

On the convergence of (ensemble) Kalman filters and smoothers onto the unstable subspace

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2 Theoretical results for linear dynamical systems

- The filter case
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- From linear to nonlinear models

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- Eigenspectrum
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Assimilation in the unstable subspace (AUS paradigm)

- ▶ Several numerical results suggest that the skills of ensemble-based data assimilation methods in chaotic systems are related to the instabilities of the underlying dynamics [Ng et al., 2011].
- ▶ Numerical evidence that some asymptotic properties of the ensemble-based covariances (rank, range) relate to the unstable modes of the dynamics [Sakov and Oke, 2008; Carrassai et al., 2009].
- ▶ This behaviour is at the basis of algorithms known as Assimilation in the Unstable Subspace [Trevisan and Ubaldi, 2004; Palatella et al. 2013], and exploited in the Iterative Ensemble Kalman Filter/Smoother [Bocquet and Sakov, 2012-2016].
- ▶ But we need formal proof with a view to a better design of reduced-order methods, and a better understanding of these results. **A formal proof could be obtained in the linear model case, while numerical evidence could be obtained in the non-Gaussian/nonlinear case.**

Characterization of model dynamics: reminder

- ▶ State and (infinitesimal) error dynamics:

$$\frac{dx(t)}{dt} = \mathcal{M}_t(x(t)), \quad \frac{de(t)}{dt} = \mathbf{M}_{x(t), t} e(t). \quad (1)$$

The time integration of the linear error dynamics yields the resolvent:

$$e(t_1) = \mathbf{M}(t_1, t_0) e(t_0). \quad (2)$$

- ▶ The Oseledec theorem tells that the limiting matrix (far future)

$$\mathbf{S}(t_0) = \lim_{t_1 \rightarrow \infty} \left\{ \mathbf{M}(t_1, t_0)^T \mathbf{M}(t_1, t_0) \right\}^{\frac{1}{2(t_1 - t_0)}}. \quad (3)$$

exists, has eigenvalues $e^{\lambda_1} \geq e^{\lambda_2} \geq \dots \geq e^{\lambda_n}$ where the λ_i are called the **Lyapunov exponents** that do not depend on t_0 , and has eigenvectors that are called the **forward Lyapunov vectors** (which depend on t_0). Symmetrically (far past)

$$\mathbf{S}(t_1) = \lim_{t_0 \rightarrow -\infty} \left\{ \mathbf{M}(t_1, t_0) \mathbf{M}(t_1, t_0)^T \right\}^{\frac{1}{2(t_1 - t_0)}}. \quad (4)$$

exists, has the same eigenvalues that do not depend on t_1 , and eigenvectors that are called the **backward Lyapunov vectors** (which depend on t_1).

Characterization of model dynamics: reminder

- ▶ The forward and backward Lyapunov vectors are orthonormal. They are norm-dependent.
- ▶ The positive Lyapunov exponents correspond to exponentially growing error/unstable modes. The negative Lyapunov exponents correspond to exponentially decaying error/stable modes. The zero Lyapunov exponents correspond to neutral modes.
- ▶ The backward Lyapunov vectors generate a sequence of embedded subspaces of \mathbb{R}^n for each t_1 such that

$$F_1^-(t_1) \subset F_2^-(t_1) \subset \cdots \subset F_n^-(t_1) = \mathbb{R}^n \quad (5)$$

where for $\mathbf{e} \in F_i^-(t_1) \setminus F_{i-1}^-(t_1)$, $\|\mathbf{M}^{-1}(t_1, t_0)\mathbf{e}\| \underset{t_0 \rightarrow -\infty}{\sim} e^{-\lambda_i(t_1 - t_0)} \|\mathbf{e}\|$.

- ▶ We define the **unstable-neutral subspace** $\mathcal{U}_{t_1} \equiv F_{n_0}^-(t_1)$ as the space generated by the n_0 backward Lyapunov vectors that are related to positive and zero Lyapunov exponents. Here, the **stable subspace** is defined as the orthogonal $\mathcal{U}_{t_1}^\perp$ of \mathcal{U}_{t_1} in \mathbb{R}^n .
- ▶ See [Legras and Vautard, 1996] for a topical introduction.

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Linear case: Degenerate Kalman filter equations

- Model dynamics and observation model:

$$\mathbf{x}_k = \mathbf{M}_k \mathbf{x}_{k-1} + \mathbf{w}_k, \quad (6)$$

$$\mathbf{y}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{v}_k. \quad (7)$$

The model and observation noises, \mathbf{w}_k and \mathbf{v}_k , are assumed mutually independent, unbiased Gaussian white sequences with statistics

$$\mathbb{E}[\mathbf{v}_k \mathbf{v}_l^T] = \delta_{k,l} \mathbf{R}_k, \quad \mathbb{E}[\mathbf{w}_k \mathbf{w}_l^T] = \delta_{k,l} \mathbf{Q}_k, \quad \mathbb{E}[\mathbf{v}_k \mathbf{w}_l^T] = \mathbf{0}. \quad (8)$$

- Forecast error covariance matrix \mathbf{P}_k recurrence of the Kalman filter (KF)

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1} (\mathbf{I} + \mathbf{P}_k \mathbf{\Omega}_k)^{-1} \mathbf{P}_k \mathbf{M}_{k+1}^T + \mathbf{Q}_{k+1}, \quad (9)$$

where

$$\mathbf{\Omega}_k \equiv \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \quad (10)$$

are the **precision matrices** and \mathbf{P}_0 can be of **arbitrary rank**.

