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► To cite this version:

Pierre Tandeo. Data-driven identification and reconstruction of partially observed dynamical systems. ISDA 2024 - 10th International Symposium on Data Assimilation, RIKEN, Oct 2024, Kobe, Japan. hal-04764759

HAL Id: hal-04764759 https://imt-atlantique.hal.science/hal-04764759v1

Submitted on 8 Nov 2024

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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:

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

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

Machine learning appears everywhere:

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

$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t), oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t), oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

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

$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t),oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t),oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

Dynamical operator (\mathcal{M}) :

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



$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t),oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t),oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

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

$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t), oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t), oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

Observation operator (\mathcal{H}) :

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



Source: Janjić et al. 2018, QJRMS

$$egin{aligned} \mathsf{x}(t+dt) &= \mathcal{M}\left(\mathsf{x}(t), oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathsf{x}(t), oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

Noisy and partial observations (y):

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



Source: Marcille et al. 2023, Wind Energy Science

$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t), oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t), oldsymbol{\epsilon}(t)
ight) \end{aligned}$$

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

General framework:

 $egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t), oldsymbol{\eta}(t)
ight) \ \mathbf{y}(t) &= \mathcal{H}\left(\mathbf{x}(t), oldsymbol{\epsilon}(t)
ight) \end{aligned}$

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:

$$egin{aligned} \mathbf{x}(t+dt) &= \mathcal{M}\left(\mathbf{x}(t), oldsymbol{\eta}(t)
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<u>Goal:</u>

- 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 x_1 *x*₂ 10 Values -10100 200 400 ò 300 Time

 $\frac{\text{State-space model:}}{\text{Estimate } \mathbf{x}(0), \dots, \mathbf{x}(\mathcal{T})}$

 $\frac{\text{Variables and matrices:}}{\mathbf{x} = [x_1, x_2]}$



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

 $\frac{\text{Variables and matrices:}}{\mathbf{M} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}}$



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

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



$$\begin{split} & \frac{\text{State-space model:}}{\textbf{x}(t+1) = \textbf{M}\textbf{x}(t) + \textbf{Q}^{1/2}\boldsymbol{\eta}(t)} \\ & \textbf{y}(t) = \textbf{H}\textbf{x}(t) \end{split}$$

Variables and matrices:

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



State-space model:

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

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

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



 $\begin{array}{l} \frac{\text{State-space model:}}{\textbf{x}(t+1) = \textbf{M}\textbf{x}(t) + \textbf{Q}^{1/2}\boldsymbol{\eta}(t)} \\ \textbf{y}(t) = \textbf{H}\textbf{x}(t) + \textbf{R}^{1/2}\boldsymbol{\epsilon}(t) \\ \Rightarrow \text{ Kalman smoother} \end{array}$

 $\begin{array}{l} & \underbrace{\text{Variables and matrices:}} \\ \hat{M}, \hat{Q}, \hat{R} = \mathop{\mathrm{argmax}}_{M,Q,R} \mathcal{L}\left(y \right) \\ \Rightarrow \text{EM algorithm} \end{array}$

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):

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

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

Initialization: M, Q, R

Expectation (DA step):

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

Maximization (ML step):

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

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

Maximization (ML step):

- fix $\mathbf{x}_{0:T}^{s}$ and $\mathbf{P}_{0:T}^{s}$
- estimation of M, Q, R
- ullet \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 $\mathcal{L}(\mathbf{y})$

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

Graphical representation of the innovation likelihood:



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

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ight)$$

Graphical representation of the innovation likelihood:



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

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

Introduction of a latent variable



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

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

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

Estimation of the latent variable



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

 $\frac{\text{Variables and matrices:}}{\text{Estimate } \hat{\mathbf{M}}, \hat{\mathbf{Q}}, \hat{\mathbf{R}}}$ Estimate $z_1(0), \dots, z_1(\mathcal{T})$

Introduction of a new latent variable



State-space model:

$$\begin{aligned} \mathbf{x}(t+1) &= \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2}\boldsymbol{\eta}(t) \\ \mathbf{y}(t) &= \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2}\boldsymbol{\epsilon}(t) \\ \mathbf{H} &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \end{aligned}$$

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

Estimation of the new latent variable



State-space model:

$$egin{aligned} & \mathbf{x}(t+1) = \mathbf{M}\mathbf{x}(t) + \mathbf{Q}^{1/2} \eta(t) \ & \mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{R}^{1/2} \epsilon(t) \ & \mathbf{H} = egin{bmatrix} 1 & 0 & 0 \ 0 & 1 & 0 & 0 \end{bmatrix} \end{aligned}$$

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 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:

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

OSSE:

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

Estimation of $\hat{\mathbf{M}}$, $\hat{\mathbf{Q}}$, $\hat{\mathbf{R}}$ 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 $\mathbf{x} = [\mathbf{x}_2, \mathbf{x}_3, \mathbf{z}_1]$
- to $\textbf{x} = [\textbf{x}_2, \textbf{x}_3, \textbf{z}_1, \dots, \textbf{z}_{20}]$

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*:

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

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 $\mathbf{M}(t)$ and $\mathbf{Q}(t)$ operators



Prediction of the FNSO 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
- between z_1 and usual transformations of x_2 and x_3



Link between latent variables and x_1



 \Rightarrow x₁ 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