

State, global and local parameter estimation using local ensemble Kalman filters: applications to online machine learning of chaotic dynamics

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Goals

- 1 Goals
- 2 Surrogate model representation
- 3 Model identification as a variational offline data assimilation problem
- 4 Online learning of state, model and forcings
- 5 Covariance localization
- 6 Augmented dynamics and the unstable/neutral subspace
- 7 Conclusions
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From model error to the absence of a model

- ▶ At crossroads between:

Data Assimilation (DA), Machine Learning (ML) and Dynamical Systems (DS)

- ▶ **Goal:** Estimate **autonomous chaotic** dynamics from **partial** and **noisy** observations

→ **Surrogate model**

- ▶ **Subgoal 1:** Develop a **Bayesian** framework for this estimation problem. ✓

- ▶ **Subgoal 2:** Estimate and minimize the errors attached to the estimation. ✓

- ▶ **Subgoal 3:** What about more complex models? learning hybrid models. ✓

- ▶ **Subgoal 4:** What about **online** (sequential) learning?

→ **This talk [ensemble methods]!**

- ▶ **References** connected to data-driven reconstruction of the dynamics in DA and ML: [Park et al. 1994; Wang et al. 1998; Paduart et al. 2010; Lguensat et al. 2017; Pathak et al. 2017; Harlim 2018; Dueben et al. 2018; Long et al. 2018; Fablet et al. 2018; Vlachas et al. 2020; Brunton et al. 2016] and many more since the beginning of 2020.

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ODE representation for the surrogate model

- Ordinary differential equations (ODEs) representation of the surrogate dynamics

$$\frac{dx}{dt} = \Phi_{\mathbf{A}}(\mathbf{x}),$$

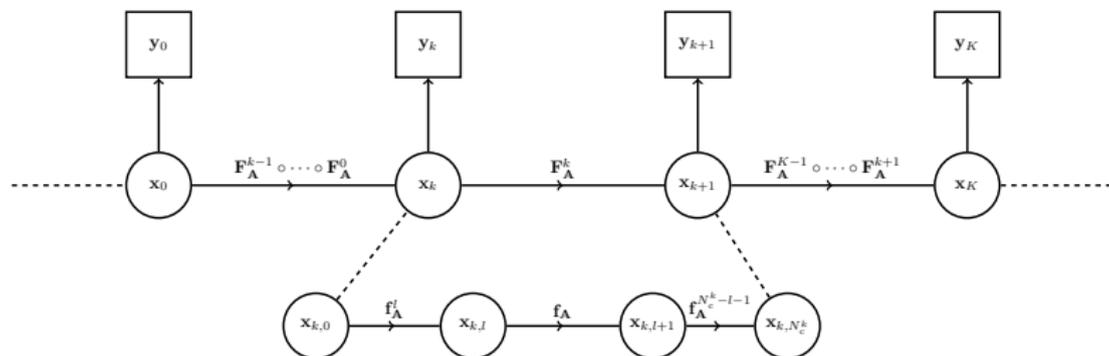
where \mathbf{A} is a set of N_p coefficients.

- We need:
 - to specify the tendency $\mathbf{x} \mapsto \Phi_{\mathbf{A}}(\mathbf{x})$,
 - to choose a numerical scheme to integrate in time the tendency $\Phi_{\mathbf{A}}$ and be able to build resolvent of the surrogate dynamics $\mathbf{x}_{k+1} = \mathbf{F}_{\mathbf{A}}(\mathbf{x}_k)$.
- Going beyond, we wish to account for (surrogate) model error, so that the surrogate model representation is actually an SDE:

$$d\mathbf{x} = \Phi_{\mathbf{A}}(\mathbf{x})dt + \sqrt{\mathbf{Q}}d\mathbf{W}(t),$$

with $\mathbf{W}(t)$ an N_x -dimensional Wiener process.

Integration scheme and cycling



- Choosing a Runge-Kutta method as **integration scheme**:

$$\mathbf{f}_{\mathbf{A}}(\mathbf{x}) = \mathbf{x} + h \sum_{i=0}^{N_{\text{RK}}-1} \beta_i \mathbf{k}_i, \quad \mathbf{k}_i = \Phi_{\mathbf{A}} \left(\mathbf{x} + h \sum_{j=0}^{i-1} \alpha_{i,j} \mathbf{k}_j \right).$$

- **Compositions** of integration schemes:

$$\mathbf{x}_{k+1} = \mathbf{F}_{\mathbf{A}}^k(\mathbf{x}_k) \quad \text{where} \quad \mathbf{F}_{\mathbf{A}}^k \equiv \underbrace{\mathbf{f}_{\mathbf{A}}^{N_c^k}}_{N_c^k \text{ times}} \equiv \mathbf{f}_{\mathbf{A}} \circ \dots \circ \mathbf{f}_{\mathbf{A}}$$

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Bayesian analysis of the joint problem

- **Bayesian view** on state and model estimation:

$$p(\mathbf{A}, \mathbf{Q}_{1:K}, \mathbf{x}_{0:K} | \mathbf{y}_{0:K}, \mathbf{R}_{0:K}) = \frac{p(\mathbf{y}_{0:K} | \mathbf{x}_{0:K}, \mathbf{A}, \mathbf{Q}_{1:K}, \mathbf{R}_{0:K}) p(\mathbf{x}_{0:K} | \mathbf{A}, \mathbf{Q}_{1:K}) p(\mathbf{A}, \mathbf{Q}_{1:K})}{p(\mathbf{y}_{0:K}, \mathbf{R}_{0:K})}.$$