- In the case $\mathbf{Q}_k \equiv \mathbf{0}$, Gurumoorthy et al. (2016) proved rigorously that the **full-rank** KF \mathbf{P}_k collapses onto the unstable subspace.
- Still in the case $\mathbf{Q}_k \equiv \mathbf{0}$, this is going to be generalised [Bocquet et al., 2016] in the following in several ways and for **degenerate** \mathbf{P}_0 required to connect to reduced-order methods such as the ensemble Kalman filter (EnKF).

Result 1: Bound of the covariance free forecast

- ▶ Simple inequality in the set of the semi-definite symmetric matrices

$$\mathbf{P}_k \leq \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T + \Xi_k. \quad (11)$$

where

$$\Xi_0 \equiv \mathbf{0} \quad \text{and for } k \geq 1 \quad \Xi_k \equiv \sum_{l=1}^k \mathbf{M}_{k:l} \mathbf{Q}_l \mathbf{M}_{k:l}^T \quad (12)$$

is known as the *controllability* matrix [Jazwinski, 1970].

- ▶ In the absence of model noise ($\mathbf{Q}_k \equiv \mathbf{0}$ for the rest of this talk), it reads

$$\mathbf{P}_k \leq \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T. \quad (13)$$

Assuming the dynamics is non-singular

$$\text{Im}(\mathbf{P}_k) = \mathbf{M}_{k:0}(\text{Im}(\mathbf{P}_0)). \quad (14)$$

If n_0 is the dimension of the unstable-neutral subspace, it can further be shown that

$$\lim_{k \rightarrow \infty} \text{rank}(\mathbf{P}_k) \leq \min \{ \text{rank}(\mathbf{P}_0), n_0 \}. \quad (15)$$

Result 2: Collapse onto the unstable subspace

- ▶ Let σ_i^k , for $i = 1, \dots, n$ denote the eigenvalues of \mathbf{P}_k ordered as $\sigma_1^k \geq \sigma_2^k \dots \geq \sigma_n^k$. We can show that

$$\sigma_i^k \leq \alpha_i \exp\left(2k\lambda_i^k\right) \quad (16)$$

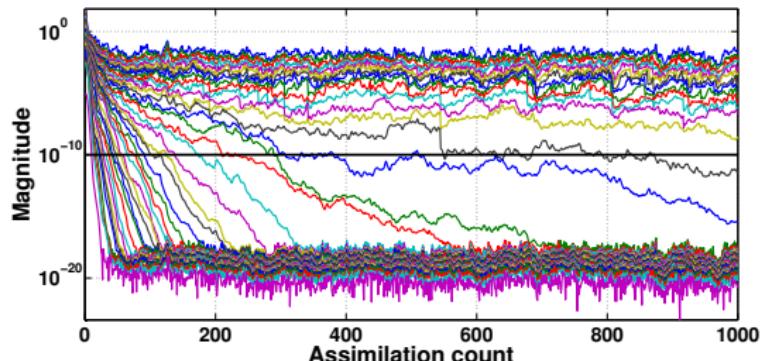
where $k\lambda_i^k$ is a log-singular value of $\mathbf{M}_{k:0}$ and $\lim_{k \rightarrow \infty} \lambda_i^k = \lambda_i$. This gives an upper bound for all eigenvalues of \mathbf{P}_k and a rate of convergence for the $n - n_0$ smallest ones.

- ▶ If \mathbf{P}_k is uniformly bounded, it can further be shown that the stable subspace of the dynamics is asymptotically in the null space of \mathbf{P}_k , i.e. for any vector $\mathbf{u}_{k:0}$ in the stable subspace

$$\lim_{k \rightarrow \infty} \|\mathbf{P}_k \mathbf{u}_{k:0}\| = 0. \quad (17)$$

Numerical illustration and verification

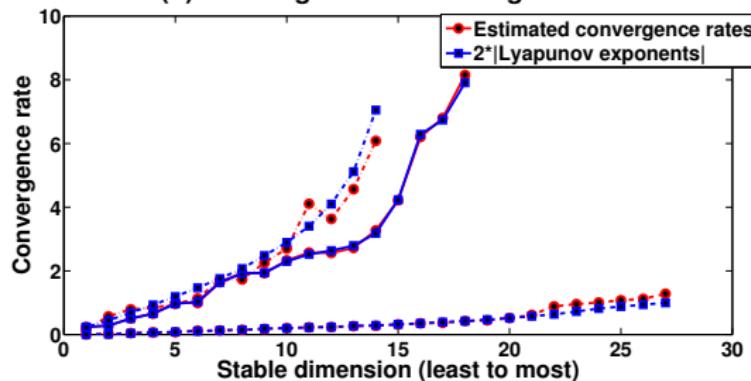
(a) Eigenvalues of analysis error covariance matrix



Linearized Lorenz-95 model
around a Lorenz-95 trajectory.

