Using machine learning and data assimilation to learn both dynamics and state

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Outline

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

  $\longrightarrow$ 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 online (sequential) learning?

- 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.

Outline

ODE representation for the surrogate model

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

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \boldsymbol{\phi}_{\mathbf{A}}(\mathbf{x}),$$

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

▶ We need:

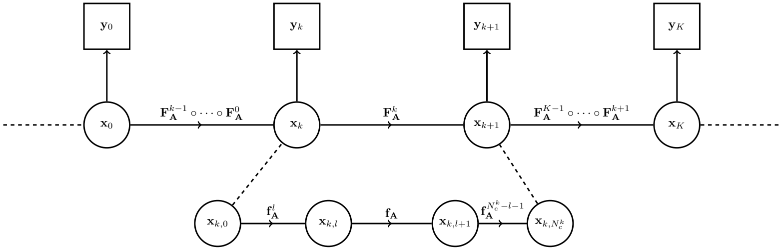
- to choose a numerical scheme to integrate in time the tendency $\boldsymbol{\phi}_{\mathbf{A}}$ and be able to build resolvent of the surrogate dynamics $\mathbf{x}_{k+1} = \mathbf{F}_{\mathbf{A}}(\mathbf{x}_k)$,
- to specify the tendency $\mathbf{x} \mapsto \boldsymbol{\phi}_{\mathbf{A}}(\mathbf{x})$.

▶ Going beyond in this work, we wish to account for (surrogate) model error, so that the surrogate model representation is actually an SDE:

$$\mathrm{d}\mathbf{x} = \boldsymbol{\phi}_{\mathbf{A}}(\mathbf{x})\mathrm{d}t + \sqrt{\mathbf{Q}}\mathrm{d}\mathbf{W}(t),$$

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

Integration scheme and cycling



- Choosing a Runge-Kutta method as integration scheme:

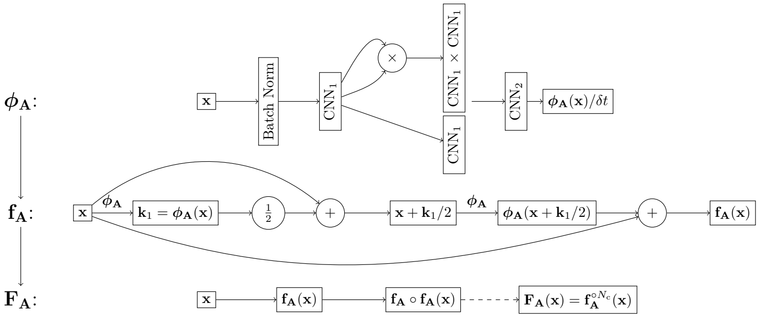
$$\mathbf{f}_\mathbf{A}(\mathbf{x}) = \mathbf{x} + h \sum_{i=0}^{N_{\mathrm{RK}}-1} \beta_i \mathbf{k}_i, \qquad \mathbf{k}_i = \boldsymbol{\phi}_\mathbf{A}\left(\mathbf{x} + h \sum_{j=0}^{i-1} \alpha_{i,j} \mathbf{k}_j\right).$$

- Compositions of integration schemes:

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

Neural network models

- We tested many simple architectures, all following the structure of N_c explicit Runge-Kutta schemes, with linear or nonlinear activation functions:
  - $\phi_{\mathbf{A}}$: minimal representation (as few parameters as possible), or based on a NN (with potentially many parameters) implemented in TensorFlow 2.x
  - Convolutional layers were used for local, homogeneous systems.
  - Locally connected convolutional layers were used for local, heterogeneous systems.



