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Data-driven identification and reconstruction of partially observed dynamical systems

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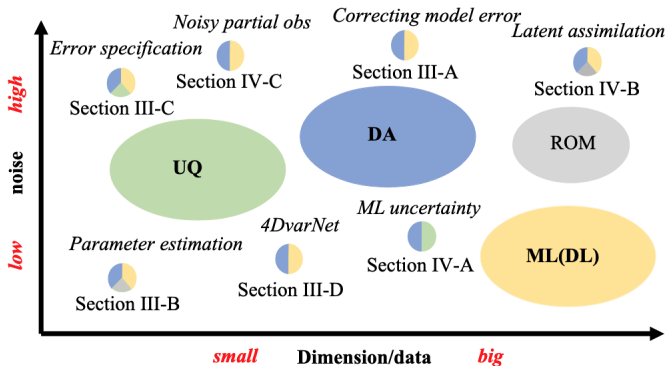
The 10th International Symposium on Data Assimilation (ISDA)
October 21-25, 2024, Kobe, Japan



DA + ML + UQ: a quick overview¹

Context:

- rapidly growing field of research
- still lot of developments to do



¹Cheng et al., *Machine Learning with Data Assimilation and Uncertainty Quantification for Dynamical Systems: a Review*, IEEE/CAA Journal of Automatica Sinica, 2023

Data assimilation formulation:

$$\begin{aligned}\mathbf{x}(t + dt) &= \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t)) \\ \mathbf{y}(t) &= \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))\end{aligned}$$

Machine learning appears everywhere:

- state \mathbf{x} and observations \mathbf{y}
- operators \mathcal{M} and \mathcal{H}
- errors $\boldsymbol{\eta}$ and $\boldsymbol{\epsilon}$
- inversion of the system $p(\mathbf{x}|\mathbf{y})$

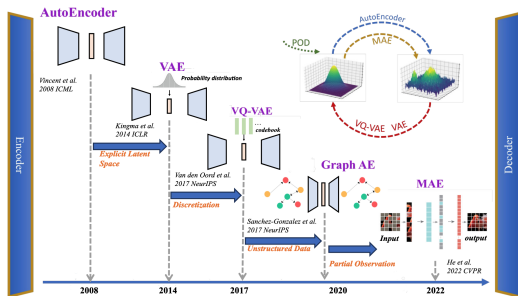
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

State of the system (\mathbf{x}):

- reduced-order modeling (principal components, VAE)
- state augmentation (parameters, latent variables)



Source: Cheng et al. 2023, IEEE/CAA Journal of Automatica Sinica

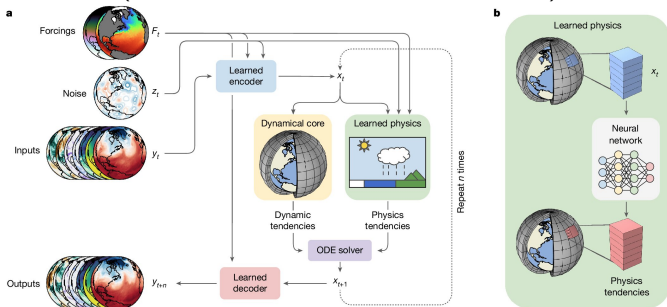
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

Dynamical operator (\mathcal{M}):

- surrogate models (AI, RNN, analogs, AR1 processes)
- hybrid models (GCM core + ML parameterization)



Source: Kochkov et al. 2024, Nature

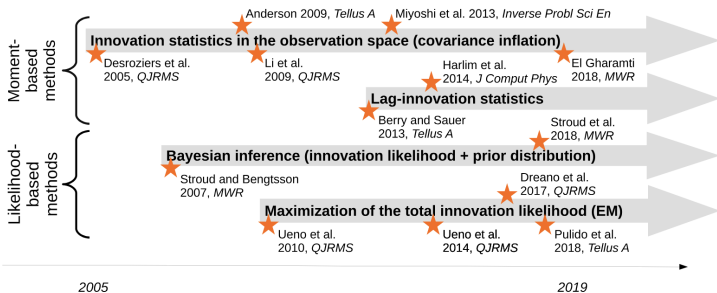
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

Model and observation errors ($\boldsymbol{\eta}$ and $\boldsymbol{\epsilon}$):

- innovation statistics, inflation methods, statistical approaches, NN
- joint estimation of error covariances \mathbf{Q} and \mathbf{R}



Source: Tandeo et al. 2020, Monthly Weather Review

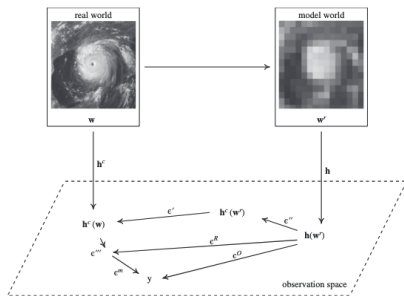
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

Observation operator (\mathcal{H}):

- emulation of transfer functions using ML (e.g., radiative)
- estimation of representativity error



Source: Janjić et al. 2018, QJRMS

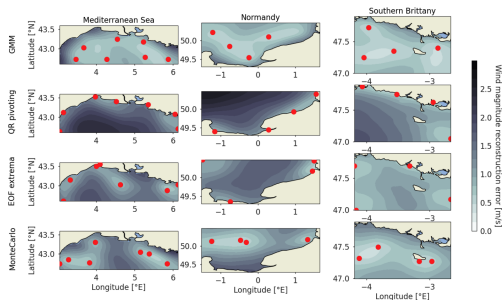
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

Noisy and partial observations (\mathbf{y}):