- **Data assimilation cost function** assuming Gaussian errors and Markovian dynamics:

$$\begin{aligned} \mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K}, \mathbf{Q}_{1:K}) &= \frac{1}{2} \sum_{k=0}^K \left\{ \|\mathbf{y}_k - \mathbf{H}_k(\mathbf{x}_k)\|_{\mathbf{R}_k}^2 + \ln |\mathbf{R}_k| \right\} \\ &\quad + \frac{1}{2} \sum_{k=1}^K \left\{ \|\mathbf{x}_k - \mathbf{F}_A^{k-1}(\mathbf{x}_{k-1})\|_{\mathbf{Q}_k}^2 + \ln |\mathbf{Q}_k| \right\} - \ln p(\mathbf{x}_0, \mathbf{A}, \mathbf{Q}_{1:K}). \end{aligned}$$

→ This is a (4D) **variational** problem.

→ Allows to rigorously handle **partial and noisy observations**.

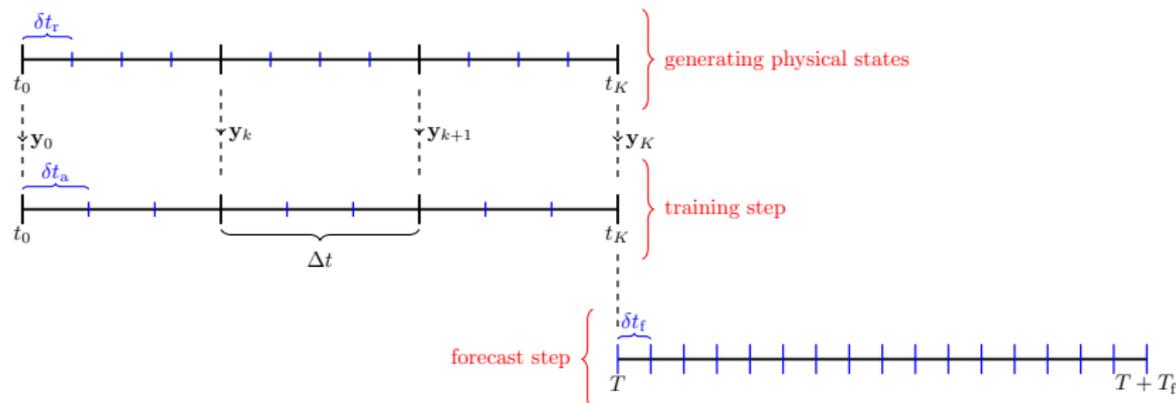
- Typical **machine learning cost function** with $\mathbf{H}_k = \mathbf{I}_k$ in the limit $\mathbf{R}_k \rightarrow \mathbf{0}$:

$$\mathcal{J}(\mathbf{A}) \approx \frac{1}{2} \sum_{k=1}^K \left\| \mathbf{y}_k - \mathbf{F}_A^{k-1}(\mathbf{y}_{k-1}) \right\|_{\mathbf{Q}_k}^2 - \ln p(\mathbf{y}_0, \mathbf{A}).$$

Similar outcome or improved upon [Hsieh et al. 1998; Abarbanel et al. 2018].

Experiment plan

► The reference model, the surrogate model and the forecasting system



► Metrics of comparison:

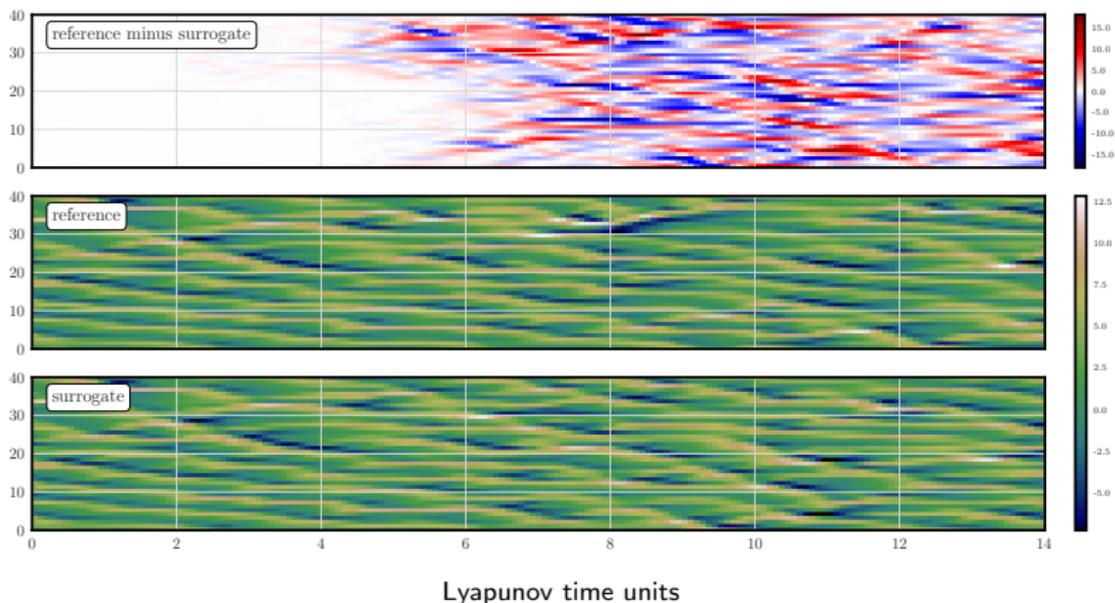
- Forecast skill [FS]: Normalized RMSE (NRMSE) between the reference and surrogate forecasts as a function of lead time (averaged over initial conditions).
- Lyapunov spectrum [LS].
- Power spectrum density [PSD].