Outline

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:

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

⟶ 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 $\mathbf{R}_k \longrightarrow \mathbf{0}$:

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

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

Bayesian analysis of the joint problem: Assuming $\mathbf{Q}_{1:K}$ is known

- If the $\mathbf{Q}_{1:K}$ are known, we look for minima of

$$\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K} | \mathbf{Q}_{1:K}) = -\ln p(\mathbf{A}, \mathbf{x}_{0:K} | \mathbf{y}_{0:K}, \mathbf{R}_{0:K}, \mathbf{Q}_{1:K})$$

which is not as general as $\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K}, \mathbf{Q}_{1:K})$.

(1) ▶ $\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K} | \mathbf{Q}_{1:K})$ can be optimized using a full variational approach:

- In [Bocquet et al. 2019], $\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K} | \mathbf{Q}_{1:K})$ is minimized using a full weak-constraint 4D-Var where both $\mathbf{x}_{0:K}$ and $\mathbf{A}$ are control variables.

Bayesian analysis of the joint problem: Assuming $\mathbf{Q}_{1:K}$ is known

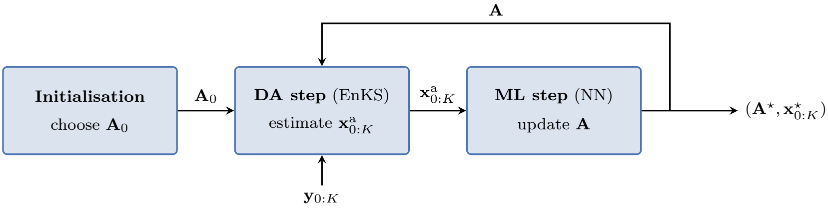
(2) ▶ $\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K}|\mathbf{Q}_{1:K})$ is minimized using a coordinate descent:

- ▶ using a weak constraint 4D-Var for $\mathbf{x}_{0:K}$ and a variational subproblem for $\mathbf{A}$ [Bocquet et al. 2019].

- ▶ using a (higher-dimensional) strong constraint 4D-Var for $\mathbf{x}_{0:K}$ and a variational subproblem for $\mathbf{A}$ [Bocquet et al. 2019].

- ▶ using an EnKF/EnKS for $\mathbf{x}_{0:K}$ and a variational subproblem for $\mathbf{A}$ [Brajard et al. 2020a; Bocquet et al. 2020b].

⟶ Combine data assimilation and machine learning techniques in a coordinate descent



Bayesian analysis of the marginal problem: Assuming $\mathbf{Q}_{1:K}$ is unknown

- Focusing on the marginal $p(\mathbf{A}, \mathbf{Q}_{1:K}|\mathbf{y}_{0:K}, \mathbf{R}_{0:K})$:

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

yields the loss function

$$\mathcal{J}(\mathbf{A}, \mathbf{Q}_{1:K}) = -\ln p(\mathbf{A}, \mathbf{Q}_{1:K}|\mathbf{y}_{0:K}, \mathbf{R}_{0:K}).$$

- A MAP solution (minimum of $\mathcal{J}$) is provided by the EM algorithm. Applying it for the reconstruction of a dynamical system has been suggested in [Ghahramani et al. 1999], using an extended Kalman smoother, or for the estimation of subgrid stochastic processes in [Pulido et al. 2018] using an ensemble Kalman smoother (EnKS).

- An EM solution based on the EnKS has been suggested by [Nguyen et al. 2019] but their approximation is in practice a coordinate descent where model error is not controlled.

Algorithm for an approximate solution of the marginal problem (1/2)

▶ The expectation step: EnKS over a long period $[t_0, t_K]$ which accounts for model error (SQRT-CORE scheme). The outputs are $\overline{\mathbf{x}}_{0:K}^{(j)}$ and $\mathbf{Q}^{(j+1)}$ computed online by accumulating over the time window.

$$\mathbf{Q}^{(j+1)} = \frac{1}{K N_\mathrm{e}} \sum_{i=1}^{N_\mathrm{e}} \sum_{k=1}^{K} \left(\mathbf{x}_{k,i}^{(j)} - \mathbf{F}_{\mathbf{A}^{(j)}}^{k-1}(\mathbf{x}_{k-1,i}^{(j)})\right) \left(\mathbf{x}_{k,i}^{(j)} - \mathbf{F}_{\mathbf{A}^{(j)}}^{k-1}(\mathbf{x}_{k-1,i}^{(j)})\right)^\top .$$

Hence this expectation step anticipates the maximization step when estimating $\mathbf{Q}^{(j+1)}$.