(a) Evolution
of the eigenvalues of \mathbf{P}_k .

(b) Convergence rates of eigenvalues



(b) Convergence rate to 0
of the eigenvalues related to
the stable modes.

Result 3: Explicit dependence of \mathbf{P}_k on \mathbf{P}_0

- ▶ Using either analytic continuation or the symplectic symmetry of the linear representation of covariances, we have proven that

$$\mathbf{P}_k = \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T \left(\mathbf{I} + \boldsymbol{\Gamma}_k \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T \right)^{-1}. \quad (18)$$

where

$$\boldsymbol{\Gamma}_k \equiv \sum_{l=0}^{k-1} \mathbf{M}_{k:l}^{-T} \boldsymbol{\Omega}_l \mathbf{M}_{k:l}^{-1}. \quad (19)$$

- ▶ An alternative is

$$\mathbf{P}_k = \mathbf{M}_{k:0} \mathbf{P}_0 [\mathbf{I} + \boldsymbol{\Theta}_k \mathbf{P}_0]^{-1} \mathbf{M}_{k:0}^T \quad (20)$$

where

$$\boldsymbol{\Theta}_k \equiv \mathbf{M}_{k:0}^T \boldsymbol{\Gamma}_k \mathbf{M}_{k:0} = \sum_{l=0}^{k-1} \mathbf{M}_{l:0}^T \boldsymbol{\Omega}_l \mathbf{M}_{l:0}. \quad (21)$$

is the *information* matrix, directly related to the *observability* of the DA system.

- ▶ Formulas theoretically enlightening!

Result 4: Asymptotics of \mathbf{P}_k

- ▶ Questions: Under which conditions does \mathbf{P}_k forget about $\mathbf{P}_0 = \mathbf{X}_0 \mathbf{X}_0^T$? Can we analytically compute its asymptotics?
- ▶ We proposed a sufficient set of conditions
 - **Condition 1:** Assume the forward Lyapunov vectors at t_0 associated to the unstable and neutral directions are the columns of $\mathbf{V}_{+,0} \in \mathbb{R}^{n \times n_0}$. The condition reads

$$\text{rank} \left(\mathbf{X}_0^T \mathbf{V}_{+,0} \right) = n_0. \quad (22)$$

- **Condition 2:** The model is sufficiently observed so that the unstable and neutral directions remain under control, that is

$$\mathbf{U}_{+,k}^T \boldsymbol{\Gamma}_k \mathbf{U}_{+,k} > \varepsilon \mathbf{I} \quad (23)$$

where $\mathbf{U}_{+,k}$ is a matrix whose columns are the backward Lyapunov vectors related to non-negative exponents and $\varepsilon > 0$ is a positive number.

- **Condition 3:** For any neutral backward Lyapunov vector \mathbf{u}_k , we have

$$\lim_{k \rightarrow \infty} \mathbf{u}_k^T \boldsymbol{\Gamma}_k \mathbf{u}_k = \infty, \quad (24)$$

i.e. the neutral modes should be sufficiently observed.

Result 4: Asymptotics of \mathbf{P}_k

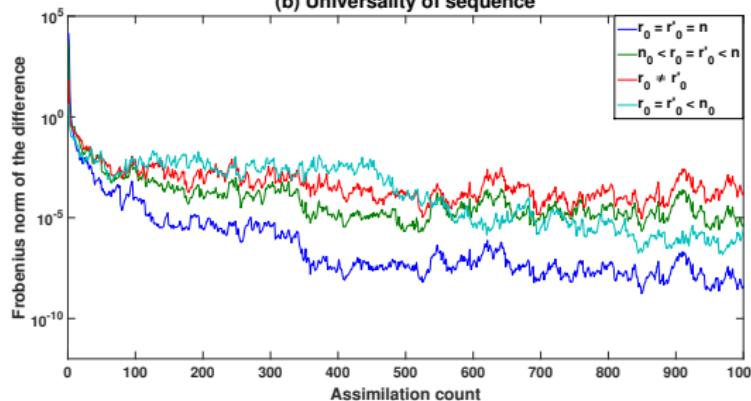
Under these three conditions, we obtain

$$\lim_{k \rightarrow \infty} \left\{ \mathbf{P}_k - \mathbf{U}_{+,k} \left[\mathbf{U}_{+,k}^T \boldsymbol{\Gamma}_k \mathbf{U}_{+,k} \right]^{-1} \mathbf{U}_{+,k}^T \right\} = \mathbf{0}. \quad (25)$$

The asymptotic sequence does not depend on \mathbf{P}_0 , only $\boldsymbol{\Gamma}_k$!

