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Pierre Tandeo

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# Data-driven identification and reconstruction of partially observed dynamical systems

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IMT Atlantique, Brest, France  
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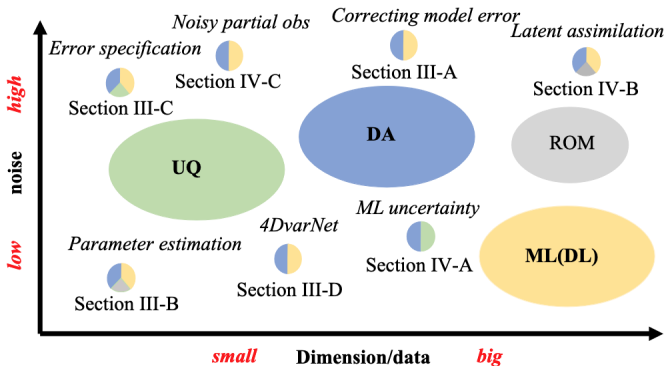




# DA + ML + UQ: a quick overview<sup>1</sup>

## Context:

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



<sup>1</sup>Cheng 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  $p(\mathbf{x}|\mathbf{y})$

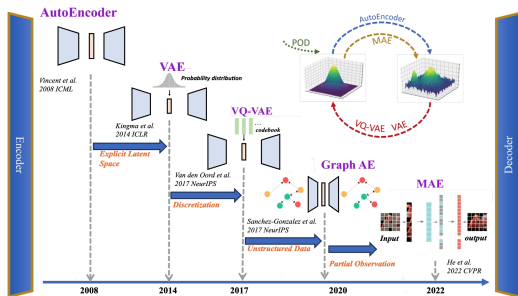
# DA + ML + UQ: a quick overview

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

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

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

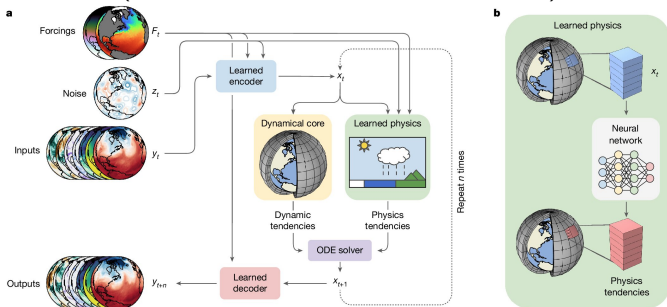
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$$\mathbf{x}(t + dt) = \mathcal{M}(\mathbf{x}(t), \boldsymbol{\eta}(t))$$

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

Dynamical operator ( $\mathcal{M}$ ):

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



Source: Kochkov et al. 2024, Nature

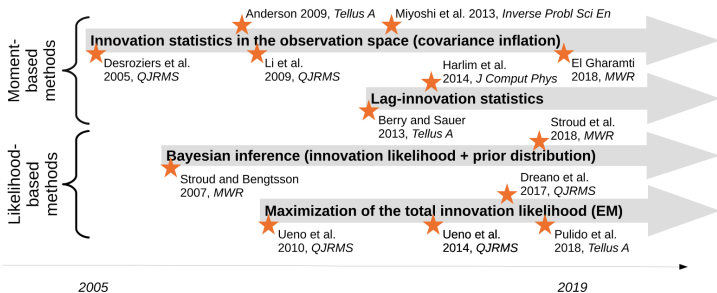
# DA + ML + UQ: a quick overview

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

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

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

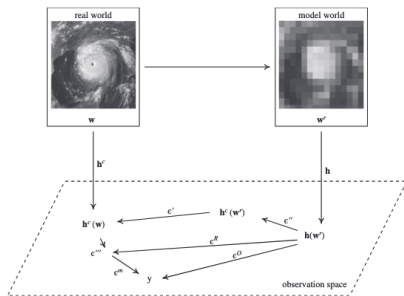
# DA + ML + UQ: a quick overview

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

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

Observation operator ( $\mathcal{H}$ ):

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



Source: Janjić et al. 2018, QJRMS

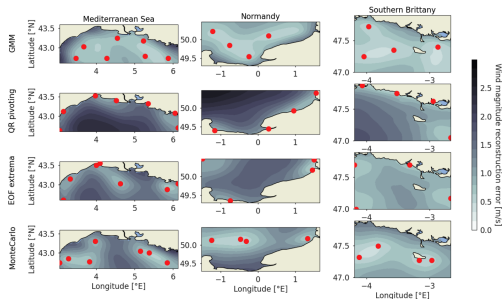
# DA + ML + UQ: a quick overview

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

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

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

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



Source: Marcille et al. 2023, Wind Energy Science

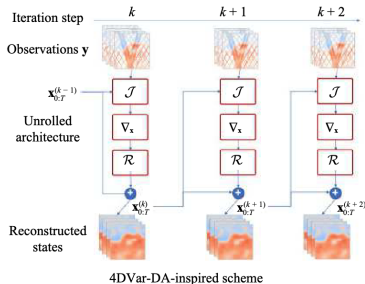
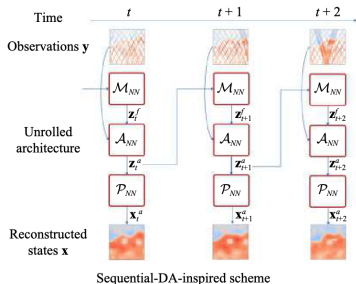
# DA + ML + UQ: a quick overview