Almost identifiable model and perfect observations

- Inferring the dynamics from dense & noiseless observations of a non-identifiable model

The Lorenz 96 model (40 variables). Surrogate model based on an RK2 scheme.

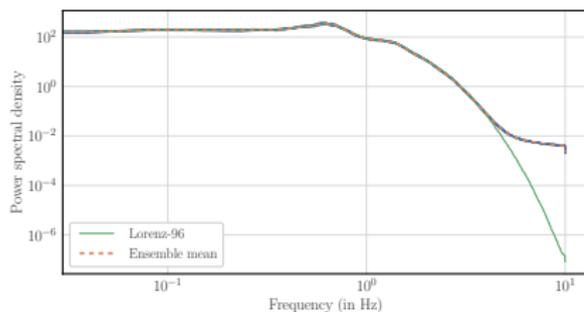
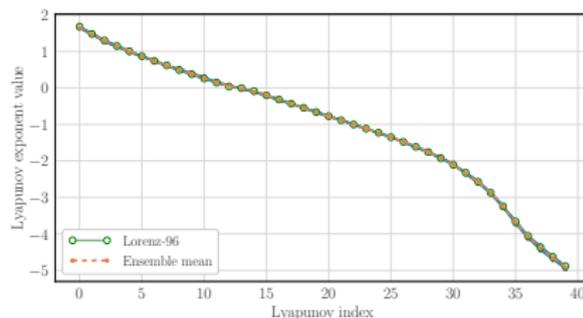
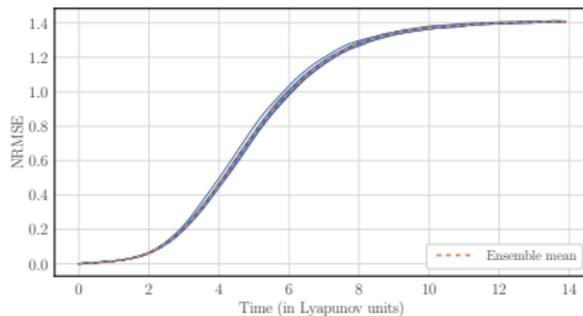
$$\frac{dx_n}{dt} = (x_{n+1} - x_{n-2})x_{n-1} - x_n + F,$$



Application to the one-scale Lorenz-96 model

- ▶ Very good reconstruction of the **long-term properties** of the model (L96 model).

- ▶ CNN+RK4
- ▶ Approximate scheme
- ▶ Fully observed
- ▶ Significantly noisy observations $\mathbf{R} = \mathbf{I}$
- ▶ Long window $K = 5000$, $\Delta t = 0.05$
- ▶ EnKS with $L = 4$
- ▶ 30 EM iterations

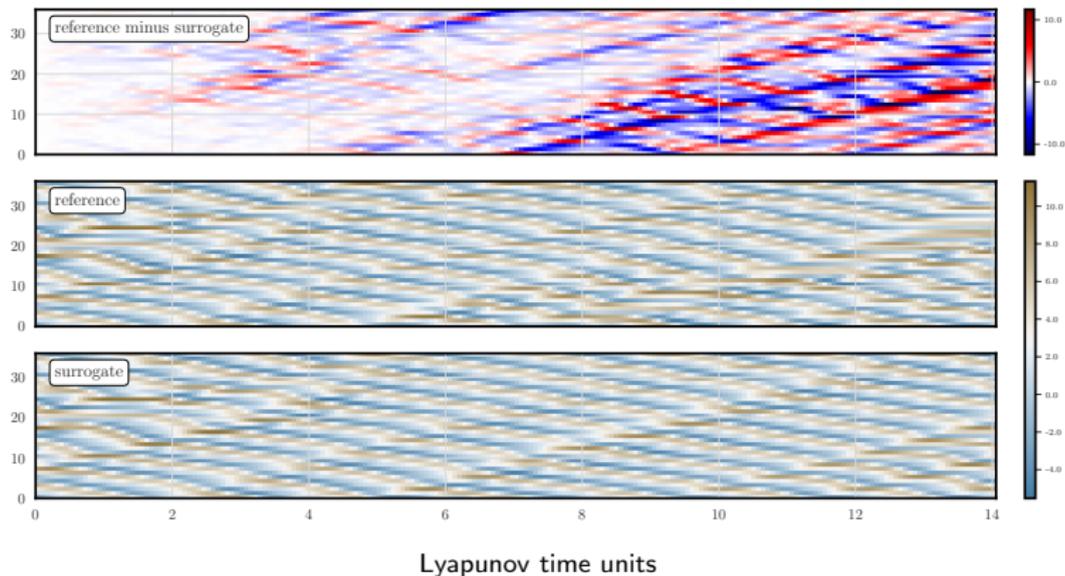


Non-identifiable model and imperfect observations

- The Lorenz 05III (two-scale) model (36 slow & 360 fast variables).

$$\frac{dx_n}{dt} = \psi_n^+(\mathbf{x}) + F - h \frac{c}{b} \sum_{m=0}^9 u_{m+10n},$$