- aggregation, fusion, and data exclusion
- optimal sampling of the observations



Source: Marcille et al. 2023, Wind Energy Science

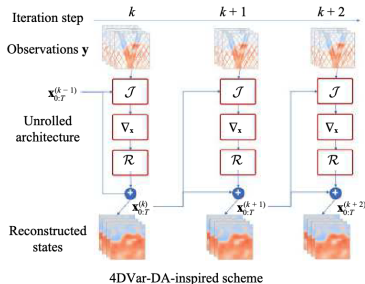
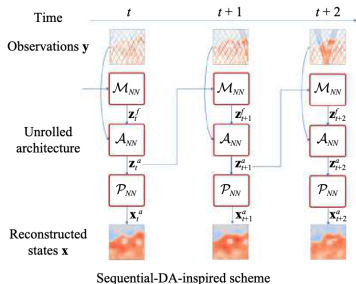
DA + ML + UQ: a quick overview

$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))$$

Full system resolution $p(\mathbf{x}|\mathbf{y})$:

- optimization problem (link between 4D-Var and NN)
- probabilistic ML using Bayesian approaches



Source: Cheng et al. 2023, IEEE/CAA Journal of Automatica Sinica

A simple combination of DA + ML + UQ¹

General framework:

$$\begin{aligned}\mathbf{x}(t + dt) &= \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t)) \\ \mathbf{y}(t) &= \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))\end{aligned}$$

Proposed framework:

$$\begin{aligned}\mathbf{x}(t + 1) &= \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t) \\ \mathbf{y}(t) &= \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)\end{aligned}$$

Assumptions:

- **linear** model and observation operators
- **Gaussian** state, observations, and error terms
- **constant** operators and error covariances

¹Tandeo et al., *Data-driven Reconstruction of Partially Observed Dynamical Systems*, Nonlinear Processes in Geophysics, 2023

A simple combination of DA + ML + UQ¹

General framework:

$$\begin{aligned}\mathbf{x}(t + dt) &= \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t)) \\ \mathbf{y}(t) &= \mathcal{H}(\mathbf{x}(t), \boldsymbol{\epsilon}(t))\end{aligned}$$

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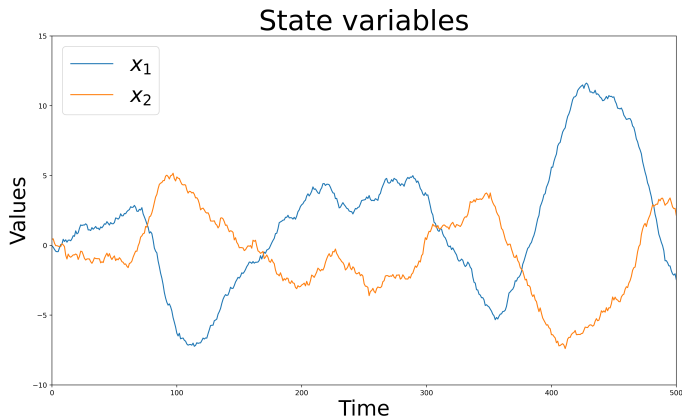
$$\begin{aligned}\mathbf{x}(t + 1) &= \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t) \\ \mathbf{y}(t) &= \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)\end{aligned}$$

Goal:

- make **probabilistic forecasts**
- purely **data-driven** approach
- **interpretation** of the retrieved model

¹Tandeo et al., *Data-driven Reconstruction of Partially Observed Dynamical Systems*, Nonlinear Processes in Geophysics, 2023

Classic approach: Kalman + EM



State-space model:

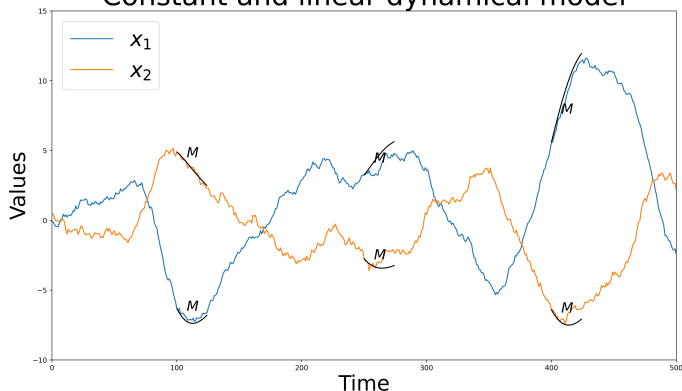
Estimate $\mathbf{x}(0), \dots, \mathbf{x}(T)$

Variables and matrices:

$\mathbf{x} = [x_1, x_2]$

Classic approach: Kalman + EM

Constant and linear dynamical model

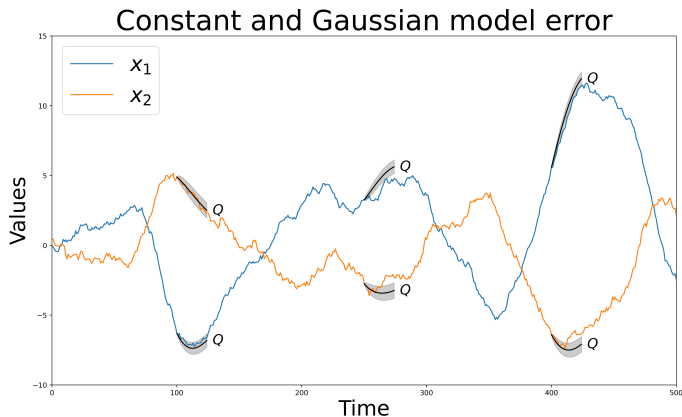


State-space model:
 $\mathbf{x}(t + 1) = \mathbf{M}\mathbf{x}(t)$

Variables and matrices:

$$\mathbf{M} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}$$

Classic approach: Kalman + EM



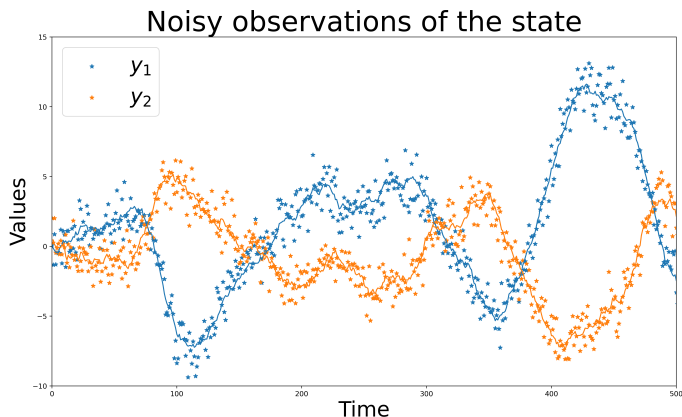
State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