- ▶ Peculiar role of the neutral modes (arithmetic convergence).
- ▶ Numerical illustration and verification

(b) Universality of sequence



Linearized Lorenz-95 model around a Lorenz-95 trajectory.

Frobenius norm of the difference between two different \mathbf{P}_0 when the conditions are satisfied, i.e. $\|\mathbf{P}_k^a - \mathbf{P}'_k^a\|$.

From the degenerate KF to the square-root EnKF

- ▶ Normalised anomaly decomposition

$$\mathbf{P}_k = \mathbf{X}_k \mathbf{X}_k^T. \quad (26)$$

- ▶ Square-root formulation; right-transform update formula

$$\mathbf{X}_k = \mathbf{M}_{k:0} \mathbf{X}_0 \left[\mathbf{I} + \mathbf{X}_0^T \boldsymbol{\Theta}_k \mathbf{X}_0 \right]^{-1/2} \boldsymbol{\Psi}_k \quad (27)$$

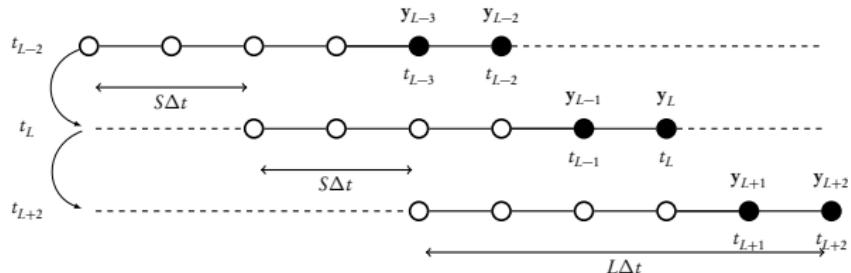
where $\boldsymbol{\Psi}_k$ is an orthogonal matrix.

- ▶ Square-root formulation; left-transform update formula

$$\mathbf{X}_k = \left[\mathbf{I} + \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T \boldsymbol{\Gamma}_k \right]^{-1/2} \mathbf{M}_{k:0} \mathbf{X}_0 \boldsymbol{\Psi}_k. \quad (28)$$

- ▶ With linear models, Gaussian observation and initial errors, the (square-root) degenerate KF is equivalent to the square-root EnKF and can serve as a **proxy to the EnKF applied to nonlinear models**.

Degenerate square root Kalman smoother



- The scheme at a glance, variational correspondence ($\mathbf{x} = \bar{\mathbf{x}}_k + \mathbf{X}_k \mathbf{w}$) :

$$\widetilde{\mathcal{J}}(\mathbf{w}) = \frac{1}{2} \sum_{l=k+L-S+1}^{k+L} \|\mathbf{y}_l - \mathbf{H}_l \mathbf{M}_{l:k} (\bar{\mathbf{x}}_k + \mathbf{X}_k \mathbf{w})\|_{\mathbf{R}_l}^2 + \frac{1}{2} \|\mathbf{w}\|^2 \quad (29)$$

- From the Hessian of $\widetilde{\mathcal{J}}$,

$$\mathbf{I}_N + \mathbf{X}_k^T \widehat{\Omega}_k \mathbf{X}_k \quad \text{where} \quad \widehat{\Omega}_k \triangleq \sum_{l=k+L-S+1}^{k+L} \mathbf{M}_{l:k}^T \mathbf{\Omega}_l \mathbf{M}_{l:k}, \quad (30)$$

we infer

$$\mathbf{X}_{k+S} = \mathbf{M}_{k+S:k} \mathbf{X}_k \left(\mathbf{I}_N + \mathbf{X}_k^T \widehat{\Omega}_k \mathbf{X}_k \right)^{-\frac{1}{2}} \mathbf{\Psi}_k. \quad (31)$$

Degenerate square root Kalman smoother: dependence on \mathbf{X}_0

- ▶ From the recurrence, we can obtain the explicit expression of the anomalies as a function of the initial anomalies.
- ▶ Left-transform update; if $k = pS$, $p = 0, 1, \dots$:

$$\mathbf{X}_k = \mathbf{M}_{k:0} \mathbf{X}_0 \left[\mathbf{I}_N + \mathbf{X}_0^T \hat{\Theta}_k \mathbf{X}_0 \right]^{-\frac{1}{2}} \mathbf{\Psi}_k \quad (32)$$

where

$$\hat{\Theta}_k \triangleq \sum_{q=0}^{p-1} \mathbf{M}_{qS:0}^T \hat{\Omega}_{qS} \mathbf{M}_{qS:0} \quad (33)$$