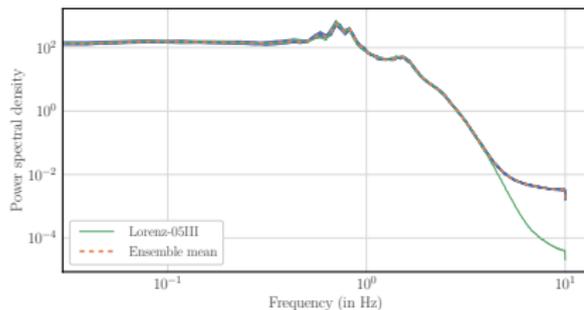
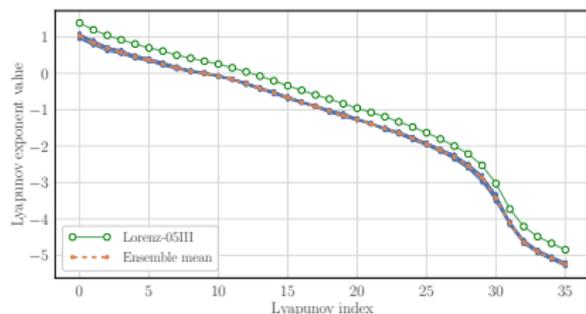
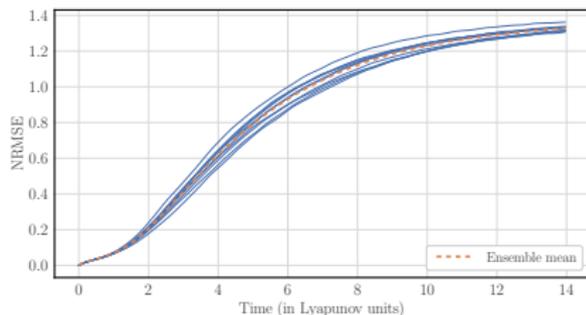
$$\frac{du_m}{dt} = \frac{c}{b} \psi_m^-(b\mathbf{u}) + h \frac{c}{b} x_{m/10}, \quad \text{with} \quad \psi_n^\pm(\mathbf{x}) = x_{n\mp 1}(x_{n\pm 1} - x_{n\mp 2}) - x_n,$$



Application to the two-scale Lorenz-05III model

- ▶ Good reconstruction of the **long-term properties** of the model (L05III model).

- ▶ CNN+RK4
- ▶ Approximate scheme
- ▶ Observation of the coarse modes only
- ▶ Significantly noisy observations $\mathbf{R} = \mathbf{I}$
- ▶ Long window $K = 5000$, $\Delta t = 0.05$
- ▶ EnKS with $L = 4$
- ▶ 30 EM iterations



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Online learning scheme: Principle

► So far, learning was **offline**, i.e. based on variational technique using all available data. Can one design a sequential (**online**) scheme that progressively updates **both the state and the model** as data are collected?

► In the following, we make the assumptions:

- (i) *autonomous* and *local* dynamics,
- (ii) *homogeneous* dynamics or *heterogeneous* dynamics, or *mixed* dynamics.

► All parameters of the model are hereafter noted:

$$\mathbf{A} \longrightarrow \mathbf{p} \in \mathbb{R}^{N_p} \text{ [Global parameters]}, \quad \mathbf{q} \in \mathbb{R}^{N_q} \text{ [local parameters]}.$$

► **Augmented state** formalism [Jazwinski 1970; Ruiz et al. 2013]:

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \\ \mathbf{q} \end{bmatrix} \in \mathbb{R}^{N_z}, \quad \text{with} \quad N_z = N_x + N_p + N_q.$$

Just a (more ambitious) parameter estimation problem!?

Online learning scheme: The problem

- ▶ We use the augmented state formalism with **ensemble Kalman filters** (EnKFs):
 - ① global deterministic EnKFs (EnSRF, ETKF),
 - ② global iterative EnKF (IEnKF), key for nonlinearity.
 - ③ local EnKFs (LEnSRF, LETKF), key for scalability.

- ▶ Adequacy and inadequacy between the main LEnKF classes and the estimation of local and global parameters.

| | Global parameters | Local parameters | Mixed set of parameters |
|--------------|--|------------------------------|-----------------------------------|
| LEnSRF CL | well suited localization in parameter space? | suited numerically costly | unclear solution proposed here |
| LETKF DL | only approximate (average) solution proposed here | well suited | unclear solution proposed here |

- ▶ We assume that the observations are **local** whenever **DL** is used.
- ▶ **Nonlocal** observations require **CL**.

Online learning scheme: Notation

- ▶ **Augmented** ensemble matrix: $\mathbf{E} \in \mathbb{R}^{N_z \times N_e}$
- ▶ Ensemble means and anomalies:

$$\bar{\mathbf{z}} \triangleq \mathbf{E}\mathbf{1}/N_e,$$

$$\mathbf{X} \triangleq (\mathbf{E} - \bar{\mathbf{z}}\mathbf{1}^\top) / \sqrt{N_e - 1},$$