Variables and matrices:

$$\boldsymbol{\eta}(t) \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \mathbf{Q} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}$$

Classic approach: Kalman + EM



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

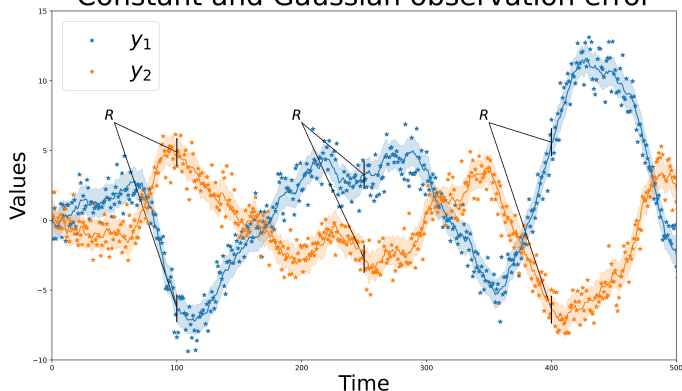
$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t)$$

Variables and matrices:

$$\mathbf{y} = [y_1, y_2], \quad \mathbf{H} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Classic approach: Kalman + EM

Constant and Gaussian observation error



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

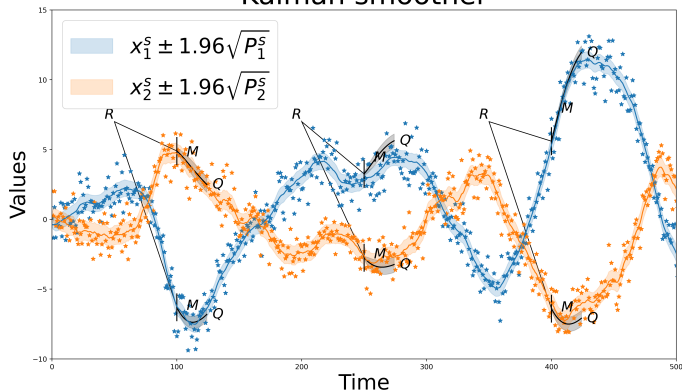
$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

Variables and matrices:

$$\boldsymbol{\epsilon}(t) \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \mathbf{R} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}$$

Classic approach: Kalman + EM

Kalman smoother



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

⇒ Kalman smoother

Variables and matrices:

$$\hat{\mathbf{M}}, \hat{\mathbf{Q}}, \hat{\mathbf{R}} = \underset{\mathbf{M}, \mathbf{Q}, \mathbf{R}}{\operatorname{argmax}} \mathcal{L}(\mathbf{y})$$

⇒ EM algorithm

The Expectation-Maximization algorithm¹

Initialization: **M, Q, R**

¹Shumway and Stoffer, *An approach to time series smoothing and forecasting using the EM algorithm*, Journal of Time Series Analysis, 1982

The Expectation-Maximization algorithm¹

Initialization: \mathbf{M} , \mathbf{Q} , \mathbf{R}

Expectation (DA step):

- fix \mathbf{M} , \mathbf{Q} , \mathbf{R}
- estimation of $\mathbf{x}_{0:T}^s$ and $\mathbf{P}_{0:T}^s$
- \Rightarrow Kalman smoother

¹Shumway and Stoffer, *An approach to time series smoothing and forecasting using the EM algorithm*, Journal of Time Series Analysis, 1982

The Expectation-Maximization algorithm¹

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- \Rightarrow Kalman smoother

Maximization (ML step):

- fix $\mathbf{x}_{0:T}^s$ and $\mathbf{P}_{0:T}^s$
- estimation of \mathbf{M} , \mathbf{Q} , \mathbf{R}
- \Rightarrow analytic solution

¹Shumway and Stoffer, *An approach to time series smoothing and forecasting using the EM algorithm*, Journal of Time Series Analysis, 1982

The Expectation-Maximization algorithm¹

Initialization: \mathbf{M} , \mathbf{Q} , \mathbf{R}

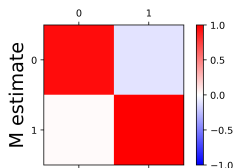
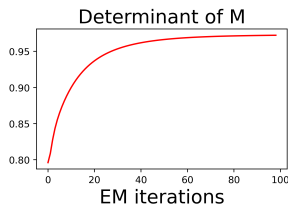
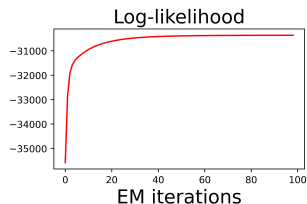
Expectation (DA step):

- fix \mathbf{M} , \mathbf{Q} , \mathbf{R}
- estimation of $\mathbf{x}_{0:T}^s$ and $\mathbf{P}_{0:T}^s$
- \Rightarrow Kalman smoother

Maximization (ML step):

- fix $\mathbf{x}_{0:T}^s$ and $\mathbf{P}_{0:T}^s$
- estimation of \mathbf{M} , \mathbf{Q} , \mathbf{R}
- \Rightarrow analytic solution

Repeat E- and M-steps until convergence of $\mathcal{L}(\mathbf{y})$



¹Shumway and Stoffer, *An approach to time series smoothing and forecasting using the EM algorithm*, Journal of Time Series Analysis, 1982

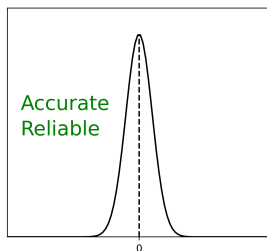
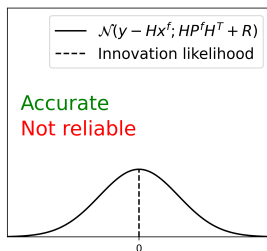
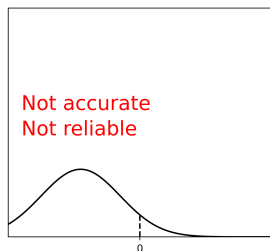
The innovation likelihood $\mathcal{L}(\mathbf{y})$

$$\mathcal{L}(\mathbf{y}) = \prod_{t=0}^T \mathcal{N}\left(0; \mathbf{y}(t) - \mathbf{H}\mathbf{x}^f(t), \mathbf{H}\mathbf{P}^f(t)\mathbf{H}^\top + \mathbf{R}\right)$$