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

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

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 + UQ<sup>1</sup>

## 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

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

# A simple combination of DA + ML + UQ<sup>1</sup>

## General framework:

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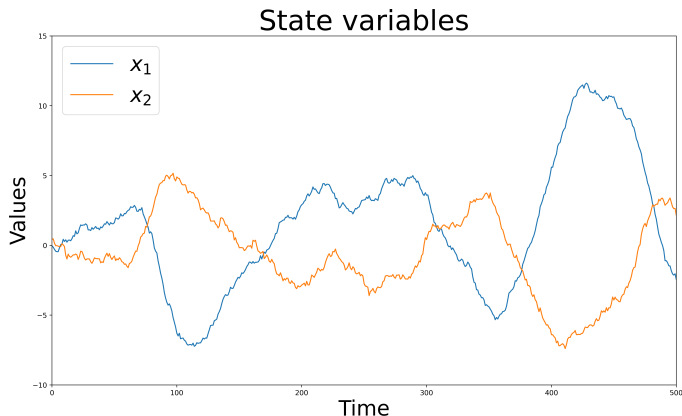
## Goal:

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

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

# Classic approach: Kalman + EM



State-space model:

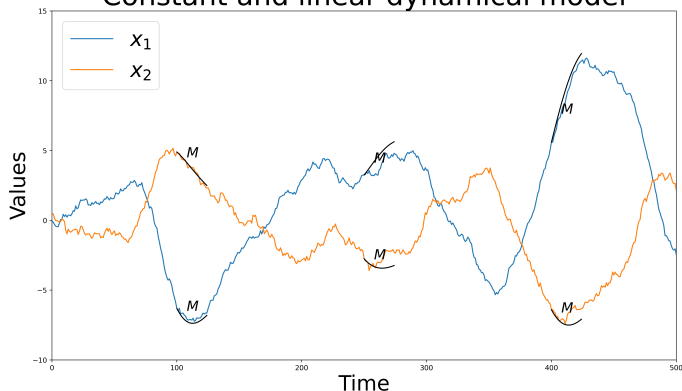
Estimate  $\mathbf{x}(0), \dots, \mathbf{x}(T)$

Variables and matrices:

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

# Classic approach: Kalman + EM

## Constant and linear dynamical model

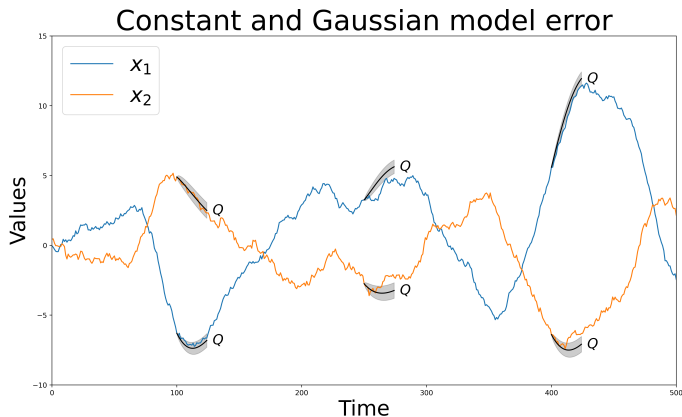


State-space model:  
 $\mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t)$

Variables and matrices:

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

# Classic approach: Kalman + EM



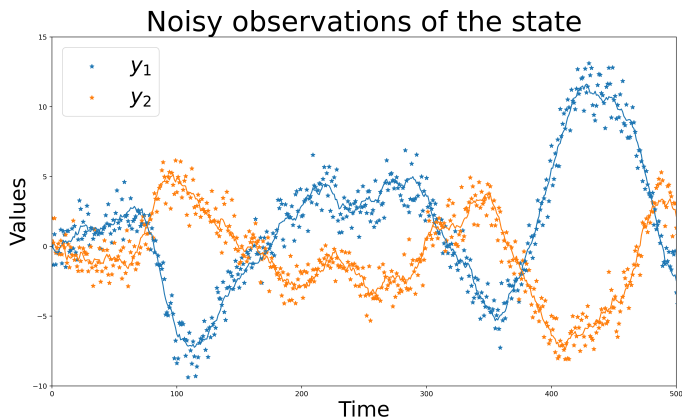
State-space model:

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

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:

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

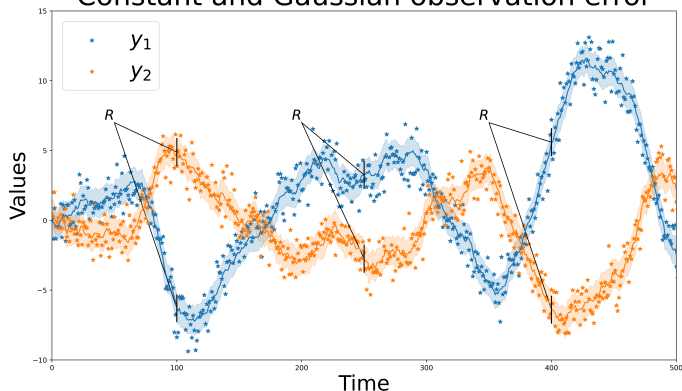
$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t)$$

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:

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

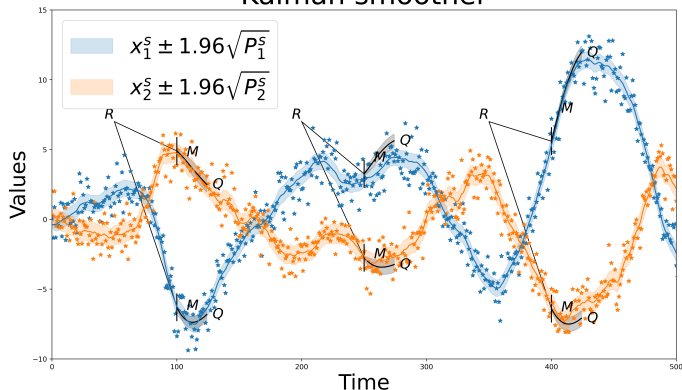
$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$$

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:

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

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

$\Rightarrow$  Kalman smoother

Variables and matrices:

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

$\Rightarrow$  EM algorithm



# The Expectation-Maximization algorithm<sup>1</sup>

Initialization: **M, Q, R**

---

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

# The Expectation-Maximization algorithm<sup>1</sup>

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

---

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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

---

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# The Expectation-Maximization algorithm<sup>1</sup>

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

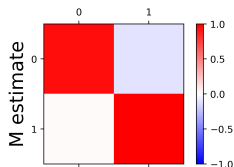
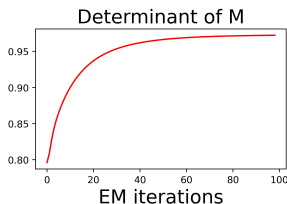
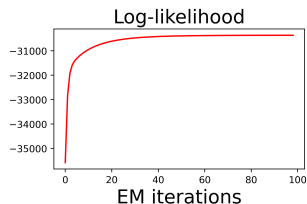
Expectation (DA step):

- 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  $\mathcal{L}(\mathbf{y})$



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

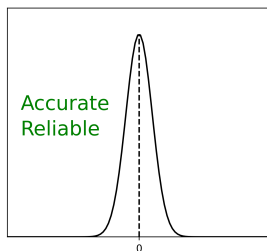
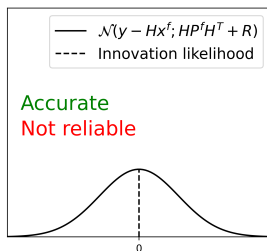
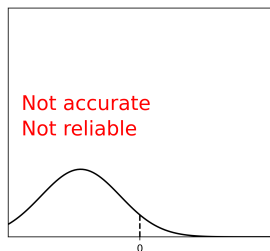
## The innovation likelihood $\mathcal{L}(\mathbf{y})$

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

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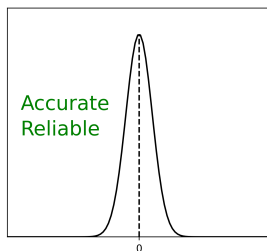
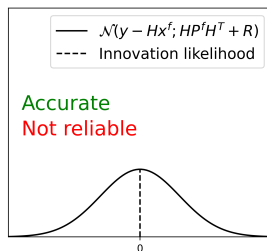
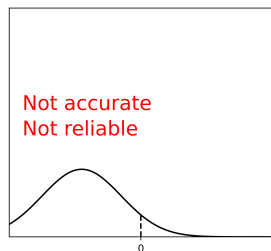
Graphical representation of the innovation likelihood:



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

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Graphical representation of the innovation likelihood:

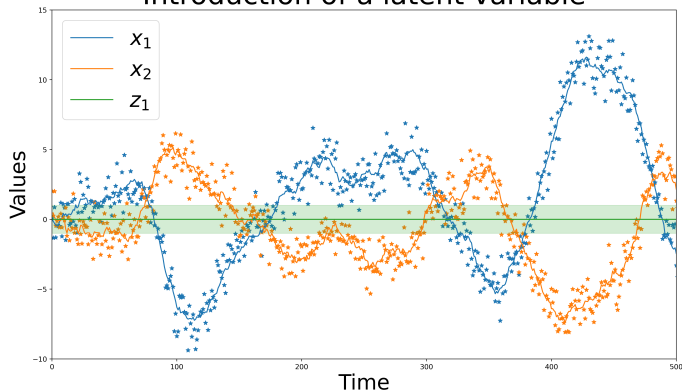


$\mathcal{L}(\mathbf{y})$  depends on  $\mathbf{M}$ ,  $\mathbf{Q}$ ,  $\mathbf{R}$ :

- $\mathbf{x}^f(t) = \mathbf{M}\mathbf{x}^a(t-1) \rightarrow$  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  $\mathbf{x} = [x_1, x_2, z_1]$

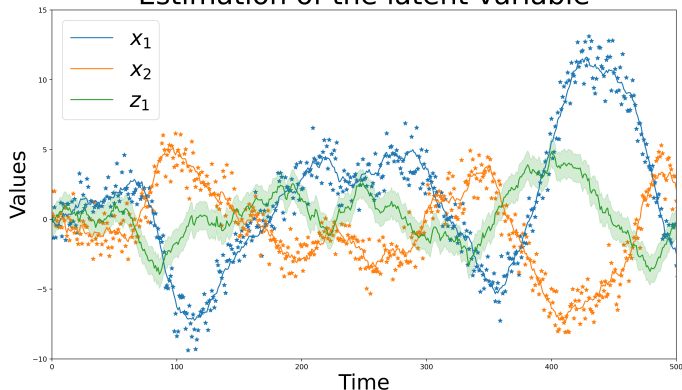
$\mathbf{M}$  and  $\mathbf{Q}$  are  $3 \times 3$

$\mathbf{R}$  is  $2 \times 2$



# Proposed approach: Kalman + EM + augmented state

## Estimation of the latent variable



State-space model:

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

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

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

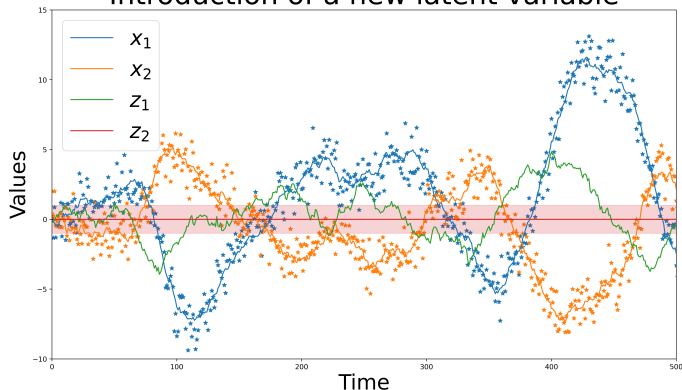
Variables and matrices:

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:

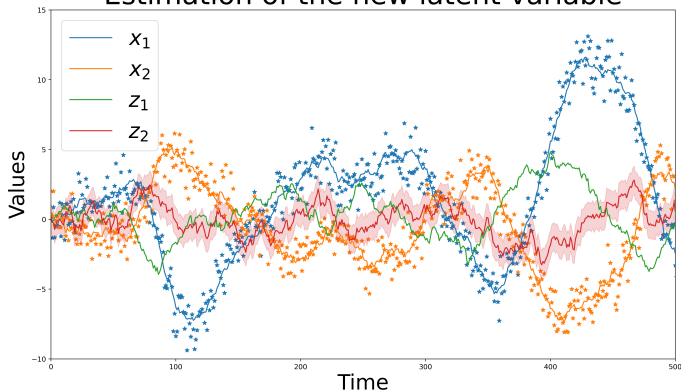
New state  $\mathbf{x} = [x_1, x_2, z_1, z_2]$

$\mathbf{M}$  and  $\mathbf{Q}$  are  $4 \times 4$

$\mathbf{R}$  is  $2 \times 2$

# 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:

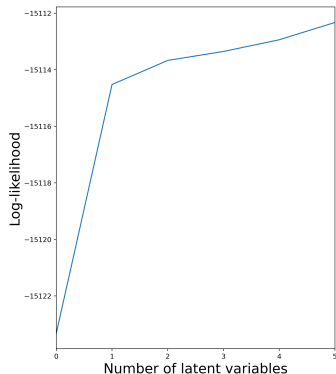
Estimate  $\hat{\mathbf{M}}, \hat{\mathbf{Q}}, \hat{\mathbf{R}}$