- ▶ Splitting state/global/local:

$$\mathbf{E} = \begin{bmatrix} \mathbf{E}_x \\ \mathbf{E}_p \\ \mathbf{E}_q \end{bmatrix}, \quad \bar{\mathbf{z}} = \begin{bmatrix} \bar{x} \\ \bar{p} \\ \bar{q} \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} \mathbf{X}_x \\ \mathbf{X}_p \\ \mathbf{X}_q \end{bmatrix}, \quad \text{and} \quad \mathbf{A} = \begin{bmatrix} \mathbf{A}_{xx} & \mathbf{A}_{xp} & \mathbf{A}_{xq} \\ \mathbf{A}_{px} & \mathbf{A}_{pp} & \mathbf{A}_{pq} \\ \mathbf{A}_{qx} & \mathbf{A}_{qp} & \mathbf{A}_{qq} \end{bmatrix}.$$

- ▶ Observation operator (**key assumption!**):

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_x \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}.$$

Online learning scheme: EnKF two-step update

► The ensemble update (analysis) can be decomposed into a **two-step** scheme:

- 1 Update the state part of the ensemble $\mathbf{E}_x^f \rightarrow \mathbf{E}_x^a$ using an EnKF.
- 2 Update the parameter part of the ensemble:

$$\mathbf{E}_p^a = \mathbf{E}_p^f + \mathbf{B}_{px} \mathbf{B}_{xx}^{-1} \left(\mathbf{E}_x^a - \mathbf{E}_x^f \right),$$

which can be computed:

- (i) solving the linear system $\mathbf{B}_{xx} \Delta = \mathbf{E}_x^a - \mathbf{E}_x^f$, and
- (ii) updating $\mathbf{E}_p^a = \mathbf{E}_p^f + \mathbf{B}_{px} \Delta$ (**linear regression!**).

► This can actually be proven for any statistical assumption provided the parameters are not directly observed. Should also remain valid for the update of local EnKFs.

[Bocquet et al. 2020b]

Covariance localization

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The EnSRF-ML update (global parameters)

- Convenient reformulation of the EnSRF update in the observation space, follows [Andrews 1968; Whitaker et al. 2002; Bocquet 2016; Malartic et al. 2021]:
- Ancillary matrices:

$$\begin{aligned}\mathbf{T} &\triangleq \mathbf{I} + \mathbf{R}^{-1/2} \mathbf{H}_x \mathbf{B}_{xx} \mathbf{H}_x^\top \mathbf{R}^{-1/2} \in \mathbb{R}^{N_y \times N_y}, \\ \mathbf{u}_x &\triangleq \mathbf{H}_x^\top \mathbf{R}^{-1/2} \mathbf{T}^{-1} \mathbf{R}^{-1/2} (\mathbf{y} - \mathbf{H}_x \bar{\mathbf{x}}^f) \in \mathbb{R}^{N_x}, \\ \mathbf{U}_x &\triangleq -\mathbf{H}_x^\top \mathbf{R}^{-1/2} (\mathbf{T} + \mathbf{T}^{1/2})^{-1} \mathbf{R}^{-1/2} \mathbf{H}_x \mathbf{X}_x^f \in \mathbb{R}^{N_x \times N_e}.\end{aligned}$$

- Updates:

$$\begin{aligned}\Delta \bar{\mathbf{x}} &= \mathbf{B}_{xx} \mathbf{u}_x, & \Delta \mathbf{X}_x &= \mathbf{B}_{xx} \mathbf{U}_x, \\ \Delta \bar{\mathbf{p}} &= \mathbf{B}_{px} \mathbf{u}_x, & \Delta \mathbf{X}_p &= \mathbf{B}_{px} \mathbf{U}_x.\end{aligned}$$

[Malartic et al. 2021]

The LEnSRF-ML update (global parameters)

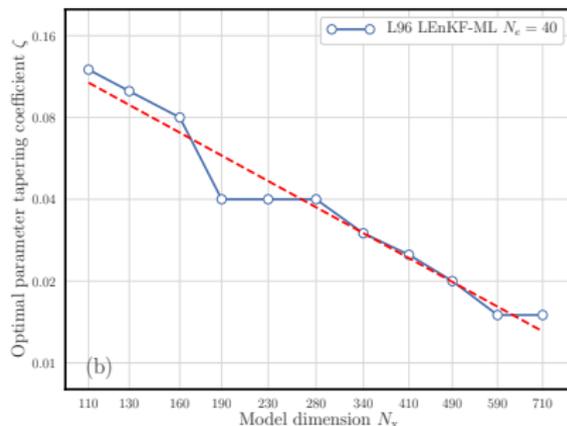
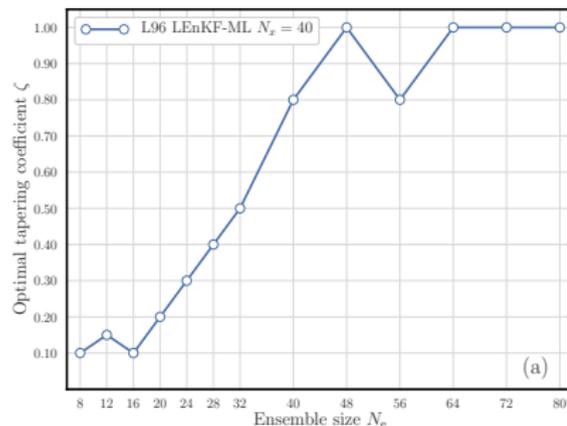
- Covariance localization in the augmented space:

$$\begin{aligned}\mathbf{B}_{xx} &= \rho_{xx} \circ \left[\mathbf{X}_x^f \left(\mathbf{X}_x^f \right)^\top \right], \\ \mathbf{B}_{px} &= \rho_{px} \circ \left[\mathbf{X}_p^f \left(\mathbf{X}_x^f \right)^\top \right] = \mathbf{B}_{xp}^\top, \\ \mathbf{B}_{pp} &= \rho_{pp} \circ \left[\mathbf{X}_p^f \left(\mathbf{X}_p^f \right)^\top \right].\end{aligned}$$