The innovation likelihood $\mathcal{L}(\mathbf{y})$

$$\mathcal{L}(\mathbf{y}) = \prod_{t=0}^T \mathcal{N}\left(0; \mathbf{y}(t) - \mathbf{H}\mathbf{x}^f(t), \mathbf{H}\mathbf{P}^f(t)\mathbf{H}^\top + \mathbf{R}\right)$$

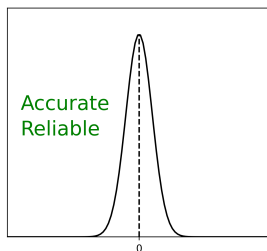
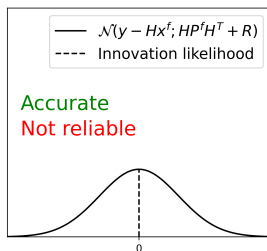
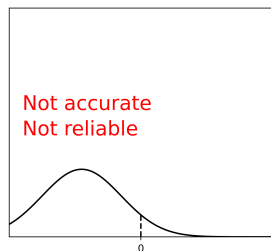
Graphical representation of the innovation likelihood:



The innovation likelihood $\mathcal{L}(\mathbf{y})$

$$\mathcal{L}(\mathbf{y}) = \prod_{t=0}^T \mathcal{N}\left(0; \mathbf{y}(t) - \mathbf{H}\mathbf{x}^f(t), \mathbf{H}\mathbf{P}^f(t)\mathbf{H}^\top + \mathbf{R}\right)$$

Graphical representation of the innovation likelihood:

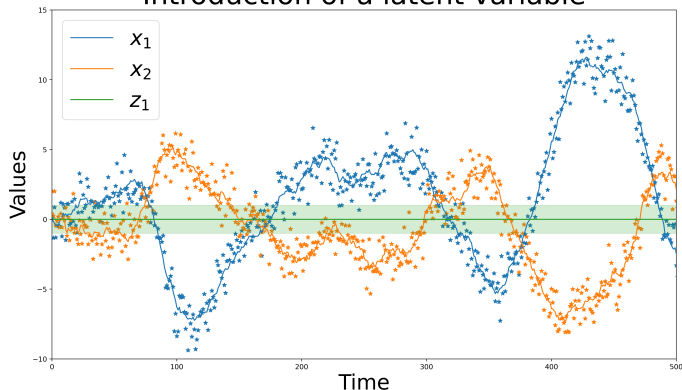


$\mathcal{L}(\mathbf{y})$ depends on \mathbf{M} , \mathbf{Q} , \mathbf{R} :

- $\mathbf{x}^f(t) = \mathbf{M}\mathbf{x}^a(t-1) \rightarrow$ forecast precision
- $\mathbf{P}^f(t) = \mathbf{M}\mathbf{P}^a(t-1)\mathbf{M}^\top + \mathbf{Q} \rightarrow$ forecast reliability
- $\mathbf{R} \rightarrow$ observation error

Proposed approach: Kalman + EM + augmented state

Introduction of a latent variable



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

$$\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Variables and matrices:

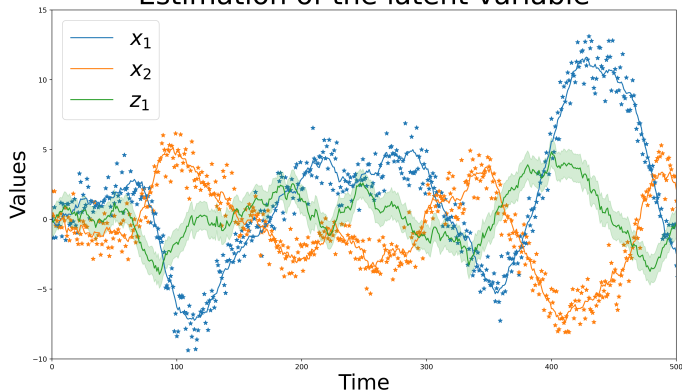
Augmented state $\mathbf{x} = [x_1, x_2, z_1]$

\mathbf{M} and \mathbf{Q} are 3×3

\mathbf{R} is 2×2

Proposed approach: Kalman + EM + augmented state

Estimation of the latent variable



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

$$\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

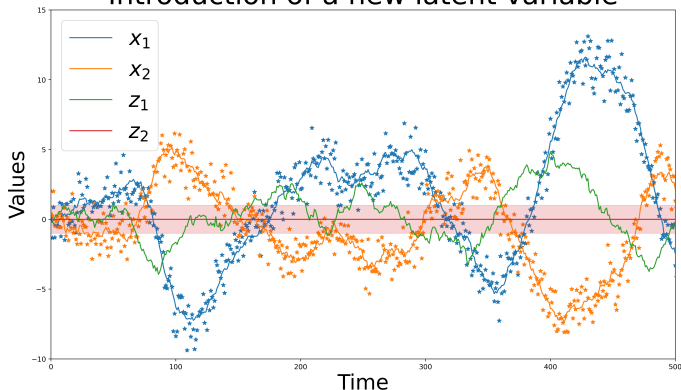
Variables and matrices:

Estimate $\hat{\mathbf{M}}, \hat{\mathbf{Q}}, \hat{\mathbf{R}}$

Estimate $z_1(0), \dots, z_1(T)$

Proposed approach: Kalman + EM + augmented state

Introduction of a new latent variable



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

$$\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Variables and matrices:

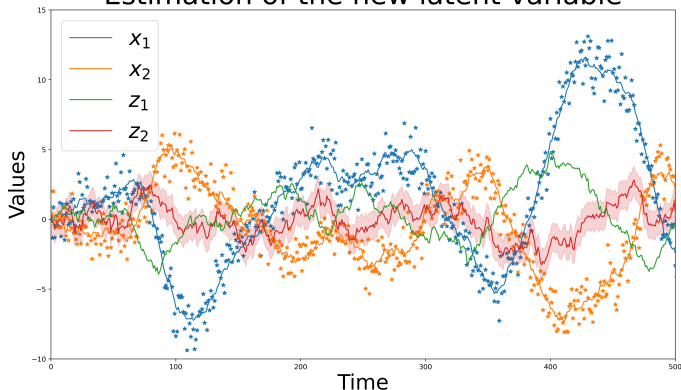
New state $\mathbf{x} = [x_1, x_2, z_1, z_2]$

\mathbf{M} and \mathbf{Q} are 4×4

\mathbf{R} is 2×2

Proposed approach: Kalman + EM + augmented state

Estimation of the new latent variable



State-space model:

$$\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t)$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

$$\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Variables and matrices:

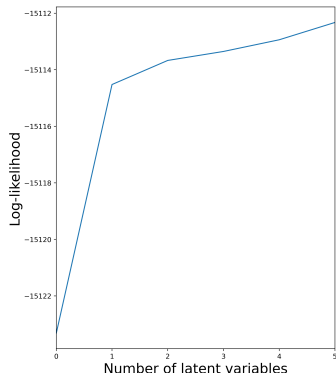
Estimate $\hat{\mathbf{M}}, \hat{\mathbf{Q}}, \hat{\mathbf{R}}$

Estimate $z_2(0), \dots, z_2(T)$

Main scientific questions

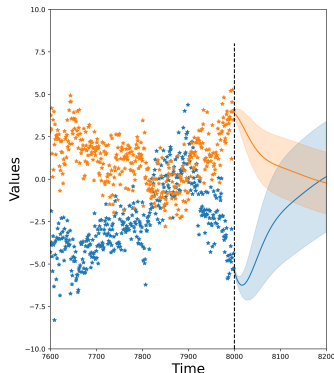
Latent variables:

- how many are needed?
- what is their meaning?
- why do we need them?

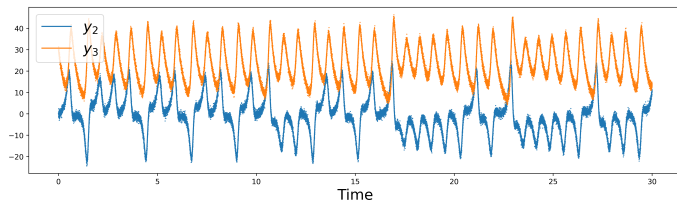


Quality of the forecasts:

- are they precise?
- are they reliable?
- how they compare?



Application to Lorenz-63: formulation and OSSE



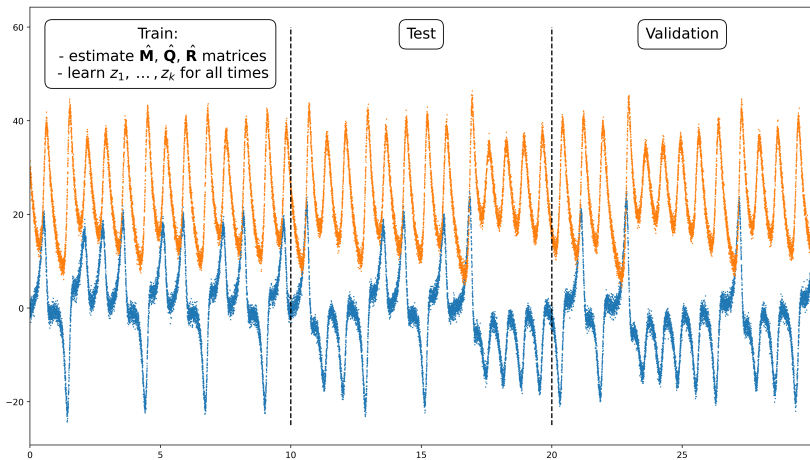
Observations, state, and latent variables:

- $\mathbf{y} = [y_2, y_3]$ → **partial observations** of the system
- $\mathbf{x} = [x_2, x_3, \mathbf{z}]$ → **augmented state** with latent variables \mathbf{z}
- $\mathbf{z} = [z_1, \dots, z_k]$ → **latent variables**

OSSE:

- $dt = 0.001$ → observation sampling
- $\text{Var}(\epsilon) = 1$ → observation error variance

Estimation of $\hat{\mathbf{M}}$, $\hat{\mathbf{Q}}$, $\hat{\mathbf{R}}$ and z_1, \dots, z_k using training data

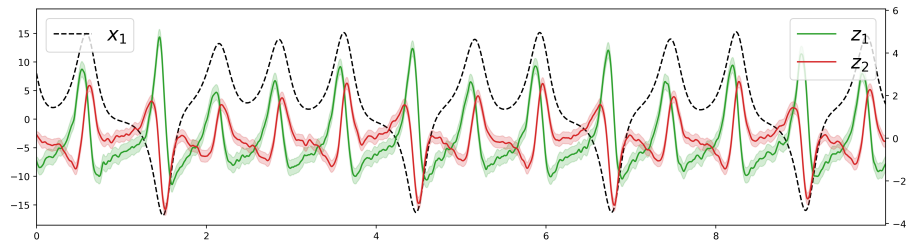


Time series are divided in three parts:

- train, test, and validation datasets
- EM algorithm is applied to the training data

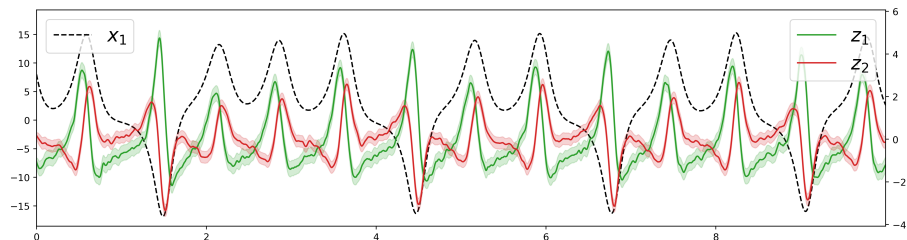
Estimation and meaning of the latent variables

