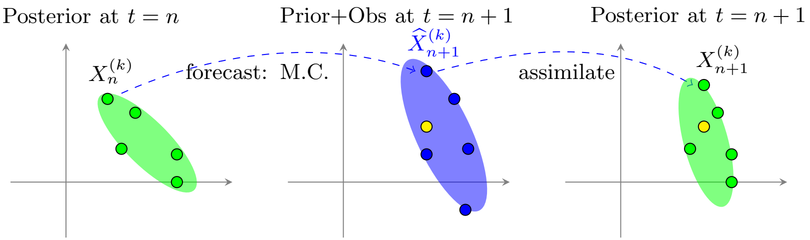
- Forecast step

$$\color{blue}{\widehat{X}^{(k)}_{n+1}} = A_n X^{(k)}_n + B_n + \zeta^{(k)}_{n+1}, \quad \widehat{C}_{n+1} = \frac{\widehat{S}_{n+1}\widehat{S}^T_{n+1}}{K-1}$$

- EAKF assimilation step, find $S_{n+1} = \mathbf{A}_{n+1}\widehat{S}_{n+1}$

$$\overline{X}_{n+1} = \overline{\widehat{X}}_{n+1} + \mathcal{G}(\widehat{C}_{n+1})(Y_{n+1} - H_n\overline{\widehat{X}}_{n+1}), \quad \mathbb{E}C_{n+1} \approx \mathcal{K}(\widehat{C}_{n+1})$$

- Complexity: $O(dK^2)$.



Nonlinear case

- Forecast step

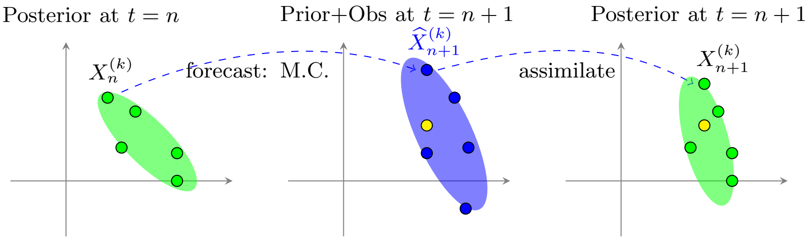
$$\widehat{X}^k_{n+1} = \Psi_n(X^k_n) + \xi^k_{n+1}, \quad Y^k_{n+1} = H_n(X^k_{n+1}) + \zeta^k_{n+1}$$

- Assimilation step

$$X^k_{n+1} = \widehat{X}^k_{n+1} + \mathcal{G}_{n+1}(Y_{n+1} - Y^k_{n+1}).$$

Gain matrix: $\mathcal{G}_{n+1} = S_X S_Y^T (I + S_Y S_Y^T)^{-1}$,
$S_X = \frac{1}{K-1}[X^{(1)}_{n+1} - \overline{X}_{n+1}, \dots, X^k_{n+1} - \overline{X}_{n+1}]$.

- Complexity $O(K^2 d)$.

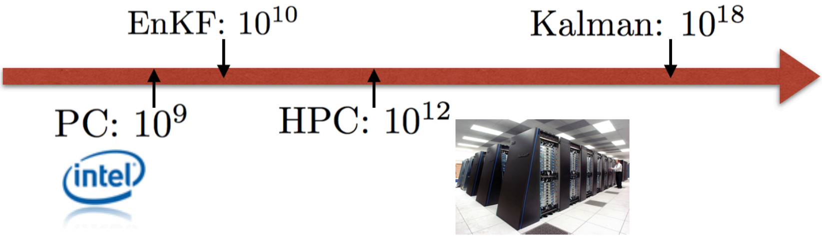


Successful applications to weather forecast

- System $d \sim 10^6$, ensemble size $K \sim 10^2$.
- Complexity of Kalman filter: $O(d^3) = O(10^{18})$.
- Complexity of EnKF: $O(K^2 d) = O(10^{10})$.
- No computation of gradient.

Also find applications in

- Oil reservoir management.
- Bayesian inverse problems.
- Deep learning.



Application:

- Successful weather forecast and oil reservoir management.
- Recently been applied to deep neural networks.
- $K = 50$ ensembles can forecast $d = 10^6$ dimensional systems.
- Extreme savings: $10^{10} = dK^2 \ll d^3 = 10^{18}$.

Literature

- Focused on showing ensemble version $(\overline{X}_n, C_n) \to (m_n, R_n)$
- Require $K \to \infty$ (Mandel, Cobb, Beezley 11)
- Fixed d sufficiently large K, $|A| < 1$ (Del Moral, Tugaut 16)
- Perturbation interpretation (Bishop, Del Moral, Pathiraja 17)
- Fixed K, well definedness $\mathbb{E}|X_n^{(k)}|^2 < \infty$ (Law, Kelly, Stuart, 14)
- Fixed K, boundedness $\sup_n \mathbb{E}|X_n^{(k)}|^2 < \infty$ (Tong, Majda, Kelly 15)
- Continuous version, stability for full obs (de Wilijes, Reich, Stannat17)

Missing: performance analysis with $K \ll d$.