- ▶ Right-transform update; if $k = pS$, $p = 0, 1, \dots$:

$$\mathbf{X}_k = \left[\mathbf{I}_n + \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^T \hat{\Gamma}_k \right]^{-\frac{1}{2}} \mathbf{M}_{k:0} \mathbf{X}_0 \mathbf{\Psi}_k \quad (34)$$

where

$$\hat{\Gamma}_k = \sum_{q=0}^{p-1} \mathbf{M}_{k:qS}^{-T} \hat{\Omega}_{qS} \mathbf{M}_{k:qS}^{-1} \quad (35)$$

Degenerate square root Kalman smoother: convergence onto the unstable-neutral subspace

- ▶ The convergence rate of the collapse of \mathbf{P}_k of the smoother is not expected to be faster than the filter's: the bounding rate is the same.
- ▶ However the accuracy of the smoother for re-analysis is expected to be better which should impact the asymptotic sequences. Indeed we have, for $k = pS$, $p = 0, 1, \dots$:

$$\lim_{k \rightarrow \infty} \left\{ \mathbf{X}_k - \mathbf{U}_{+,k} \left[\mathbf{U}_{+,k}^T \widehat{\boldsymbol{\Gamma}}_k \mathbf{U}_{+,k} \right]^{-\frac{1}{2}} \boldsymbol{\Psi}_k \right\} = \mathbf{0}. \quad (36)$$

- ▶ The only difference is in the observability matrix $\widehat{\boldsymbol{\Gamma}}_k$, for $k = pS$, $p = 0, 1, \dots$:

$$\widehat{\boldsymbol{\Gamma}}_k = \boldsymbol{\Gamma}_k + \sum_{l=k}^{k+L-S} \mathbf{M}_{k:l}^{-T} \boldsymbol{\Omega}_l \mathbf{M}_{k:l}^{-1}. \quad (37)$$

which guarantees that

$$\mathbf{U}_{+,k} \left[\mathbf{U}_{+,k}^T \widehat{\boldsymbol{\Gamma}}_k \mathbf{U}_{+,k} \right]^{-1} \mathbf{U}_{+,k}^T \leq \mathbf{U}_{+,k} \left[\mathbf{U}_{+,k}^T \boldsymbol{\Gamma}_k \mathbf{U}_{+,k} \right]^{-1} \mathbf{U}_{+,k}^T. \quad (38)$$

From linear to nonlinear models

- Nonlinear model dynamics and nonlinear observation model:

$$\mathbf{x}_k = \mathcal{M}_{k:k-1}(\mathbf{x}_{k-1}), \quad (39)$$

$$\mathbf{y}_k = \mathcal{H}_k(\mathbf{x}_k) + \mathbf{v}_k \quad (40)$$

- Square root degenerate Kalman filter \rightarrow Square root ensemble Kalman filter (EnKF)
- Square root degenerate Kalman smoother \rightarrow Iterative ensemble Kalman smoother (IEnKS)
- The IEnKS follows the square root degenerate Kalman smoother that we inferred from a variational principle, but from the cost function

$$\widetilde{\mathcal{J}}(\mathbf{w}) = \frac{1}{2} \sum_{l=k+L-S+1}^{k+L} \|\mathbf{y}_l - H_l \circ \mathcal{M}_{l:k}(\bar{\mathbf{x}}_k + \mathbf{X}_k \mathbf{w})\|_{\mathbf{R}_l}^2 + \frac{1}{2} \|\mathbf{w}\|^2. \quad (41)$$

The this archetype of the so-called four-dimensional EnVar method (4DEnVar) which avoid the need to use an adjoint model, but with a proper ensemble update, and an outer loop. The IEnKS is systematically more accurate for smoothing and filtering than 4D-Var, the EnKF, and the EnKS.

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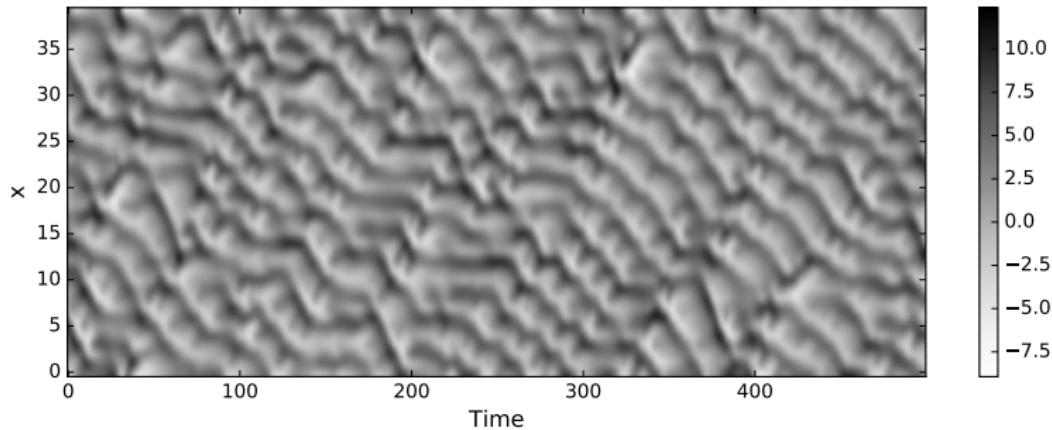
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Nonlinear chaotic models: the Lorenz-95 low-order model