- The localization matrix ρ_{xx} is the usual localization matrix and almost certainly makes \mathbf{B}_{xx} positive definite.
- The localization matrix ρ_{px} has to be **uniform** because the parameters are global. The most natural choice is to use $\rho_{px} = \zeta \mathbf{\Pi}_{px}$, where $\mathbf{\Pi}_{px} \in \mathbb{R}^{N_p \times N_x}$ is the matrix full of ones, and where ζ is a tuning parameter [Ruckstuhl et al. 2018].
- For simplicity, we assume $\rho_{px} = \mathbf{\Pi}_{px}$ and enforce the **tapering coefficient** ζ in the update:

$$\Delta \bar{\mathbf{p}} = \zeta \mathbf{B}_{px} \mathbf{u}_x, \quad \Delta \mathbf{X}_p = \zeta \mathbf{B}_{px} \mathbf{U}_x.$$

Numerics: Optimal tapering coefficient (global parameters)



- ▶ Mathematical constraint: \mathbf{B} must be positive definite \rightarrow constraint on ζ .
- ▶ Optimal scaling of the tapering consistent with [Ruckstuhl et al. 2018; Bocquet et al. 2020a]:

$$\zeta < \sqrt{\frac{\lambda_{\min}}{N_x}}.$$

[Bocquet et al. 2020b]

The LEnSRF-HML update (mixed parameters)

- ▶ Updating both global and local parameters (hybrid updating). We simply add:

$$\Delta \bar{\mathbf{q}} = \mathbf{B}_{\mathbf{q}\mathbf{x}} \mathbf{u}_{\mathbf{x}}, \quad \Delta \mathbf{X}_{\mathbf{q}} = \mathbf{B}_{\mathbf{q}\mathbf{x}} \mathbf{U}_{\mathbf{x}}.$$

- ▶ Without localization, there is no distinction between local and global parameters.
- ▶ With localization we define

$$\mathbf{B}_{\mathbf{q}\mathbf{x}} = \rho_{\mathbf{q}\mathbf{x}} \circ \left[\mathbf{X}_{\mathbf{q}}^{\mathbf{f}} \left(\mathbf{X}_{\mathbf{x}}^{\mathbf{f}} \right)^{\top} \right] = \mathbf{B}_{\mathbf{x}\mathbf{q}}^{\top},$$

$$\mathbf{B}_{\mathbf{q}\mathbf{p}} = \rho_{\mathbf{q}\mathbf{p}} \circ \left[\mathbf{X}_{\mathbf{q}}^{\mathbf{f}} \left(\mathbf{X}_{\mathbf{p}}^{\mathbf{f}} \right)^{\top} \right] = \mathbf{B}_{\mathbf{p}\mathbf{q}}^{\top},$$

$$\mathbf{B}_{\mathbf{p}\mathbf{p}} = \rho_{\mathbf{q}\mathbf{q}} \circ \left[\mathbf{X}_{\mathbf{q}}^{\mathbf{f}} \left(\mathbf{X}_{\mathbf{q}}^{\mathbf{f}} \right)^{\top} \right].$$

- ▶ Neither $\rho_{\mathbf{q}\mathbf{p}}$, nor $\rho_{\mathbf{q}\mathbf{q}}$ have to be specified.
- ▶ As opposed to $\rho_{\mathbf{p}\mathbf{x}}$, $\rho_{\mathbf{q}\mathbf{x}}$ has to reflect the geometry of the local parameters and state variables.

Augmented dynamics and the unstable/neutral subspace

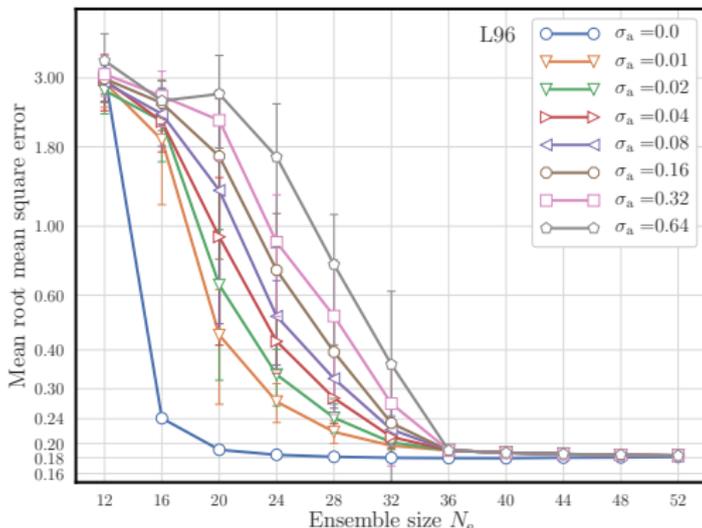
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The augmented dynamics

- **Augmented dynamics** (model persistence or Brownian motion):