Application and theory of EnKF

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Challenges

Ensemble size K to represent uncertainty of dimension d:

- Rank deficiency: $C_n = \frac{\sum_{k=1}^{K}(X_n^{(k)}-\overline{X}_n)(X_n^{(k)}-\overline{X}_n)^T}{K-1}$
  Has rank(C_n)$\leq K-1$, see as $\begin{bmatrix} C_n & 0 \\ 0 & 0 \end{bmatrix}$ } K-1 } d-K+1
- Instability of the dynamics: $\widehat{C}_{n+1} = A_n C_n A_n^T + \Sigma_n$
  What if span(C_n) does not cover expanding directions?
- Covariance decay by random sampling: $C_{n+1} = \mathcal{K}(\widehat{C}_{n+1})$
  $\mathcal{K}$: concave, monotone: $\mathbb{E}C_{n+1} = \mathbb{E}\mathcal{K}(\widehat{C}_{n+1}) \preceq \mathcal{K}(\mathbb{E}\widehat{C}_{n+1})$
- Spurious correlation in high dimension.
  Suppose $X_n^{(k)} \sim \mathcal{N}(0, I_d)$ i.i.d, by Bai-Yin's law

$$\|C_n - I_d\| \approx \sqrt{d/K} \quad \text{with large probability}$$

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Heuristic answers

We need conditions! One of two will help us

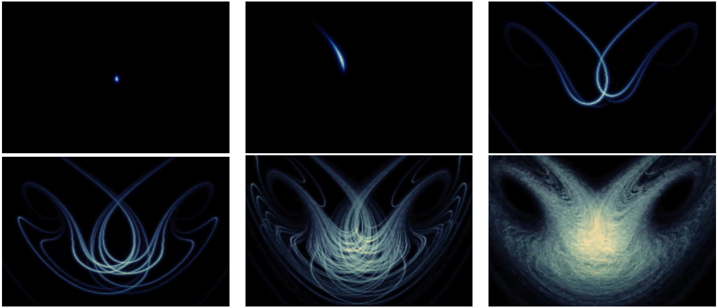
- Low effective dimension.
- Localized covariance structure.

Compared with high dimensional matrix computation

- Low rank matrices.
- Sparse matrices.

Low effective dimension

Simulation of Lorenz 63:



Lorenz system propagation. Video: MIT Aero Astro

Exploited by the UQ community for various purpose.
Assume there is a effective dimension $p < K \ll d$

- Most uncertainty lies in p directions, others below a threshold ρ,

$$\begin{bmatrix} C_n & 0 \\ 0 & 0 \end{bmatrix} \approx \begin{bmatrix} C_n & O(\rho) \\ O(\rho) & O(\rho) \end{bmatrix} \begin{array}{l} \} \text{ K-1} \\ \} \text{ d-K+1} \end{array}$$

Main results

Theorem (Majda, T. 16)

Suppose the system has a low effective filter dimension p, there is a variant of EnKF with a constant C, such that the EnKF reaches its proclaimed performance if $K > Cp$.

Next, we explain

- What variant of EnKF?
- How to define a low effective dimension?
- What does proclaimed performance mean?

Texas Hold'em,

Board: $\clubsuit 4$ $\spadesuit K$ $\heartsuit 4$ $\spadesuit 8$ $\spadesuit 7$

Your hand: $\heartsuit K$ $\diamondsuit K$ All in?

Alice's hand: $\diamondsuit 4$ $\spadesuit 4$!

- Chance of losing: 1 out of $C_{45}^{2} = 990$.
- Overconfidence makes you lose.
- Safer strategy: never all in (if possible).

For EnKF, confidence is described by the covariance matrix C_n.

- Large covariance: less confidence in estimation.
- Zero covariance: the estimator is the truth.
- An "overconfidence": filter divergence.

An illustrative example

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EnKF variant for enhanced fidelity

Techniques to enhance fidelity

- Rank deficiency: additive inflation ρI_d

$$C_n^\rho = \rho I_d + \frac{\sum_{k=1}^K (X_n^{(k)} - \overline{X}_n)(X_n^{(k)} - \overline{X}_n)^T}{K-1} = \begin{bmatrix} C_n + \rho I_{K-1} & 0 \\ 0 & \rho I_{d-K+1} \end{bmatrix}$$

The under represented direction: assume error strength is ρ.

- Instability of the dynamics. Increase noise strength

$$\widehat{X}_{n+1}^k = A_{n+1} X_n^{(k)} + \xi_{n+1}^{(k)}, \quad \xi_{n+1}^{(k)} \sim \Sigma_n^+$$
$$\Sigma_n \to \Sigma_n^+ = [\rho A_n A_n^T + \Sigma_n - \rho/r I_d],$$

Σ_n^+ indicates the system instability.