Estimation of z_1 and z_2 :



Estimation and meaning of the latent variables

Estimation of z_1 and z_2 :

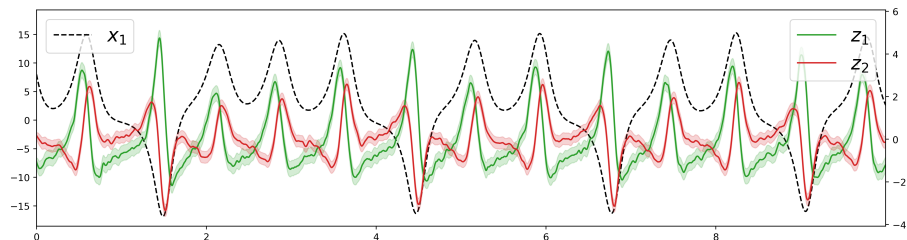


Meaning of z_1 :

$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

Estimation and meaning of the latent variables

Estimation of z_1 and z_2 :



Meaning of z_1 :

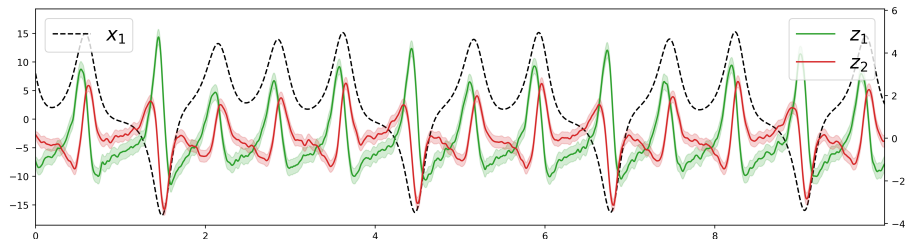
$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

Meaning of z_2 :

$$\begin{aligned} z_2 &= b_1 \dot{z}_1 + b_2 \dot{x}_2 + b_3 \dot{x}_3 \\ &= b_2 \dot{x}_2 + b_3 \dot{x}_3 + b_1 a_2 \ddot{x}_2 + b_1 a_3 \ddot{x}_3 \end{aligned}$$

Estimation and meaning of the latent variables

Estimation of z_1 and z_2 :



Meaning of z_1 :

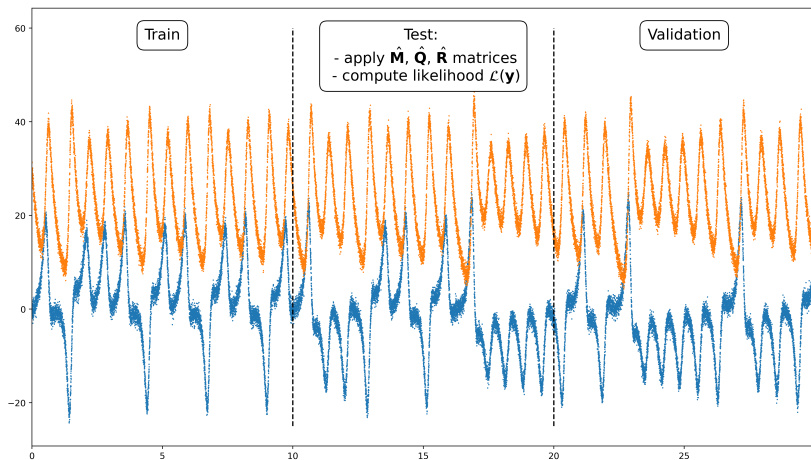
$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

Meaning of z_2 :

$$\begin{aligned} z_2 &= b_1 \dot{z}_1 + b_2 \dot{x}_2 + b_3 \dot{x}_3 \\ &= b_2 \dot{x}_2 + b_3 \dot{x}_3 + b_1 a_2 \ddot{x}_2 + b_1 a_3 \ddot{x}_3 \end{aligned}$$

⇒ latent variables take into account **time delays** of x_2 and x_3

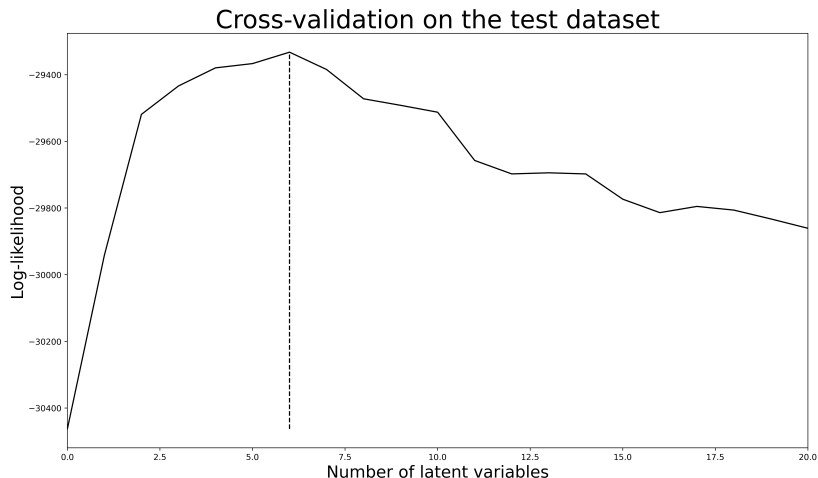
Number of latent variables to retain



Different models are tested:

- from $\mathbf{x} = [\mathbf{x}_2, \mathbf{x}_3, \mathbf{z}_1]$
- to $\mathbf{x} = [\mathbf{x}_2, \mathbf{x}_3, \mathbf{z}_1, \dots, \mathbf{z}_{20}]$