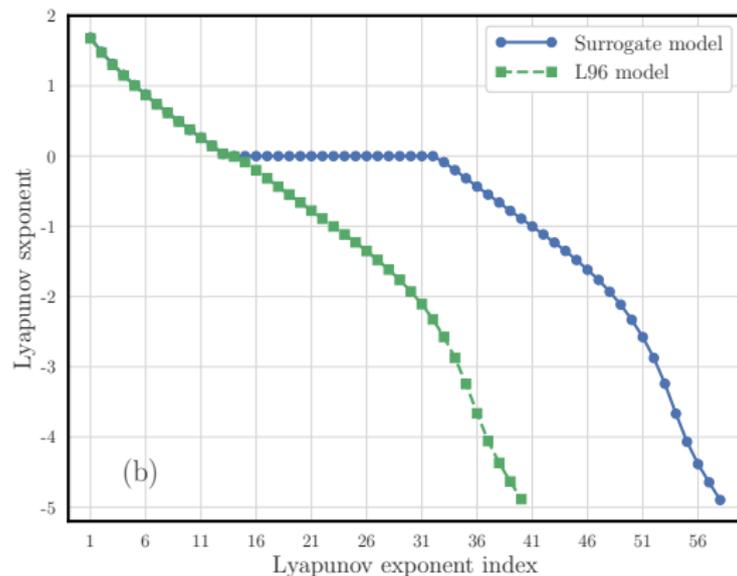
$$\begin{bmatrix} \mathbf{x}_k \\ \mathbf{p}_k \end{bmatrix} \mapsto \begin{bmatrix} \mathbf{F}^k(\mathbf{x}_k, \mathbf{p}_k) \\ \mathbf{p}_k \end{bmatrix}$$

- Assuming (i) N_0 is the dimension of the *unstable neutral subspace* of the reference dynamics, (ii) N_e is the size of the ensemble, then, in order for the augmented global EnKF (EnKF-ML) to be stable, we must have: $N_e \gtrsim N_0 + N_p + 1$.



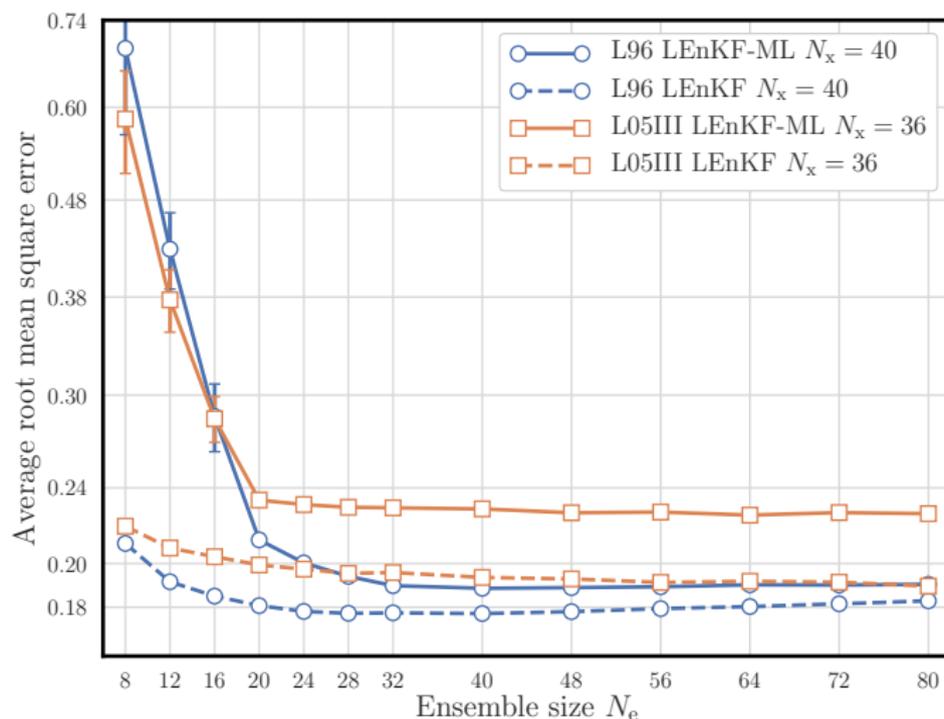
The augmented dynamics: Asymptotic properties

- Lyapunov spectra for the true and augmented L96.



Numerics (global parameters)

- LEnSRF and LEnSRF-ML applied to the L96 and L05III models.



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Conclusions

The main results presented here are from [Bocquet et al. 2020a; Malartic et al. 2021], with preliminaries from [Bocquet et al. 2019]

► Main messages:

- **Bayesian** DA view on state and model estimation.
DA can address goals assigned to **ML** but with **partial & noisy observations**.
- **Online** EnKFs-ML can also be used to sequentially estimate both state and model.
- **Rigorous** ensemble solutions for joint state var./local par./global par. estimation.
- **Theoretical** results (backed by numerics):

| LEnKF\Parameters | Global | Local | Mixed |
|------------------|------------------|----------|------------------|
| CL | clarified | existing | clarified |
| DL | new and improved | existing | new and improved |

- Successful on 1D low-order models (L96, L05III).

► Open questions and technical hardships (non-exhaustive):

- Non-autonomous dynamics?
- More complex models?
- A 2D case with the mL96 model for radiances like-observations, that **mixes CL and DL, local and global parameters and nonlocal observations** is under test.