- Covariance decay by random sampling.
  Multiplicative inflation: $\widehat{C}_{n+1} = r\widehat{C}_{n+1}$
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Algorithm 1 EnKF variant

for $n \leftarrow 0$ to $T-1$ **do**

   $\Sigma_n^+ \leftarrow$ The positive part of $\rho A_n A_n^T + \Sigma_n - \rho/r I_d$.

   Generate $\xi_{n+1}^{(k)} \sim \mathcal{N}(0, \Sigma_n^+), k = 1, \dots, K$.

   $\overline{\widehat{X}}_{n+1} \leftarrow A_n \overline{X}_n + B_n + \frac{1}{K}\sum_{k=1}^K \xi_{n+1}^{(k)}$.

   $\widehat{S}_{n+1} \leftarrow \sqrt{r}(A_n S_n + [\Delta\xi_{n+1}^{(1)}, \dots, \Delta\xi_{n+1}^{(K)}])$.

   $\widehat{C}_{n+1} \leftarrow \frac{1}{K-1}\widehat{S}_{n+1}\widehat{S}_{n+1}^T$.

   $G_{n+1} \leftarrow \widehat{C}_{n+1}^{\rho} H_n^T (I_q + H_n \widehat{C}_{n+1}^{\rho} H_n^T)^{-1}$.

   $\overline{X}_{n+1} \leftarrow \overline{\widehat{X}}_{n+1} + G_{n+1}(Y_{n+1} - H_n \overline{\widehat{X}}_{n+1})$

   $P_{n+1} \leftarrow$Projection to the largest p eigenvectors of $\mathcal{K}(\widehat{C}_{n+1}^{\rho})$.

   $S_{n+1} \leftarrow \mathbf{A}_n \widehat{S}_{n+1}$ so $\frac{S_{n+1}S_{n+1}^T}{K-1} = P_{n+1}(\mathcal{K}(\widehat{C}_{n+1}^{\rho}) - \rho I_d)P_{n+1}$

   Return: $\mathcal{N}(\overline{X}_{n+1}, \frac{S_{n+1}S_{n+1}^T}{K-1} + \rho I_d)$

end for

Kalman filter reference

Effective dimension: hard to define through physical parameters.
Use a comparison principle between Kalman filters.
Original signal observation system:

$$\text{Signal:}\quad X_{n+1} = A_n X_n + B_n + \xi_{n+1}, \quad \xi_{n+1} \sim \mathcal{N}(0, \Sigma_n)$$
$$\text{Observation:}\quad Y_{n+1} = H_n X_{n+1} + \zeta_{n+1}, \quad \zeta_{n+1} \sim \mathcal{N}(0, I_q)$$

An inflated version:

$$\text{Signal}: X'_{n+1} = rA_n X'_n + B_n + \xi'_{n+1}, \quad \xi'_{n+1} \sim \mathcal{N}(0, \Sigma'_n)$$
$$\text{Observation}: Y'_{n+1} = H_n X'_{n+1} + \zeta'_{n+1}, \quad \zeta'_{n+1} \sim \mathcal{N}(0, I_q)$$

Noise is also inflated $\Sigma'_n = r^2 \Sigma_n^+ + r^2 \rho I_d$.
When $r \approx 1, \rho \approx 0$, two systems are similar to each other.

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$$\text{Signal}: X'_{n+1}=rA_nX'_n+B_n+\xi'_{n+1},\quad \xi'_{n+1}\sim\mathcal{N}(0,\Sigma'_n)$$
$$\text{Observation}: Y'_{n+1}=H_nX'_{n+1}+\zeta'_{n+1},\quad \zeta'_{n+1}\sim\mathcal{N}(0,I_q)$$

Noise is also inflated $\Sigma'_n=r^2\Sigma_n^{+}+r^2\rho I_d$.
When $r\approx 1,\rho\approx 0$, two systems are similar to each other.

Low effective dimension

(X'_n, Y'_n) has its own Kalman filter (m'_n, R'_n), with covariance update

$$R'_{n+1} = \mathcal{K}(r^2 A_n R'_n A_n^T + \Sigma'_n)$$

Such update often has a stationary solution $\widetilde{R}_n$ (Bougerol 93)

$$C_n \preceq R'_n \quad \text{with large probability}$$

Assumption (*Low effective dimension*)

The original system has an effective dimension p if

- *A covariance sequence $\widetilde{R}_n$ has at most p eigenvalues above ρ*
- *Rank$(\Sigma_n^+) \leq p \Leftrightarrow A_n A_n^T + \Sigma_n/\rho$ has at p eigenvalues above $1/r$*

Assumption (*Uniform observability*)

- $A_n^{-1}, A_n, \Sigma_n, \widetilde{R}_n, \widetilde{R}_n^{-1}$ *are all bounded in operator norm.*
- *The m step observability Gramian $\sum_{k=1}^m A_{k,1}^T H_k^T H_k A_{k,1} \succeq c_m I_d$*

You are driving along a sub-optimal path.
vs.
Your speedometer and break are not working.