Algorithm for an approximate solution of the marginal problem (2/2)

▶ The maximization step: Minimize ($\mathbf{Q}^{(j+1)}$ is fixed):

$$\begin{aligned}\mathcal{L}^{(j)}(\mathbf{A},\mathbf{Q}^{(j+1)}) =& -\ln p(\overline{\mathbf{x}}^{(j)}_{0:K},\mathbf{y}_{0:K},\mathbf{A},\mathbf{Q}^{(j+1)},\mathbf{R}_{0:K}) \\ =& \frac{1}{2}\sum_{k=1}^{K}\left\{\left\|\overline{\mathbf{x}}^{(j)}_{k}-\mathbf{F}^{k-1}_{\mathbf{A}}(\overline{\mathbf{x}}^{(j)}_{k-1})\right\|^2_{\mathbf{Q}^{(j+1)}{}^{-1}}+\ln\left|\mathbf{Q}^{(j+1)}\right|\right\} \\ & -\ln p(\overline{\mathbf{x}}^{(j)}_{0},\mathbf{A},\mathbf{Q}^{(j+1)})+\cdots.\end{aligned}$$

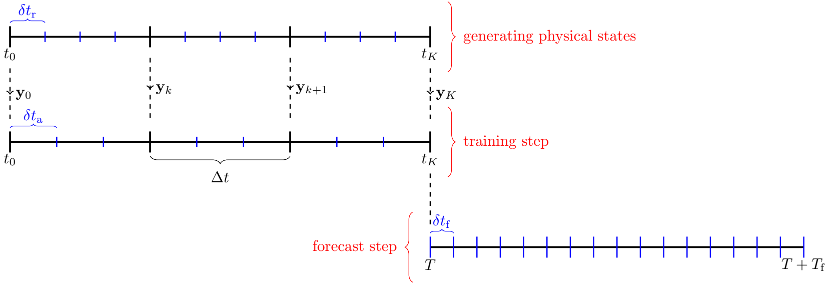
Note the use of the ensemble mean instead of the ensemble (main approximation).

▶ No iteration in the maximization step over $\mathbf{A}$ and $\mathbf{Q}$ (should be fine if $\mathbf{Q}=q\mathbf{I}_{\mathrm{x}}$).

▶ In practice, almost numerically equivalent to the full EM scheme (see [Bocquet et al. 2020b] for details).

Experiment plan

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

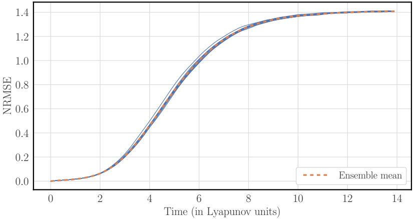


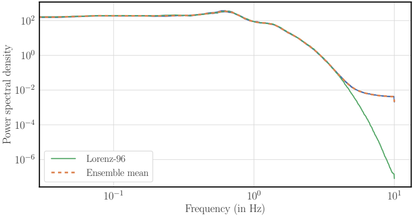
- Metrics of comparison:
  - Forecast skill [FS]: Normalized RMSE (NRMSE) between the reference and surrogate forecasts as a function of lead time (averaged over initial conditions).
  - Lyapunov spectrum [LS].
  - Power spectrum density [PSD].

