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Pierre Tandeo

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Data-driven identification and reconstruction of partially observed dynamical systems

Dr. Pierre Tandeo, associate professor

IMT Atlantique, Brest, France RIKEN Cluster for Pioneering Research, Kobe, Japan

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$DA + ML + UQ$: a quick overview¹

Context:

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

 1 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:

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

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

Machine learning appears everywhere:

- \bullet state **x** and observations **y**
- operators M and H
- \bullet errors η and ϵ
- inversion of the system $p(x|y)$

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

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

State of the system (x) :

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

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

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

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

Dynamical operator (M) :

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

Source: Kochkov et al. 2024, Nature

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

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

Model and observation errors (η and ϵ):

• innovation statistics, inflation methods, statistical approaches, NN • joint estimation of error covariances Q and R

Source: Tandeo et al. 2020, Monthly Weather Review

\overline{DA} + ML $\overline{+}$ 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

\overline{DA} + ML $\overline{+}$ UQ: a quick overview

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

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

Noisy and partial observations (y) :

• aggregation, fusion, and data exclusion o optimal sampling of the observations

Source: Marcille et al. 2023, Wind Energy Science

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

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

Full system resolution $p(x|y)$:

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

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

General framework:

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

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

Proposed framework:

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

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

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

General framework:

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

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

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

State variables ī. x_1 x_2 10 Values -10 200 100 300 400 Time

State-space model: Estimate $x(0), \ldots, x(T)$

Variables and matrices: $x = [x_1, x_2]$

 $\overline{\mathbf{x}(t+1)} = \mathbf{M}\mathbf{x}(t)$

Variables and matrices: $M =$ $\vert \cdot$ $\begin{bmatrix} . & . \ . & . \end{bmatrix}$

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ Variables and matrices: $\boldsymbol{\eta}(t) \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \ \ \mathbf{Q} = \begin{bmatrix} \cdot & \cdot \ \cdot \end{bmatrix}$

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ $y(t) = Hx(t)$

$$
\begin{aligned}\n\text{Variables and matrices:} \\
\mathbf{y} = [y_1, y_2], \ \mathbf{H} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\n\end{aligned}
$$

State-space model:

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

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

$$
\frac{\text{Variables and matrices:}}{\epsilon(t) \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \ \ \mathbf{R} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}}
$$

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$

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

Variables and matrices: $\hat{\mathsf{M}}, \hat{\mathsf{Q}}, \hat{\mathsf{R}} = \arg\!\max \mathcal{L}(\mathsf{y})$ M,Q,R \Rightarrow EM algorithm

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

Initialization: M, Q, R

Expectation (DA step):

- \bullet fix M, Q, R
- estimation of $\mathsf{x}_{0:\mathcal{T}}^s$ and $\mathsf{P}_{0:\mathcal{T}}^s$
- ⇒ Kalman smoother

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

Initialization: M, Q, R

Expectation (DA step):

- \bullet fix M, Q, R
- estimation of $\mathsf{x}_{0:\mathcal{T}}^s$ and $\mathsf{P}_{0:\mathcal{T}}^s$
- ⇒ Kalman smoother

Maximization (ML step):

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

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

Initialization: M, Q, R

Expectation (DA step):

- \bullet fix M, Q, R
- estimation of $\mathsf{x}_{0:\mathcal{T}}^s$ and $\mathsf{P}_{0:\mathcal{T}}^s$
- ⇒ Kalman smoother

Maximization (ML step):

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

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

Graphical representation of the innovation likelihood:

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

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

Introduction of a latent variable

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ $\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$ $H =$ \lceil 1 0 0 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$

Variables and matrices: Augmented state $\mathbf{x} = [x_1, x_2, z_1]$ **M** and **Q** are 3×3 **R** is 2×2

Estimation of the latent variable

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ $\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$ $H =$ \lceil 1 0 0 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$

Variables and matrices: Estimate $\hat{\mathsf{M}}, \hat{\mathsf{Q}}, \hat{\mathsf{R}}$ Estimate $z_1(0), \ldots, z_1(T)$

Introduction of a new latent variable

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ $\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$ $H =$ \lceil 1 0 0 0 $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$

Variables and matrices: New state $x = [x_1, x_2, z_1, z_2]$ **M** and **Q** are 4×4 **R** is 2×2

Estimation of the new latent variable

State-space model: $\mathsf{x}(t+1) = \mathsf{M}\mathsf{x}(t) + \mathsf{Q}^{1/2}\eta(t)$ $\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t)$ $H =$ \lceil $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$

Variables and matrices: Estimate $\hat{\mathsf{M}}$, $\hat{\mathsf{Q}}$, $\hat{\mathsf{R}}$ Estimate $z_2(0), \ldots, z_2(T)$

Main scientific questions

Latent variables:

- how many are needed?
- what is there 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:

- $y = [y_2, y_3] \rightarrow$ partial observations of the system
- $x = [x_2, x_3, z] \rightarrow$ augmented state with latent variables z
- $z = [z_1, \ldots, z_k] \rightarrow$ latent variables

OSSE:

- \bullet dt = 0.001 \rightarrow observation sampling
- $Var(\epsilon) = 1 \rightarrow$ observation error variance

Estimation of \hat{M} , \hat{Q} , \hat{R} and z_1, \ldots, 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 of z_1 and z_2 :

Estimation of z_1 and z_2 :

Meaning of z_1 :

$$
z_1=a_2\dot{x_2}+a_3\dot{x_3}
$$

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 :

$$
z_2 = b_1 \dot{z_1} + b_2 \dot{x_2} + b_3 \dot{x_3}
$$

= $b_2 \dot{x_2} + b_3 \dot{x_3} + b_1 a_2 \ddot{x_2} + b_1 a_3 \ddot{x_3}$

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 :

$$
z_2 = b_1 \dot{z_1} + b_2 \dot{x_2} + b_3 \dot{x_3}
$$

= $b_2 \dot{x_2} + b_3 \dot{x_3} + b_1 a_2 \ddot{x_2} + b_1 a_3 \ddot{x_3}$

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

Number of latent variables to retain

Different models are tested:

- from $x = [x_2, x_3, z_1]$
- 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 ${\bf x} = [{\bf x}_2, {\bf x}_3, {\bf z}_1, \ldots, {\bf z}_6]$
- six latent variables are necessary

Probabilistic forecasts using testing data

Recursive predictions, starting from an initial time t:

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

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

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

Performance metrics (data- VS model-driven)

Performance metrics (data- VS model-driven)

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:

- \bullet 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 $M(t)$ and $Q(t)$ operators

Prediction of the ENSO index

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>
- <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
- \bullet between z_1 and usual transformations of x_2 and x_3

Link between latent variables and x_1

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

Non-unique solution

Meaning of z_1 :

$$
z_1=a_2x_2+a_3x_3
$$

 \Rightarrow two clusters of solutions ($a_2 \approx 0$ and $a_3 \approx 0$) \Rightarrow x₃ more important than x₂ in the Lorenz-63 system