Source: internet

Proclaimed performance

Classical criterion: difference between (m_n, R_n) and $(\overline{X}_n, C_n)$.

Proclaimed performance

- Filter estimates its error/uncertainty by covariance C_n.
- Does the estimation captures variance of $e_n = \overline{X}_n - X_n$?

$$\mathbb{E}C_n \succeq \mathbb{E}e_n \otimes e_n? \quad \mathbb{E}e_n^T C_n^{-1} e_n < D$$

- Mahalanobis distance $\|v\|_C^2 = v^T [C]^{-1} v$.

The effective filter covariance $C_n^\rho = C_n + \rho I = \begin{bmatrix} C_n + \rho I & 0 \\ 0 & \rho I \end{bmatrix}$

- $\|e_n\|_{C_n^\rho}^2 = e_n^T C_n^{-1} e_n$ punishes errors on the represented directions.
- $\|e_n\|_{C_n^\rho}^2 \approx d$ if $e_n \sim \mathcal{N}(0, C_n^\rho)$.

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Mahalanobis distance $\|v\|_C = v^T[C]^{-1}v$

- Definition for Kalman update:

$$m_n = \arg\min_x \left(\|x - \hat{m}_n\|^2_{\widehat{R}_n} + \|Y_n - H_n x\|^2_{\Sigma_n} \right)$$

- Stable dissipation for Kalman filter errors

$$e_{n+1} = (I - K_{n+1}H_n)A_n e_n + K_{n+1}H_n\zeta_{n+1}$$

$$A_n^T(I - K_{n+1}H_n)^T R_{n+1}^{-1}(I - K_{n+1}H_n)A_n \preceq A_n^T \widehat{R}_{n+1}^{-1} A_n \preceq R_n^{-1}$$

$$e_{n+1}^T R_{n+1}^{-1} e_{n+1} \le e_n^T R_n^{-1} e_n$$

Stability results for Kalman filters (Bougerol 93, Reif et al. 99)

Main theorem

Theorem (Majda, T. 16)

Suppose the signal observation system is uniformly observable with m steps, and has a effective dimension p. Then for any c, there are C, F, D_F, M_n, so that if $K > Cp$

$$\mathbb{E}\|e_n\|_{C_n^\rho} \leq r^{-\frac{n}{6}}\mathbb{E}F(C_0)\sqrt{\|e_0\|^2_{C_0} + 2m} + M_n\sqrt{d}$$

With the constants bounded by

$$F(C) \leq D_F \exp(D_F \log^3 \|C\|), \quad \limsup_{n\to\infty} M_n \leq \frac{1+c}{1-r^{-\frac{m}{6}}}.$$

Cor1: exponential stability: the difference in mean converges to zero.
Cor2: ϵ scale noises lead to ϵ scale error for EnKF.

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How to apply it

Starting with a system

$$\text{Signal:} \quad X_{n+1} = A_n X_n + B_n + \xi_{n+1}, \quad \xi_{n+1} \sim \mathcal{N}(0, \Sigma_n)$$
$$\text{Observation:} \quad Y_{n+1} = H_n X_{n+1} + \xi_{n+1}, \quad \zeta_{n+1} \sim \mathcal{N}(0, I_q)$$

1. Find the proper error threshold, inflation strength ρ, r
2. Construct the inflated system (X'_n, Y'_n)
3. Check whether its Kalman filter has a low dimension p
4. Choose $K > Cp$ ensemble size, the Mahalonobis error is bounded.

Apply to a stochastic partial differential equation

$$\partial u(x,t) = \Omega(\partial_x)u(x,t) - \gamma(\partial_x)u(x,t) + F(x,t) + dW(x,t)$$

With Kolmogorov energy spectrum, $p = 10 - 30$ depending on observation.

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Apply to a stochastic partial differential equation

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With Kolmogorov energy spectrum, $p = 10 - 30$ depending on observation.