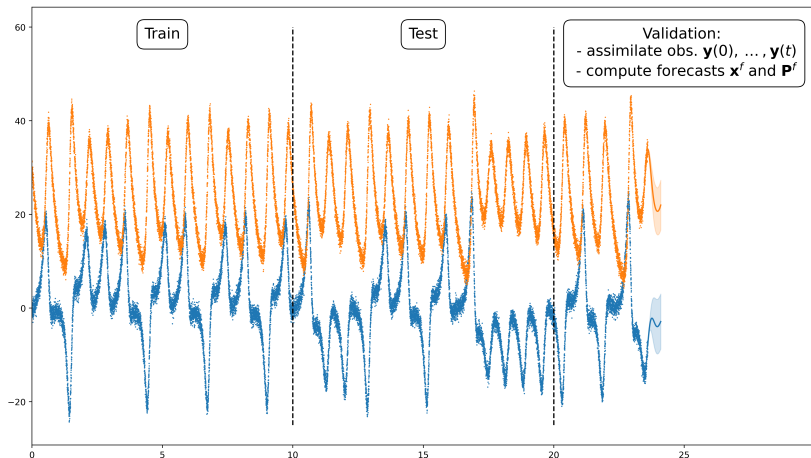
Number of latent variables to retain



Optimal model in terms of likelihood:

- with $\mathbf{x} = [\mathbf{x}_2, \mathbf{x}_3, \mathbf{z}_1, \dots, \mathbf{z}_6]$
- six latent variables are necessary

Probabilistic forecasts using testing data



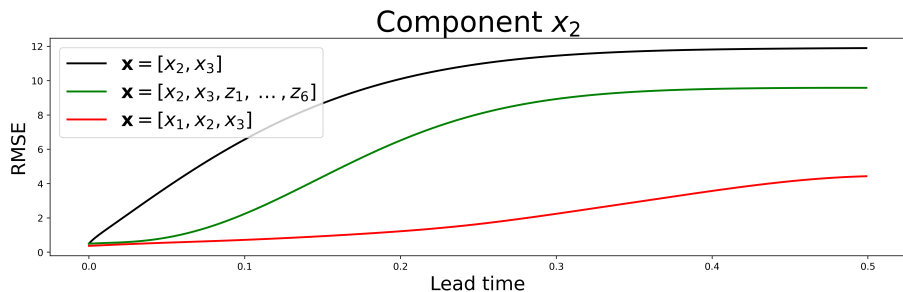
Recursive predictions, starting from an initial time t :

$$\mathbf{E}[\mathbf{x}_{t+1} | \mathbf{y}_1, \dots, \mathbf{y}_t] = \mathbf{M}\mathbf{E}[\mathbf{x}_t | \mathbf{y}_1, \dots, \mathbf{y}_t]$$

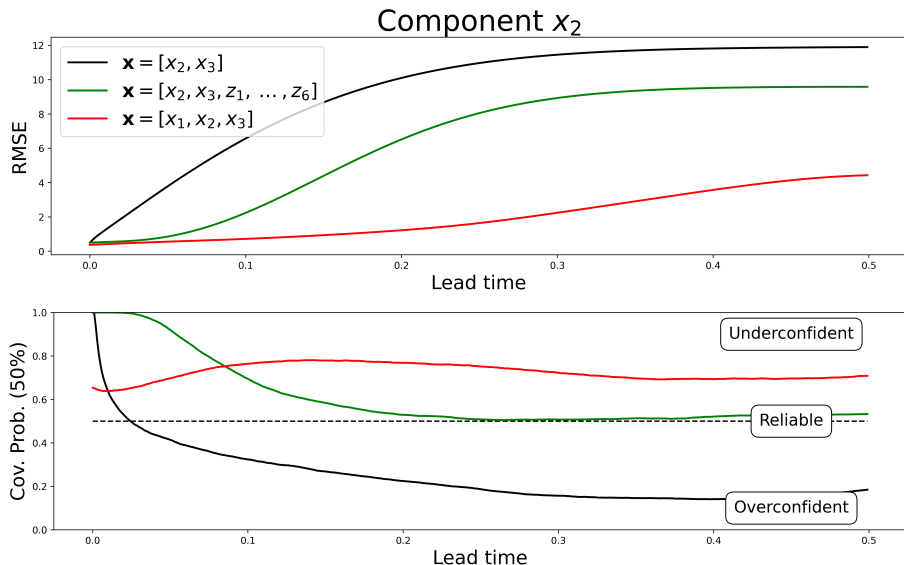
$$\text{Cov}[\mathbf{x}_{t+1} | \mathbf{y}_1, \dots, \mathbf{y}_t] = \mathbf{M}\text{Cov}[\mathbf{x}_t | \mathbf{y}_1, \dots, \mathbf{y}_t]\mathbf{M}^T + \mathbf{Q}$$

Example of probabilistic forecasts (data- VS model-driven)

Performance metrics (data- VS model-driven)



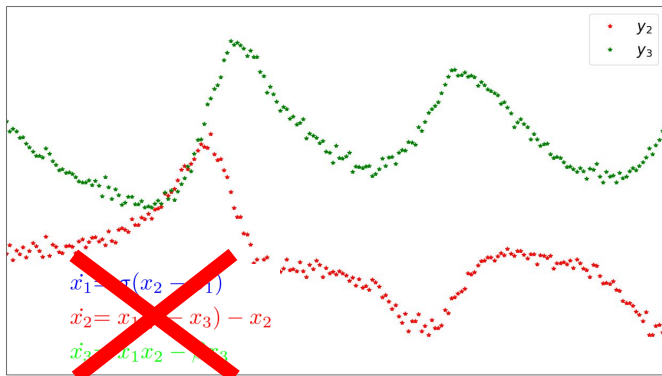
Performance metrics (data- VS model-driven)



Conclusions and perspectives

Context:

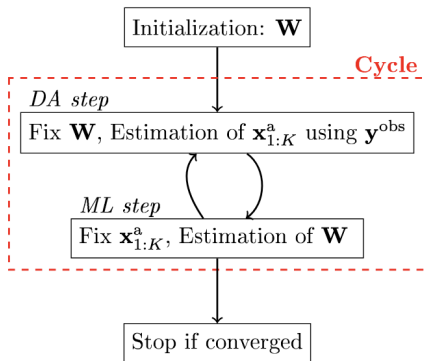
- pure data-driven predictions (i.e., without physical equations)
- missing components of the system (e.g., x_1 of Lorenz-63)
- simple assumptions (linearity, Gaussianity, constant operators)