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

# Main scientific questions

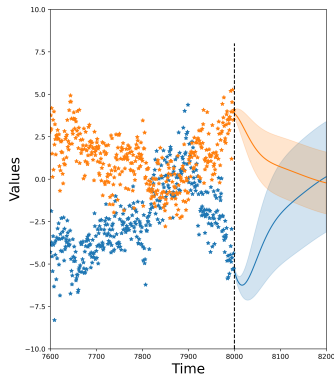
## Latent variables:

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

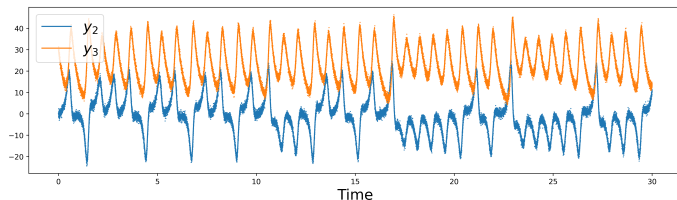


## Quality of the forecasts:

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



# Application to Lorenz-63: formulation and OSSE



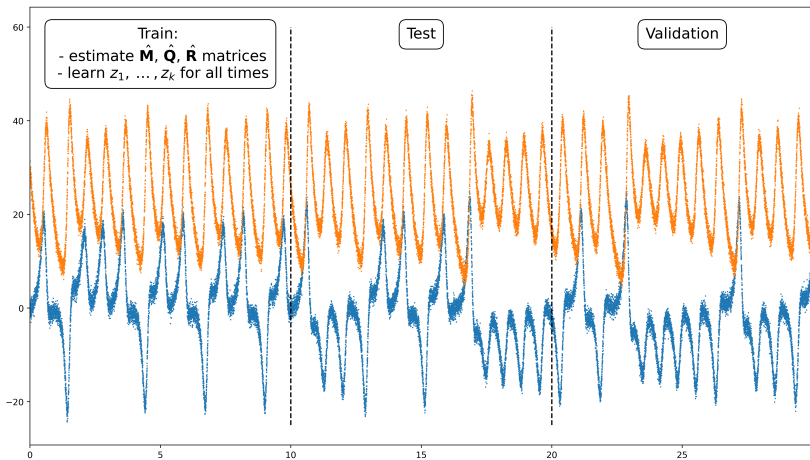
## Observations, state, and latent variables:

- $\mathbf{y} = [y_2, y_3]$  → **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

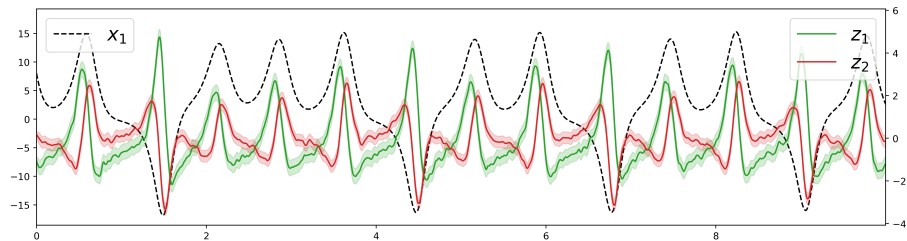


Time series are divided in three parts:

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

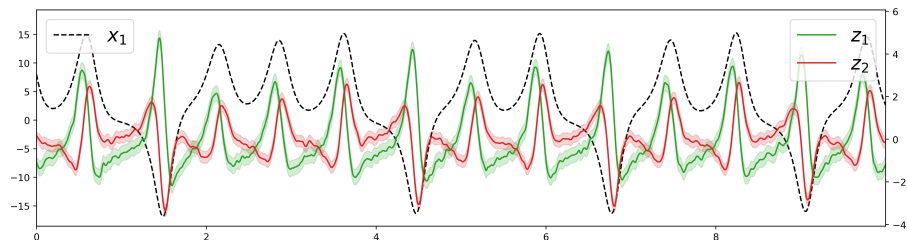
# Estimation and meaning of the latent variables

## Estimation of $z_1$ and $z_2$ :



# Estimation and meaning of the latent variables

## Estimation of $z_1$ and $z_2$ :



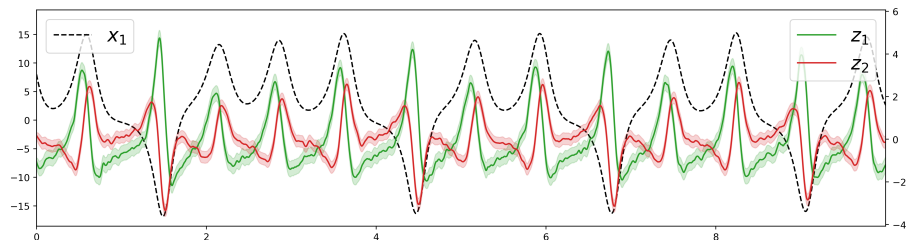
## Meaning of $z_1$ :