Concentration of Random sampling matrix

Let $\{a_k\}$ be any K vectors of rank p, $\xi_k \sim \mathcal{N}(0, \Sigma)$ with $\text{rank}(\Sigma) = p$.

$$C = \frac{1}{K-1}\sum_{k=1}^{K} a_k \otimes a_k, \quad Z = \frac{1}{K-1}\sum_{k=1}^{K}(a_k + \Delta\xi_k) \otimes (a_k + \Delta\xi_k).$$

Z concentrates around $D = \mathbb{E}Z = C + \Sigma$ in both ways if $K > Cp$.

$$\mu = \text{inf}\{u \geq 0 : [Z + \rho I_d]^{-1} \preceq u[D + \rho I_d]^{-1}\}$$

$$\lambda = \text{inf}\{u \geq 0 : Z \preceq u[D + \rho I_d]\}.$$

Then with Q being the condition number of $C + \rho I_d$:

$$\mathbb{P}(\mu > 1 + \delta \text{ or } \lambda > 1 + \delta) \leq (\log Q + 1)\exp(C_\delta p - c_\delta K)$$

The forecast covariance concentrates around its mean with high probability.

The reference Kalman filter gives control

$$
\begin{tikzcd}
C_n \arrow[d, "\text{Forecast}"'] & \text{Controlled by} & R'_n \arrow[d, "\text{Forecast}"] \\
\widehat{C}_{n+1} \arrow[d, "\text{Assimilation}"'] \arrow[r, phantom, "\approx"] & A_n C_n A_n^T + \Sigma_n^+ & \widehat{R}'_{n+1} = A_n R'_n A'_n + \Sigma'_n \arrow[l, Rightarrow] \arrow[d, "\text{Assimilation}"] \\
\mathcal{K}(\widehat{C}_{n+1}) \arrow[d, "\text{PCA}"'] \arrow[r, phantom, "\approx"] & \mathcal{K}(\mathbb{E}\widehat{C}_{n+1}) & \mathcal{K}(\widehat{R}'_{n+1}) \arrow[l, Rightarrow] \arrow[d, equal] \\
C_{n+1} & \text{Controlled by} & R'_{n+1}
\end{tikzcd}
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- Dissipation of Mahalanobis error on R'_n transfers to C_n.
- Small probability set, controlled by Lyapunov function, uniform observability.

Comparison with reference

The reference Kalman filter gives control

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- Small probability set, controlled by Lyapunov function, uniform observability.

Importance of the EnKF techniques

Our proof reveals importance of EnKF techniques:

Techniques	Application	Theoretical
Additive inflation $C_n + \rho I_d$	Under-represented directions	$[C_n + \rho I_d]^{-1}$ Well-defined
Multiplicative inflation $r\widehat{C}_n$	Covariance decay	Concentration $[r\widehat{C}_n + \rho I_d]^{-1} \preceq \mathbb{E}\widehat{C}_n$
Spectral projection: POD	Spurious correlation	Concentration: rank$(C_n) \leq p$

Summary

Main theorem:

- A variant of EnKF:
  - Inflations for covariance decay.
  - PCA: spurious correlation.
- With an effective dimension p:
  Number of significant dimensions in an inflated Kalman filter.
- Reaches proclaimed performance:
  $\mathbb{E}\|e_n\|^2_{C_n^\rho}$ converges to a constant independent of initial condition.

Heuristic answers

We need conditions! One of two will help us

- Low effective dimension.
- Localized covariance structure.

Compared with high dimensional matrix computation

- Low rank matrices.
- Sparse matrices.

Local interaction

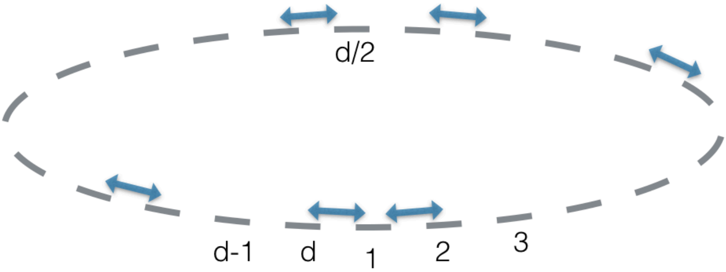
- High dimension often comes from dense grids.
- Interaction often is local: PDE discritization:

$$\partial_x x(t) \Rightarrow \frac{1}{2h}(x_{i+1}(t) - x_{i-1}(t)).$$

- Example: Lorenz 96 model

$$\dot{x}_i(t) = (x_{i+1} - x_{i-2})x_{i-1} - x_i dt + F, \quad i = 1, \cdots, d$$

- Information travels along interaction, and is dissipated.

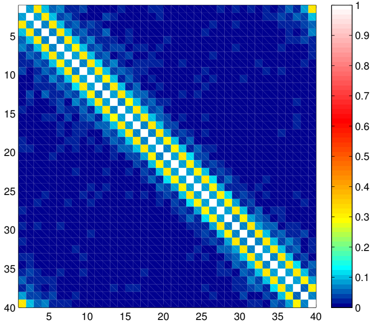


Sparsity: local covariance

- Correlation depends on information propagation.
- Correlation decays quickly with the distance.
- Covariance is localized with a structure Φ, e.g. $\Phi(x) = \rho^x$

$$[\widehat{C}_n]_{i,j} \propto \Phi(|i-j|)$$

$\Phi(x) \in [0,1]$ is decreasing. Distance can be general.