Conclusions and perspectives

Key messages:

- fruitful combination of DA + ML
- inference of latent variables (interesting physical meaning)
- precise and reliable probabilistic forecasts

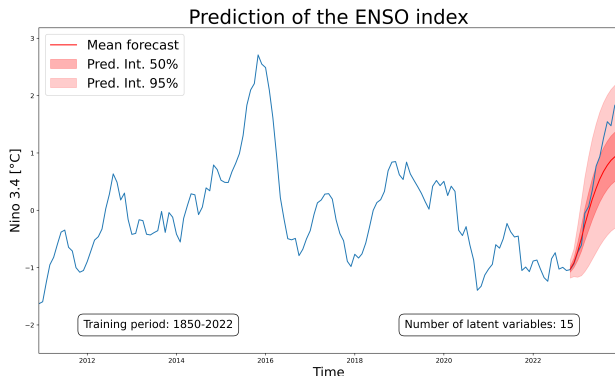


Source: Brajard et al. 2020, Journal of Computational Science

Conclusions and perspectives

Perspectives:

- application to climate indices (e.g., ENSO, AMO, NAO, etc.)
- application to high-dimensional data
- learn time-dependent $\mathbf{M}(t)$ and $\mathbf{Q}(t)$ operators



ありがとうございます (arigatō gozaimasu)!

Interested in this topic? Collaborations are welcome!

Contact:

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- www.tandeo.wordpress.com

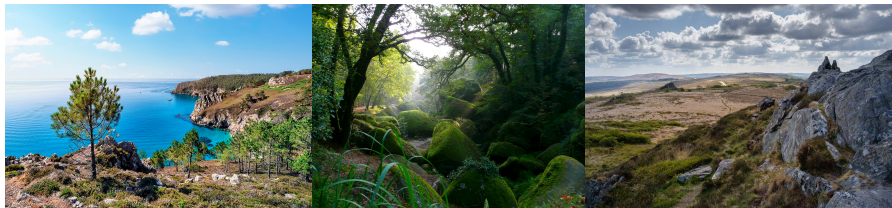


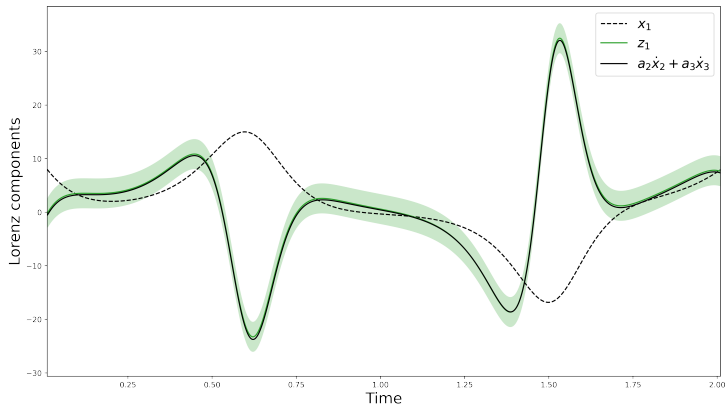
Figure: Nice places to visit near Brest, Bretagne, France

Meaning of z_1

Meaning of z_1 :

- revealed by **symbolic regression**
- between z_1 and usual transformations of x_2 and x_3

z_1	x_2	x_3	x_2x_3	x_2^2	x_3^2	$\sqrt{x_2}$	$\sqrt{x_3}$...	\dot{x}_2	\dot{x}_3
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Link between latent variables and x_1

Expression of z_1 :

$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

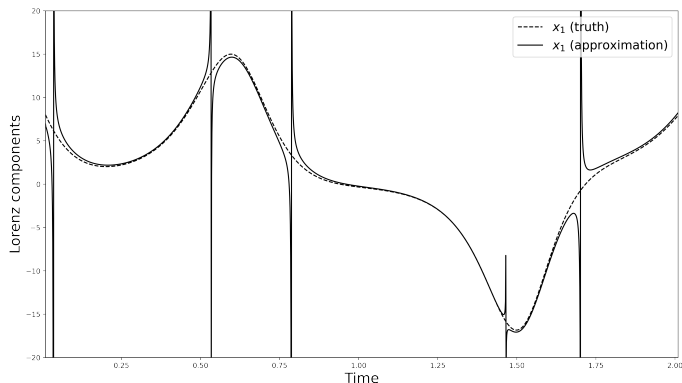
Lorenz-63 system:

$$\dot{x}_2 = x_1(\rho - x_3) - x_2$$

$$\dot{x}_3 = x_1 x_2 - \beta x_3$$

Approximation of x_1 :

$$\hat{x}_1 = \frac{z_1 + a_2 x_2 + a_3 \beta x_3}{a_2 \rho - a_2 x_3 + a_3 x_2}$$

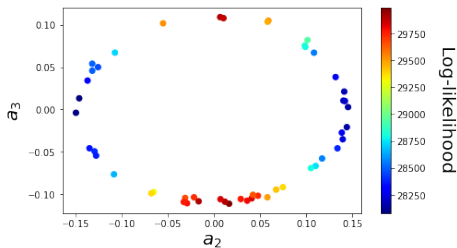
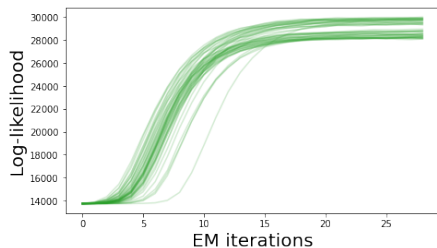


$\Rightarrow x_1$ is partially retrieved (division by zero in specific regions)

Non-unique solution

Meaning of z_1 :

$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$



⇒ **two clusters** of solutions ($a_2 \approx 0$ and $a_3 \approx 0$)

⇒ x_3 **more important** than x_2 in the Lorenz-63 system