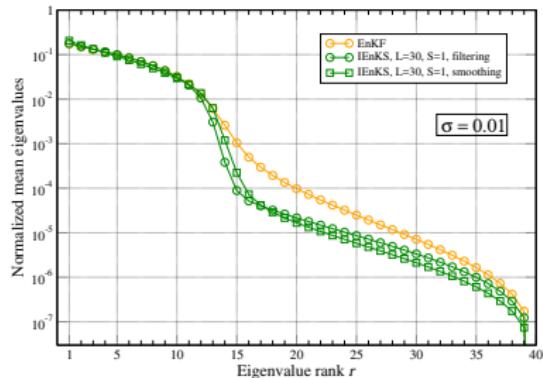
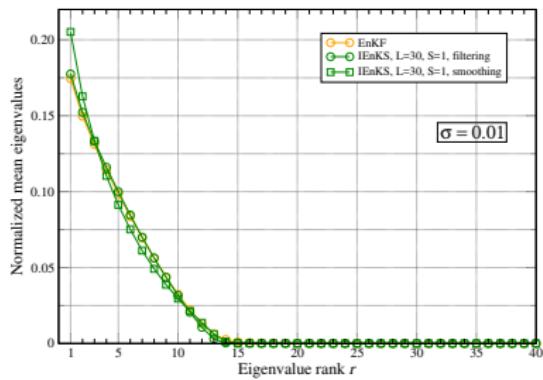
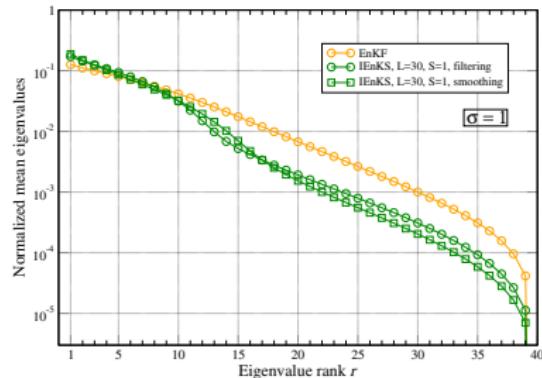
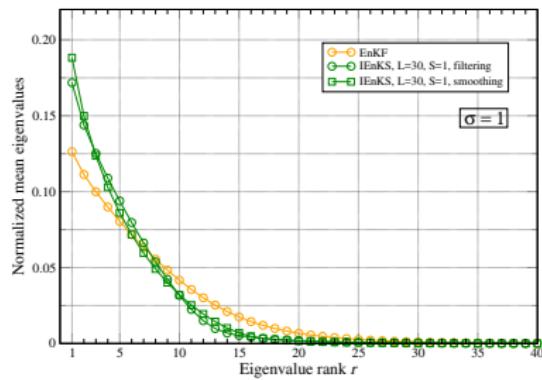
- ▶ It represents a mid-latitude zonal circle of the global atmosphere.
- ▶ Set of $M = 40$ ordinary differential equations [Lorenz and Emmanuel 1998]:

$$\frac{dx_m}{dt} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F, \quad (42)$$

where $F = 8$, and the boundary is cyclic.

- ▶ Conservative system except for a forcing term F and a dissipation term $-x_m$.
- ▶ Chaotic dynamics, 13 positive and 1 neutral Lyapunov exponents, a doubling time of about 0.42 time units.

Spectrum of the analysis error covariance matrix



► Time-average spectra of \mathbf{P}_k^a : A visible transition at $r = 15$.

Geometry of the anomaly simplex and unstable-neutral subspace

► Anomaly to perturbation:

- Anomaly: $\mathbf{v}_k^n = [\mathbf{X}_k]_n$ with $1 \leq n \leq N$. Lyapunov vector: \mathbf{u}_k^p at t_k , $1 \leq p \leq P$.
- Projection of \mathbf{v}_k^n onto \mathbf{u}_k^p : $\|\mathbf{v}_k^n\| \cos(\theta_k^{n,p})$
where $\theta_k^{n,p}$ is the angle between the vectors (recall $\|\mathbf{u}_k^p\| = 1$.)