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Domain localization

- 1 Goals
- 2 Surrogate model representation
- 3 Model identification as a variational offline data assimilation problem
- 4 Online learning of state, model and forcings
- 5 Covariance localization
- 6 Augmented dynamics and the unstable/neutral subspace
- 7 Conclusions
- 8 References
- 9 Domain localization**

The ensemble transform Kalman filter (domain localization)

- **Generic** ETKF update (incremental)

$$\Delta \bar{\mathbf{z}} = \mathbf{X}^f \mathbf{w}^a, \quad \Delta \mathbf{X} = \mathbf{X}^f (\mathbf{T}^{-1/2} - \mathbf{I}).$$

with the definitions:

$$\begin{aligned} \mathbf{Y} &\triangleq \mathbf{H}\mathbf{X}^f, \\ \mathbf{T} &\triangleq \mathbf{I} + \mathbf{Y}^\top \mathbf{R}^{-1} \mathbf{Y}, \\ \mathbf{w}^a &\triangleq \mathbf{T}^{-1} \mathbf{Y}^\top \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\bar{\mathbf{z}}^f). \end{aligned}$$

- Now, assume that the observations are **local**. The domain localization (DL) of the ETKF (LETKF) uses for each augmented state variable $n \in \{1, \dots, N_z\}$:

$$\mathbf{R}_n^{-1} \triangleq \boldsymbol{\rho}_n \circ \mathbf{R}^{-1},$$

where $\boldsymbol{\rho}_n \in \mathbb{R}^{N_y \times N_y}$ is the localization matrix in observation space for the n -th variable.

The LETKF-ML (global parameters)

- Update of the ETKF-ML

$$\begin{aligned}\Delta\bar{\mathbf{x}} &= \mathbf{X}_x^f \mathbf{w}^a, & \Delta\mathbf{X}_x &= \mathbf{X}_x^f \left(\mathbf{T}^{-1/2} - \mathbf{I} \right), \\ \Delta\bar{\mathbf{p}} &= \mathbf{X}_p^f \left(\mathbf{X}_x^f \right)^\top \mathbf{u}_x, & \Delta\mathbf{X}_p &= \mathbf{X}_p^f \left(\mathbf{X}_x^f \right)^\top \mathbf{U}_x,\end{aligned}$$

with the definition (on the right/local version):

$$\begin{aligned}\mathbf{u}_x &= \mathbf{H}_x^\top \mathbf{R}^{-1} \left(\mathbf{y} - \mathbf{H}_x \bar{\mathbf{x}}^f - \mathbf{Y} \mathbf{w}^a \right), \\ \mathbf{U}_x &= -\mathbf{H}_x^\top \mathbf{R}^{-1} \mathbf{Y} \left(\mathbf{T} + \mathbf{T}^{1/2} \right)^{-1}.\end{aligned}$$

- This global parameter update is fully consistent with the DL framework.

This is an improvement over the [Aksoy et al. 2006; Fertig et al. 2009; Hu et al. 2010] average semi-empirical technique!

- With the tapering coefficient:

$$\Delta\bar{\mathbf{p}} = \zeta \mathbf{X}_p^f \left(\mathbf{X}_x^f \right)^\top \mathbf{u}_x, \quad \Delta\mathbf{X}_p = \zeta \mathbf{X}_p^f \left(\mathbf{X}_x^f \right)^\top \mathbf{U}_x,$$

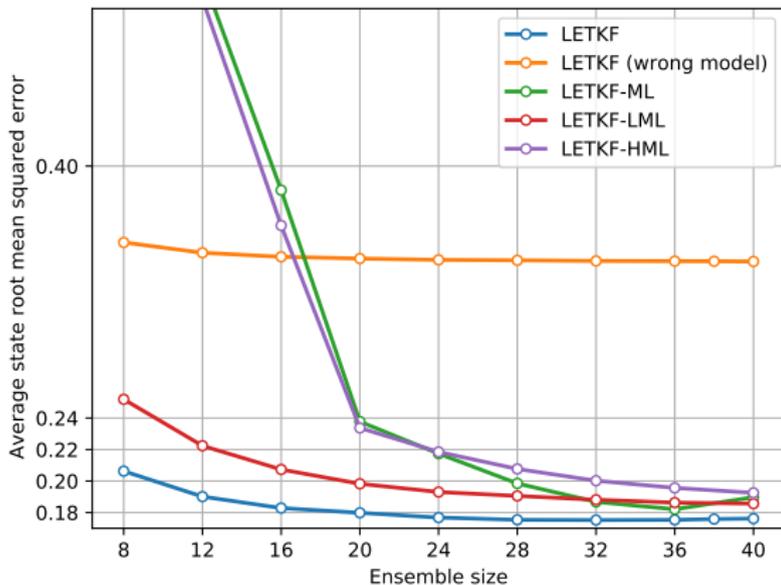
The LETKF-HML (mixed parameters)

- ▶ To account for local parameters, a very simple addition to the LETKF-ML scheme:

$$\begin{aligned}\Delta \bar{\mathbf{q}} &= \mathbf{X}_q^f \mathbf{w}^a, \\ \Delta \mathbf{X}_q &= \mathbf{X}_q^f (\mathbf{T}^{-1/2} - \mathbf{I}).\end{aligned}$$

Numerics (assorted LETKFs-ML)

- L96 model where the forcing is **inhomogeneous**: $F = 8 + \sin(2\pi n/N_x)$



- LETKF (wrong model): known dynamics except for $F = 8$.
- LETK-ML: unknown dynamics but known forcing
- LETKF-LML: known dynamics but unknown forcing
- LETKF-HML: unknown dynamics, unknown forcing