Correlation of Lorenz 96

Covariance Localization

- Spurious correlation may exist for far away terms.
- Localization: simply ignore far away correlations.
- Implementation: Schur product with a mask

$$[\widehat{C}_n \circ \mathbf{D}_L]_{i,j} = [\widehat{C}_n]_{i,j} \cdot [\mathbf{D}_L]_{i,j}$$

  Use $\widehat{C}_n \circ \mathbf{D}_L$ to describe uncertainty
- $[\mathbf{D}_L]_{i,j} = \phi(|i-j|)$, with a radius L.
  Gaspari-Cohn matrix: $\phi(x) = \exp(-4x^2/L^2)\mathbf{1}_{|i-j|\leq L}$.
  Cutoff/Branding matrix: $\phi(x) = \mathbf{1}_{|i-j|\leq L}$.
- Also resolves rank deficiency, e.g.

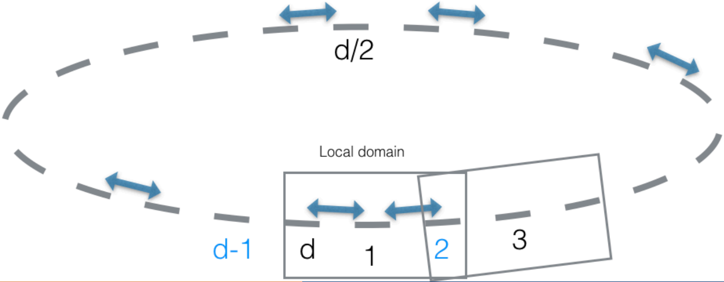
$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \circ \begin{bmatrix} 1 & 0.2 & 0 \\ 0.2 & 1 & 0.2 \\ 0 & 0.2 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0.2 & 0 \\ 0.2 & 1 & 0.2 \\ 0 & 0.2 & 1 \end{bmatrix}.$$

Domain localization

Two types LEnKF: Domain localization and covariance tempering.

Domain localization with radius l:
Assume H is a partial observation matrix
Use information in $\mathcal{I}_i = \{j : |i-j| \le l\}$ to update component i

$$C^i = P_{\mathcal{I}_i} C P_{\mathcal{I}_i}, \quad \mathcal{G}^i(C) = C^i H^T(\sigma_o^2 I_q + HC^i H^T)^{-1}$$
$$\mathcal{G}^L(C) = \sum e_i e_i^T \mathcal{G}^i(C)$$
$$X_n^{(k)} = \widehat{X}_n^{(k)} + \mathcal{G}^L(\widehat{C}_n)(Y_n - H\widehat{X}_n^{(k)} + \zeta_n^{(k)}).$$



Advantage with localization

Intuitively, ignoring the long distance covariance terms, reduces the sampling difficulty, and necessary sampling size.

Theorem (Bickel, Levina 08)

If $X^{(1)}, \dots, X^{(K)} \sim \mathcal{N}(0, \Sigma)$, denote $C = \frac{1}{K}\sum_{k=1}^{K} X^{(k)} \otimes X^{(k)}$. $\|\mathbf{D}_L\|_1 = \max_i \sum_j |\mathbf{D}_L|_{i,j}$. There is a constant c, and for any $t > 0$

$$\mathbb{P}(\|C \circ \mathbf{D}_L - \Sigma \circ \mathbf{D}_L\| > \|\mathbf{D}_L\|_1 t) \leq 8 \exp(2 \log d - cK \min\{t, t^2\})$$

This indicates that $K \propto \|\mathbf{D}_L\|_1^2 \log d$ is the necessary sample size.

$\|\mathbf{D}_L\|$ is independent of d, e.g, the cut-off/branding matrix, $[\mathbf{D}_{cut}^L]_{i,j} = \mathbf{1}_{|i-j|\leq L}$, $\|\mathbf{D}_{cut}^L\|_1 \approx 2L$.

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Main result: localized EnKF

Theorem (T. 18)

Suppose the system coefficients have bandwidth l, and the LEnKF ensemble covariance admits a stable localized structure, then for any $\delta > 0$, LEnKf reaches its proclaimed performance with high probability $1 - O(\delta)$:

$$1 - \frac{1}{T}\sum_{t=1}^{T} \mathbb{P}(\mathbb{E}_S \hat{e}_n \otimes \hat{e}_n \preceq (1+\delta)(\widehat{C}_n \circ \mathbf{D}_{cut}^{4l} + \rho I_d)) \leq \frac{1}{T} D_0 + D_1 \delta,$$

if the sample size $K > D_{l,\delta} \log d$.

$\mathbb{E}_S$ conditioned on the information of the sampling noise realization.