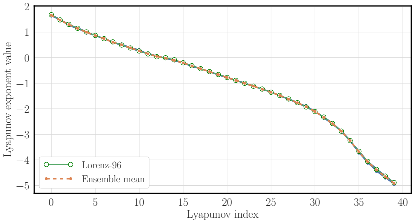
Application to the one-scale Lorenz-96 model

- 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



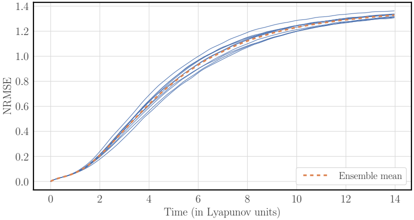


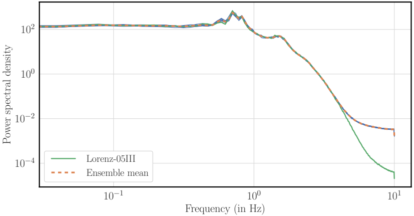


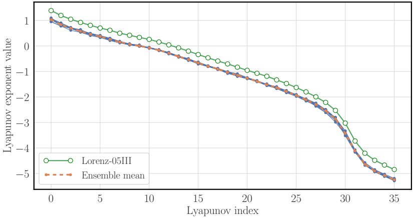
Application to the two-scale Lorenz-05III model

- 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







Outline

Online learning scheme: principle

▶ So far, the 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.
A few hypotheses could be relaxed.
All parameters of the model are hereafter noted $\mathbf{A} \longrightarrow \mathbf{p} \in \mathbb{R}^{N_\mathrm{p}}$.

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

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} \in \mathbb{R}^{N_\mathrm{z}}, \qquad \text{with} \quad N_\mathrm{z} = N_\mathrm{x} + N_\mathrm{p}.$$

Just a (more ambitious) parameter estimation problem!?

Online learning scheme: EnKF update

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

- The ensemble update (analysis) can be decomposed into a two-step scheme:
  1. Update the state part of the ensemble $\mathbf{E}_\mathrm{x}^\mathrm{f} \longrightarrow \mathbf{E}_\mathrm{x}^\mathrm{a}$ using an EnKF.
  2. Update the parameter part of the ensemble:

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

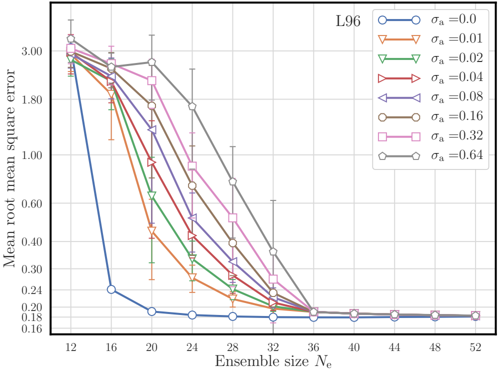
  which can be computed:
  (i) solving the linear system $\mathbf{B}_\mathrm{xx}\boldsymbol{\Delta} = \mathbf{E}_\mathrm{x}^\mathrm{a} - \mathbf{E}_\mathrm{x}^\mathrm{f}$, and
  (ii) updating $\mathbf{E}_\mathrm{p}^\mathrm{a} = \mathbf{E}_\mathrm{p}^\mathrm{f} + \mathbf{B}_\mathrm{px}\boldsymbol{\Delta}$.

The augmented dynamics

▶ Augmented dynamics (model persistence or Brownian motion):

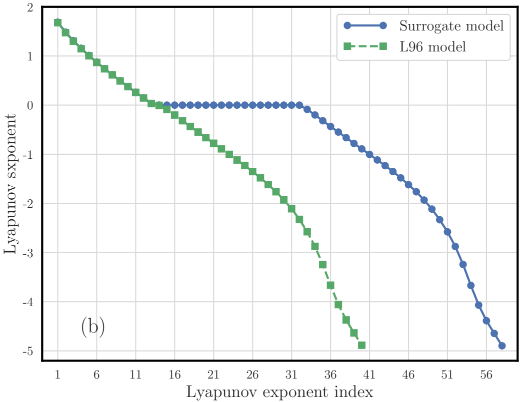
$$\begin{bmatrix} \mathbf{x}_k \\ \mathbf{p}_k \end{bmatrix} \mapsto \begin{bmatrix} \mathbf{F}^k(\mathbf{x}_k, \mathbf{p}_k) \\ \mathbf{p}_k \end{bmatrix}$$