► Anomaly to the unstable-neutral subspace:

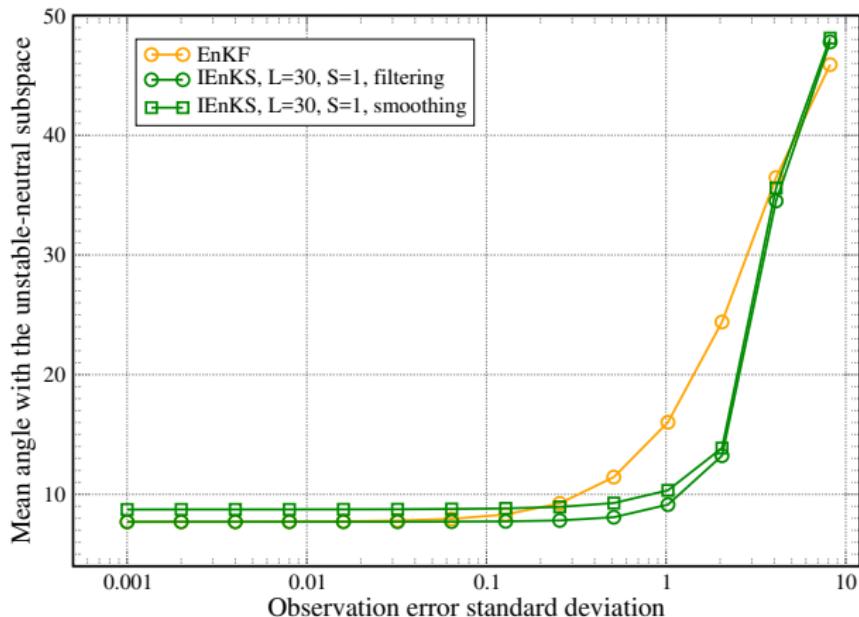
- Consider the relative position of an anomaly with respect to the unstable-neutral subspace \mathcal{U}_k , where $\mathcal{U}_k = \text{Span} \{ \mathbf{u}_k^1, \mathbf{u}_k^2, \dots, \mathbf{u}_k^{n_0} \}$.
- Square cosine of the angle between the anomaly \mathbf{v}_k^n and \mathcal{U}_k is obtained as

$$\cos^2(\theta_k^n) = \sum_{p=1}^{n_0} \cos^2(\theta_k^{n,p}) = \sum_{p=1}^{n_0} \frac{\{(\mathbf{u}_k^p)^T \mathbf{v}_k^n\}^2}{\|\mathbf{v}_k^n\|^2}. \quad (43)$$

► Anomaly simplex to the unstable-neutral subspace:

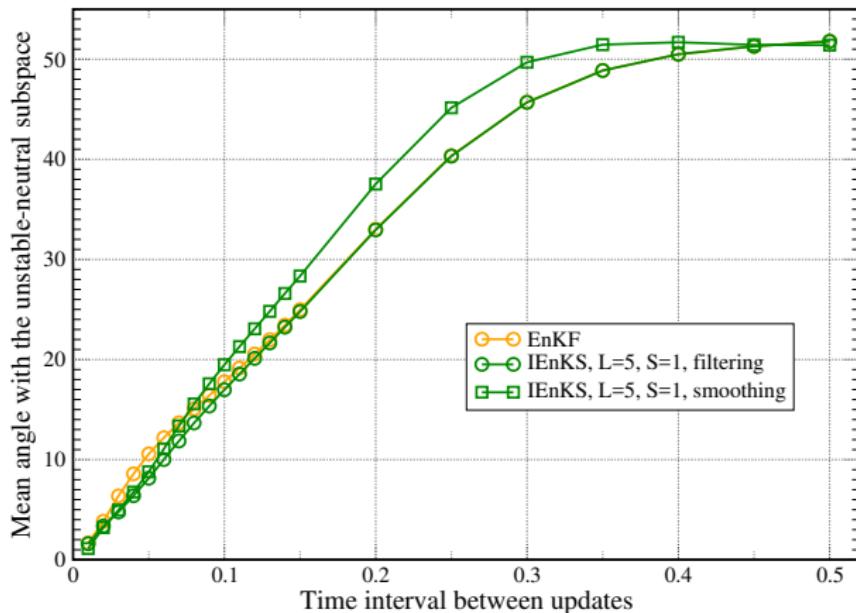
A complete characterization of the relative orientation can be achieved by a set of angles, called **principal angles**, whose number is given by the minimum of the dimensions of both subspaces. These angles are intrinsic and do not depend on the parameterization of both subspaces.