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



# Estimation and meaning of the latent variables

## Estimation of $z_1$ and $z_2$ :



## Meaning of $z_1$ :

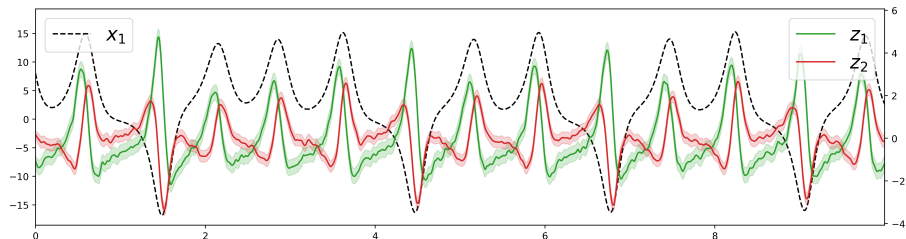
$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

## 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 $z_1$ :

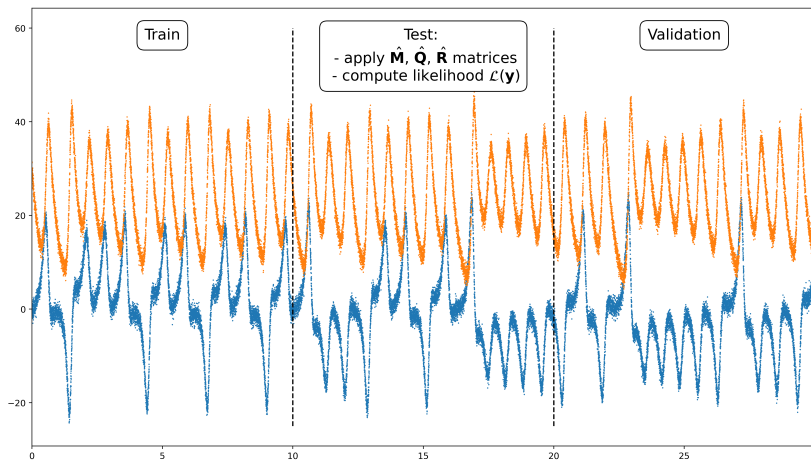
$$z_1 = a_2 \dot{x}_2 + a_3 \dot{x}_3$$

## 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  $x_3$

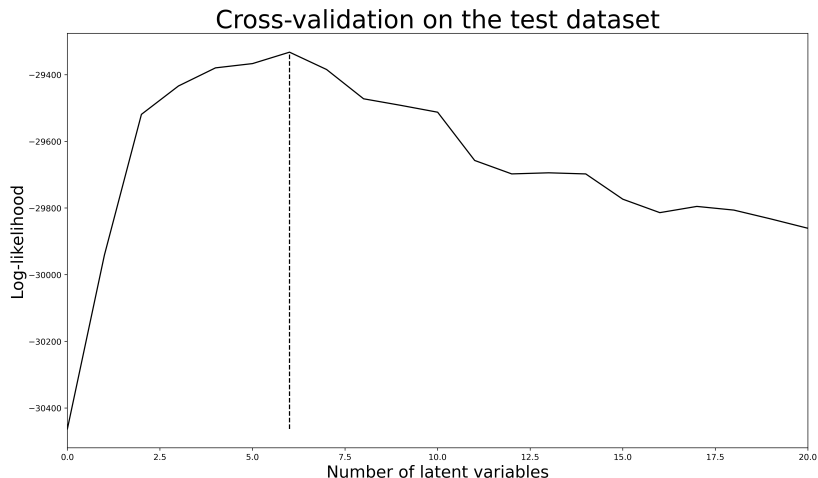
# Number of latent variables to retain



Different models are tested:

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

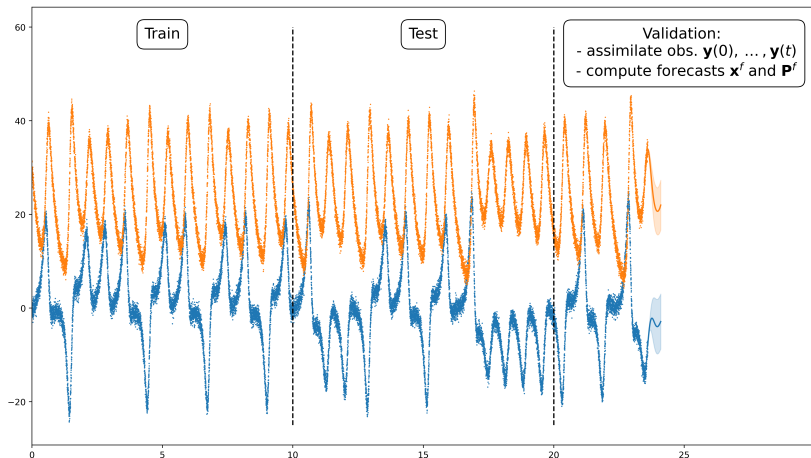
# Number of latent variables to retain



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



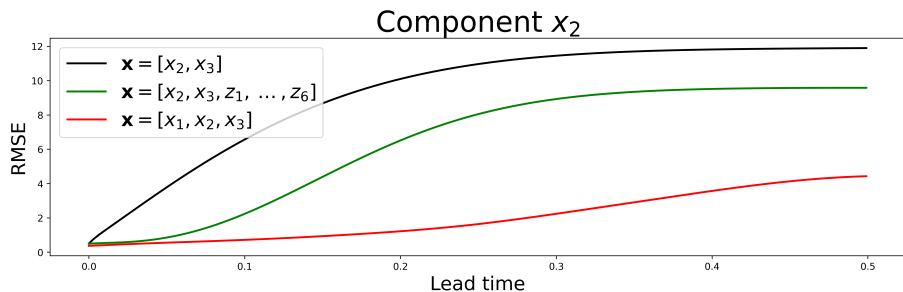
Recursive predictions, starting from an initial time  $t$ :

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

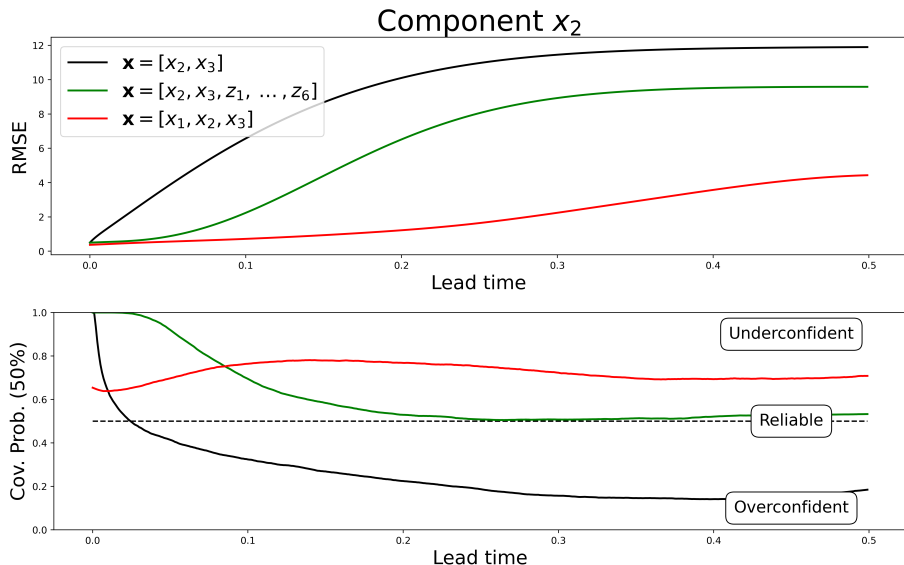
$$\text{Cov}[\mathbf{x}_{t+1} | \mathbf{y}_1, \dots, \mathbf{y}_t] = \mathbf{M}\text{Cov}[\mathbf{x}_t | \mathbf{y}_1, \dots, \mathbf{y}_t]\mathbf{M}^T + \mathbf{Q}$$

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

# Performance metrics (data- VS model-driven)



# Performance metrics (data- VS model-driven)

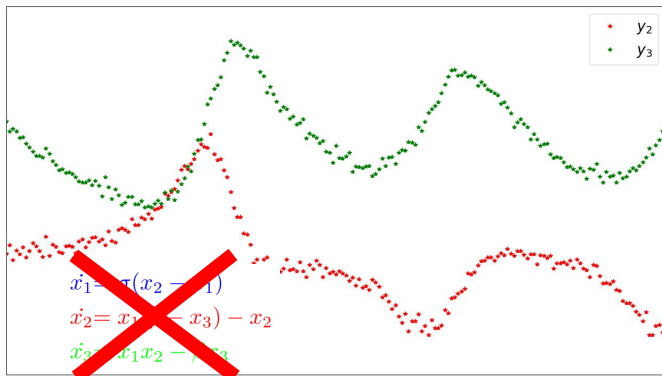




# Conclusions and perspectives

## Context:

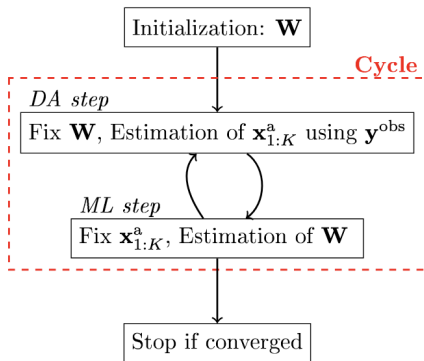
- pure data-driven predictions (i.e., without physical equations)
- missing components of the system (e.g.,  $x_1$  of Lorenz-63)
- simple assumptions (linearity, Gaussianity, constant operators)