▶ 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: $N_\mathrm{e} \gtrapprox N_0 + N_\mathrm{p} + 1.$



The augmented dynamics: Asymptotic properties

- Lyapunov spectra for the true and augmented L96.



Local EnKF-ML

- Covariance localisation/LEnSRF:

$$\mathbf{E}_\mathrm{x}^\mathrm{f} \mapsto \mathbf{E}_\mathrm{x}^\mathrm{a} \quad \text{(LEnSRF)}, \qquad \mathbf{E}_\mathrm{p}^\mathrm{a} = \mathbf{E}_\mathrm{p}^\mathrm{f} + \mathbf{B}_\mathrm{px}\mathbf{B}_\mathrm{xx}^{-1}\left(\mathbf{E}_\mathrm{x}^\mathrm{a} - \mathbf{E}_\mathrm{x}^\mathrm{f}\right) \quad \text{(global)},$$

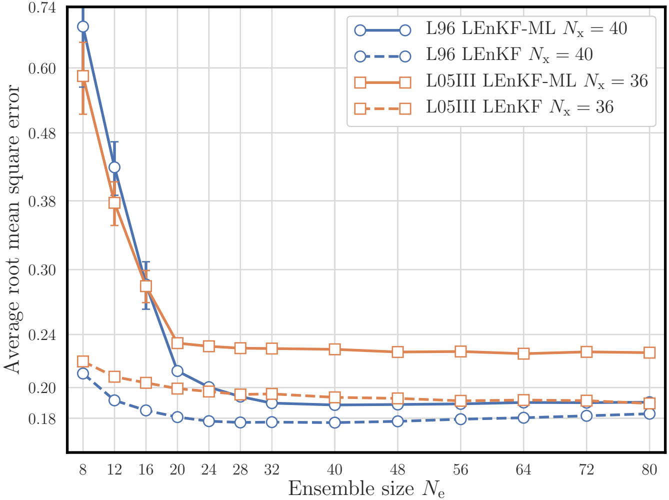
which can be computed:
(i) solving the linear system $\mathbf{B}_\mathrm{xx}\boldsymbol{\Delta} = \mathbf{E}_\mathrm{x}^\mathrm{a} - \mathbf{E}_\mathrm{x}^\mathrm{f}$, and
(ii) updating $\mathbf{E}_\mathrm{p}^\mathrm{a} = \mathbf{E}_\mathrm{p}^\mathrm{f} + \mathbf{B}_\mathrm{px}\boldsymbol{\Delta}$,
with $\mathbf{B}_\mathrm{xx} = \mathbf{C}_\mathrm{xx} \circ \left(\mathbf{X}_\mathrm{x}^\mathrm{f}\left(\mathbf{X}_\mathrm{x}^\mathrm{f}\right)^\top\right)$, $\mathbf{B}_\mathrm{px} = \zeta\mathbf{X}_\mathrm{p}^\mathrm{f}\left(\mathbf{X}_\mathrm{x}^\mathrm{f}\right)^\top$,
and ζ is the *tapering state/parameter coefficient* [Ruckstuhl et al. 2018].