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Proclaimed performance

Proclaimed/estimated performance

- EnKF estimates X_n by $\overline{X}_n = \frac{1}{K}\sum X_n^{(k)}$.
- Error $e_n = \overline{X}_n - X_n$. Covariance : $\mathbb{E}e_n e_n^T = \mathbb{E}e_n \otimes e_n$.
- EnKF estimates its performance by ensemble covariance C_n^ρ.
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Stable localized structure

- Intuitively, we need some conditions on the covariance structure.
- Stable localized structure: with local structure function Φ, e.g. $\Phi(x) = \lambda^x$,

$$[\widehat{C}_n]_{i,j} \leq M_n \Phi(|i-j|), \quad \sum_{n=1}^{T} \mathbb{E} M_n \leq T M_*.$$

  M_n describes how localized the sample covariance matrix is.
- Why is this necessary?

LEnKF inconsistency

An intrinsic bias/inconsistency in LEnKF.

- Localization creates a bias.
- Target covariance by Bayes formula

$$(I - \mathcal{G}^L(\widehat{C}_n)H)[\widehat{C}_n \circ \mathbf{D}_L](I - \mathcal{G}^L(\widehat{C}_n)H)^T + \sigma_o^2 \mathcal{G}^L(\mathcal{G}^L)^T.$$

- LEnKF implementation

$$X_n^{(k)} = \widehat{X}_n^{(k)} + \mathcal{G}^L(\widehat{C}_n)(Y_n - H\widehat{X}_n^{(k)} + \zeta_n^{(k)})$$

- Average ensemble covariance

$$C_n \circ \mathbf{D}_L = [(I - \mathcal{G}^L(\widehat{C}_n)H)\widehat{C}_n(I - \mathcal{G}^L(\widehat{C}_n)H)^T + \sigma_o^2 \mathcal{G}^L(\mathcal{G}^L)^T] \circ \mathbf{D}_L.$$

- Difference: commuting the localization and Kalman update.
- Previously investigated numerically by Nerger 2015, the inconsistency can lead to error growth.

When is the inconsistency small?

- localization is applied, covariance is assumed localized.
- Given localized structure Φ, find M_n so that

$$[\widehat{C}_n]_{i,j} \leq M_n \Phi(|i-j|).$$

- Interestingly, when $\mathbf{D}_L$ is $\mathbf{D}_{4l}^{cut}$, the

$$\text{Localization inconsistency} \leq C M_n \Phi(2l).$$

  If $2l$ is large, $\Phi(x) = \lambda^x$, this difference can be controlled.
- Localized covariance leads to small localization inconsistency.
- Therefore, we need M_n to be a stable sequence,

$$\sum_{n=1}^{T} \mathbb{E} M_n \leq T M_*.$$

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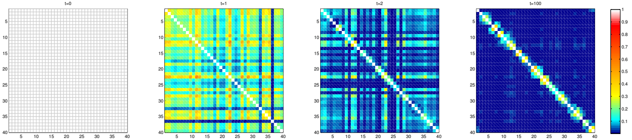
Practical perspective

- Simply assumed.
- Numerically checked.

Theoretical perspective: does covariance localize for any stochastic system?

- Linear system: covariance can be computed.
- Nonlinear: difficult, e.g. Lorenz 96.
- LEnKF: difficult since assimilation is nonlinear.
- Under strong conditions:
  - Weak local interaction, strong dissipation.
  - Sparse observation for simplicity.
- Also scales with the noise strength.



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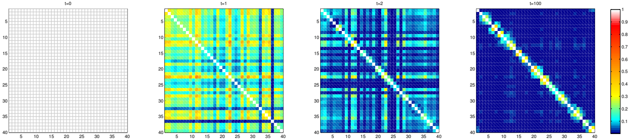


Stable local structure

Theorem

Suppose the following, then a stable localized structure with $\Phi(x) = \lambda_A^x$

1) *The system noise is diagonal and the observations are sparse* $\Sigma_n = \sigma_\xi^2 I_d, \quad \mathbf{d}(o_i, o_j) > 2l, \ \forall i \neq j.$
2) *There is a* $\lambda_A < r^{-1}$, $\max_i \left\{ \sum_{k=1}^d |[A_n]_{i,k}| \lambda_A^{-\mathbf{d}(i,k)} \right\} \leq \lambda_A$.
3) *There are constants such that* $\psi_{\lambda_A}(M_*, \delta_*) \leq M_*$

$$0 < \delta_* < \min\{0.25, \tfrac{1}{2}(\lambda_A^{-1} - r)\}, \quad M_* \geq \frac{(r + 2\delta_*)\sigma_\xi^2}{1 - \lambda_A},$$

$$\psi_{\lambda_A}(M, \delta) = (r+\delta) \max \left\{ \lambda_A M \left(1 + \sigma_o^{-2} M\right)^2 + \lambda_A \sigma_o^{-2} M^2, \lambda_A^2 M + \sigma_\xi^2 \right\}.$$