# Conclusions and perspectives

## Key messages:

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

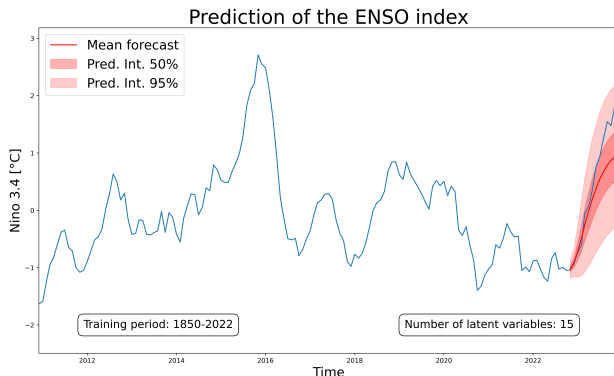


Source: Brajard et al. 2020, Journal of Computational Science

# 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

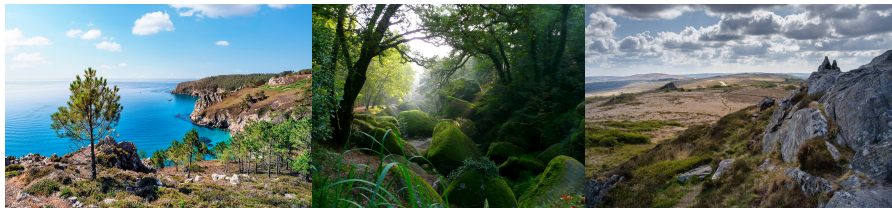


ありがとうございます (arigatō gozaimasu)!

**Interested in this topic? Collaborations are welcome!**

Contact:

- [pierre.tandeo@imt-atlantique.fr](mailto:pierre.tandeo@imt-atlantique.fr)
- [www.tandeo.wordpress.com](http://www.tandeo.wordpress.com)



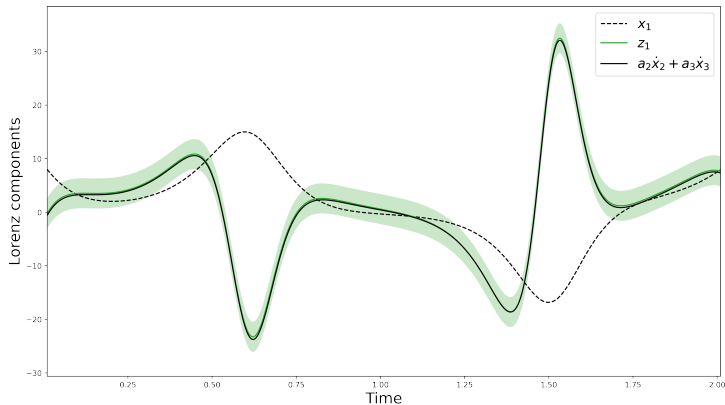
**Figure:** Nice places to visit near Brest, Bretagne, France

# 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  $z_1$ :

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

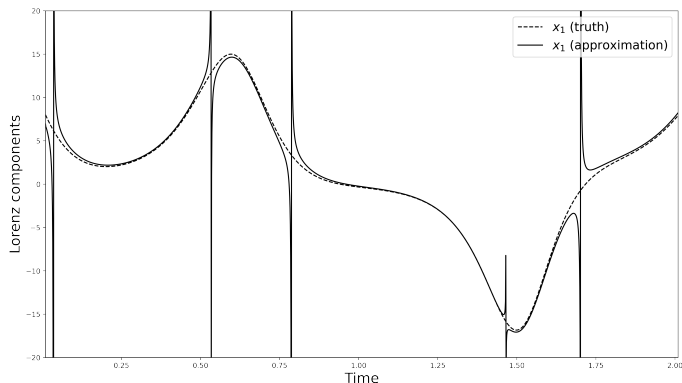
Lorenz-63 system:

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

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

Approximation of  $x_1$ :

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

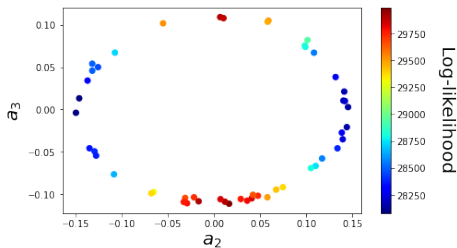
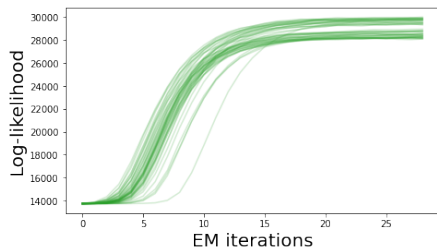


$\Rightarrow x_1$  is partially retrieved (division by zero in specific regions)

# 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