- Domain localisation/LETKF:

$$\mathbf{E}_\mathrm{x}^\mathrm{f} \mapsto \mathbf{E}_\mathrm{x}^\mathrm{a} \quad \text{(LETKF)}, \qquad \mathbf{E}_\mathrm{p}^\mathrm{a} = \mathbf{E}_\mathrm{p}^\mathrm{f} + \zeta\mathbf{X}_\mathrm{p}^\mathrm{f}\left(\mathbf{X}_\mathrm{x}^\mathrm{f}\right)^\dagger\left(\mathbf{E}_\mathrm{x}^\mathrm{a} - \mathbf{E}_\mathrm{x}^\mathrm{f}\right) \quad \text{(local)},$$

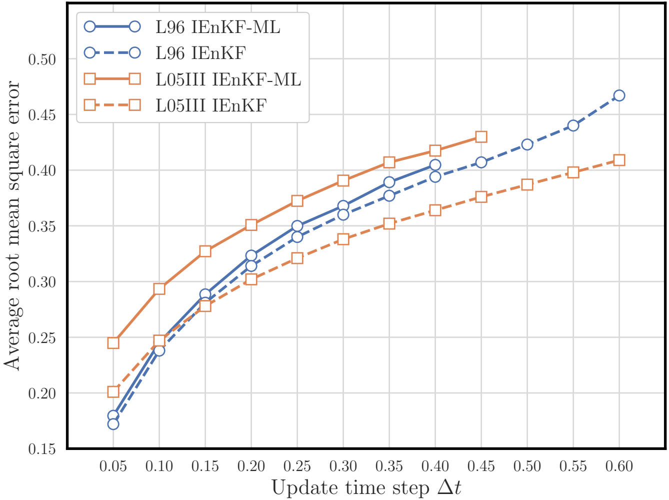
Numerics:

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



Numerics:

▶ To deal with stronger model nonlinearities, we developed the IEnKF-ML variant of the IEnKF [Sakov et al. 2012; Bocquet et al. 2012; Sakov et al. 2018].

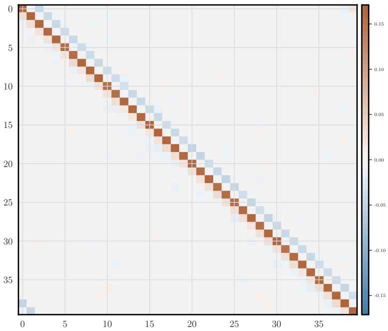


Outline

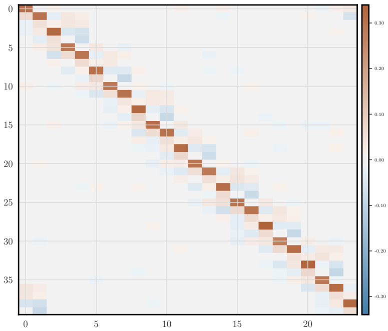
Learning 3D-Var

▶ The Bayesian formalism presented earlier can be extended to learning some key elements of the DA scheme (observed but unknown state, model known or unknown).

▶ Application to learning the Kalman gain equivalent for a 3D-Var scheme applied to the (known here) L96 model, using significantly noisy and partial observations of the state trajectory (24/40).



Fully observed



Partially observed

Outline

Conclusions

Almost all results presented here are from [Bocquet et al. 2019; Brajard et al. 2020a; Bocquet et al. 2020b; Bocquet et al. 2020a].

- Main messages:
  - Bayesian DA view on state and model estimation.
    DA can address goals assigned to ML but with partial & noisy observations.
  - The EM technique, full or approximate, is successful. Only coordinate minimization was shown to be successful so far in such context.
  - The method can handle very long training windows within a variational framework.
  - Online EnKFs-ML can also be used to sequentially estimate both state and model.
  - Successful on various 1D low-order models (L63, L96, KS, L05III).
  - Part of the DA scheme itself could additionally be learned.

- Open questions and technical hardships (non-exhaustive):
  - Non-autonomous dynamics?
  - Implicit integration schemes?
  - More complex models?
  - Surrogate model=knowledge-based+NN? $\longrightarrow$ A. Carrassi talk + A. Farchi poster.

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