4) *Denote* $n_* = 2L + \lceil \frac{\log 4\delta_*^{-1}}{\log \lambda_A^{-1}} \rceil$. *The sample size* K *exceeds*

$$K > \max \left\{ -\frac{1}{c\delta_*^2 \lambda_A^{2L}} \log(16 d^2 n_* \delta_*^{-2}), \Gamma(2r\delta_*^{-1}, d) \right\}.$$

A real example

A stochastically forced dissipative advection equation:

$$\frac{\partial u(x,t)}{\partial t} = c\frac{\partial u(x,t)}{\partial x} - \nu u(x,t) + \mu \frac{\partial^2 u(x,t)}{\partial x^2} + \sigma_x \dot{W}(x,t).$$

Discretization

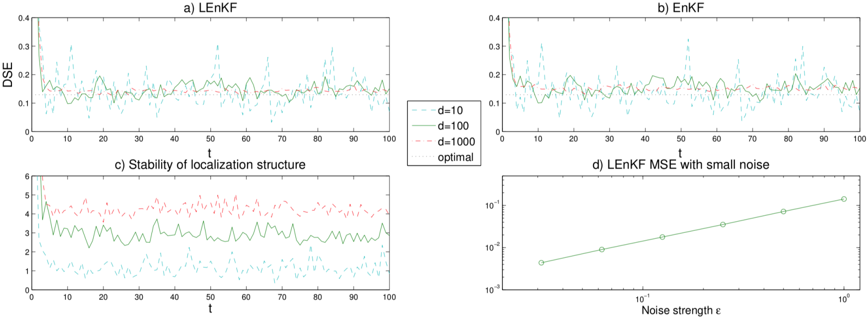
$$X_{n+1,i} = a_- X_{n,i-1} + a_0 X_{n,i} + a_+ X_{n,i+1} + \sigma_x \sqrt{\Delta t} W_{n+1,i}, \quad i = 1, \dots, d;$$
$$a_- = \tfrac{\mu \Delta t}{h^2} - \tfrac{c\Delta t}{2h}, \quad a_0 = 1 - \tfrac{2\mu\Delta t}{h^2} - \nu \Delta t, \quad a_+ = \tfrac{\mu\Delta t}{h^2} + \tfrac{c\Delta t}{2h}.$$

Observe $Y_{n,k} = X_{n,p(k-1)+1} + \sigma_o B_{n,k}$.

Strong damping+weak advection

$$h = 1, \quad \Delta t = 0.1, \quad p = 5, \quad \nu = 5, \quad c = 0.1, \quad \mu = 0.1, \quad \sigma_x = \sigma_o = 1.$$

Direct verification of the conditions is possible.

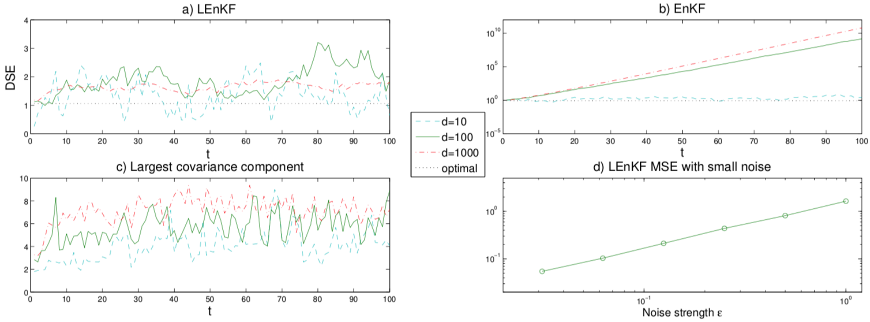


Strong advection regime

Weak damping+strong advection

$$h = 0.2, \quad \Delta t = 0.1, \quad p = 5, \quad \nu = 0.1, \quad c = 2, \quad \mu = 0.1, \quad \sigma_x = \sigma_o = 1.$$

Direct verification of the conditions is not possible.



Extension of localization

- Localization has made EnKF very effective for high dimensional DA problems.
- Various generalization to particle filters.
- Often relies on Gaspari Cohn matrices.
- Makes non-Gaussian application difficult.
- Non-ad hoc ways generalize localization to PF?
- Can we apply localization to other UQ problem?

Reference

- Robustness and Accuracy of finite Ensemble Kalman filters in large dimensions. Comm. Pure Appl. Math., 71(5), 892-937, (2018)
- Rigorous accuracy and robustness analysis for two-scale reduced random Kalman filters in high dimensions. accepted by CMS.
- Performance analysis of local ensemble Kalman filter. J. Nonlinear Sci. 2018, Vol 28, No. 4. p1397-1442.

Links and slides can be found at www.math.nus.edu.sg/∼mattxin.

Thank you!