Nonlinear chaotic model



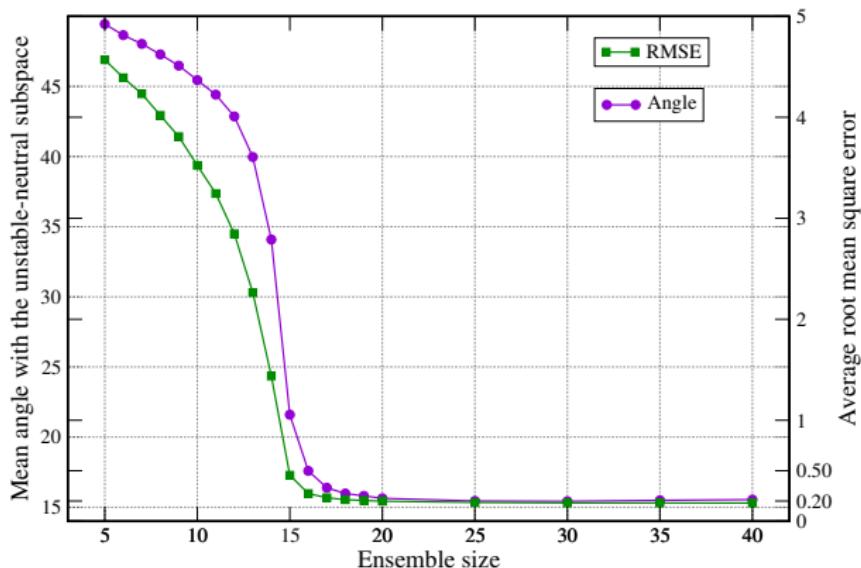
- Average angle (in degrees) between an anomaly (from the ensemble) and the unstable-neutral subspace as a function of the observation error (EnKF and IEnKS, Lorenz-95, $\Delta t = 0.05$, $\mathbf{R} = \sigma^2 \mathbf{I}$ $N = 20$).

Nonlinear chaotic model



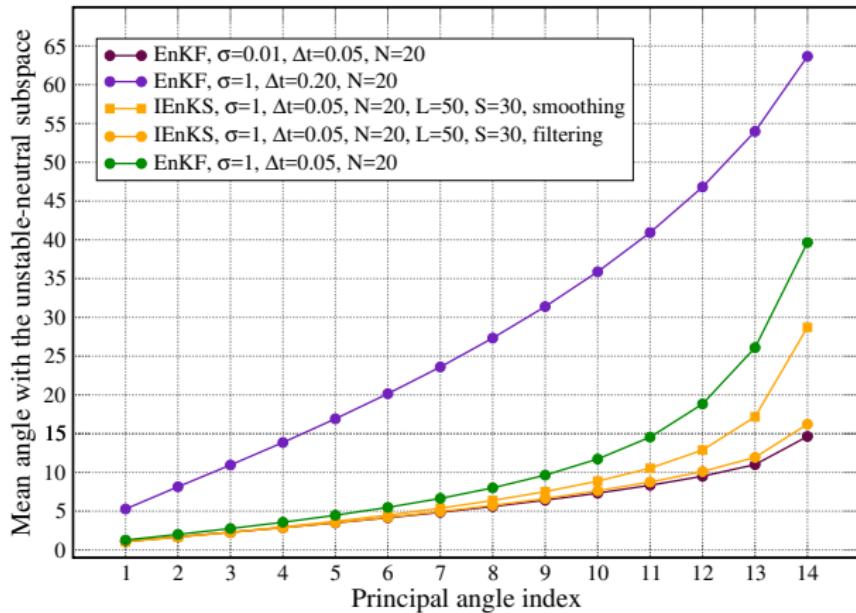
- Average angle (in degrees) between an anomaly (from the ensemble) and the unstable-neutral subspace as a function of the interval between updates (EnKF and IEnKS, Lorenz-95, $\mathbf{R} = 10^{-4} \mathbf{I}$, $N = 20$).

Nonlinear chaotic model



- Average angle (in degrees) between an anomaly (from the ensemble) and the unstable-neutral subspace as a function of the DAW length (IEnKS, Lorenz-95), as well as the corresponding RMSE of the analysis.

Nonlinear chaotic model



- Average principle angles (in degrees) between the anomalies simplex and the unstable-neutral subspace as a function of the angle index (IEnKS, Lorenz-95, $S = 1$, $\mathbf{R} = \mathbf{I}$, $N = 15$) at the end of the DAW (filtering).

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Conclusions

- We proved that if the models are linear and the initial and observation error statistics are Gaussian, the (degenerate) KF, or (deterministic) EnKF in this case, collapse onto the unstable subspace. We provided a rate of convergence.
- We showed that under specific observability conditions and for \mathbf{P}_0 of sufficiently large column space, \mathbf{P}_k asymptotics is independent from \mathbf{P}_0 and can be computed analytically.
- These results can be extrapolated to the case of smoothers.
- These degenerate KF/KS serve as proxies for the EnKF and the IEnKS (for filtering and smoothing).
- We numerically studied the collapse onto the unstable-neutral subspace of those nonlinear filter/smoothers using a geometrical description of the relative position of the unstable-neutral subspaces with the set of filter anomalies.

Final word

Thank you for your attention!

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