Estimating Dynamical Models using Machine Learning and Data Assimilation

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Data assimilation (graphical representation)



Principle:

- mix between a dynamical model and observations
- taking into account their uncertainties

<u>Goal:</u>

- to estimate accurately the initial condition
- in order to get the **best forecast**

State-space model:

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \eta$$

 $\mathbf{y} = h(\mathbf{x}) + \epsilon$

- $\mathbf{y} \rightarrow \text{observations}$ (what is provided)
- $\mathbf{x} \rightarrow$ state (what is unknown)
- *h* → link between **x** and **y**
- $f \rightarrow$ dynamical model
- η and $\epsilon
 ightarrow$ additive Gaussian errors

Data assimilation

State-space model:

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \eta$$
$$\mathbf{y} = h(\mathbf{x}) + \epsilon$$



Source: [Carrassi et al., 2018]

Examples of dynamical models

The Lorenz system:

$$\dot{x_1} = \sigma(x_2 - x_1)$$

 $\dot{x_2} = x_1(\rho - x_3) - x_2$
 $\dot{x_3} = x_1x_2 - \beta x_3$

with x_1 the rate of convection, x_2 the horizontal temperature gradient, and x_3 the vertical temperature gradient.



Examples of dynamical models

Lotka–Volterra equations:

$$\dot{x_1} = \alpha x_1 - \beta x_1 x_2$$
$$\dot{x_2} = \delta x_1 x_2 - \gamma x_2$$

with x_1 the **preys** and x_2 the **predators**.



Dynamical model f:

$$\dot{\mathbf{x}} = f(\mathbf{x})$$

Questions:

- when equations are available, is it possible to improve f?
- when equations are not available, is it possible to learn f?

Answers:

- yes, using available observations (i.e., noisy and partial)
- combining data assimilation and machine learning

Combine DA and ML to estimate f

Different case studies:

• *f* is available but **parameters are unknown**

I is approximated using a catalog of the full system

$$\dot{\mathbf{x}} = \tilde{f}(\mathbf{x})$$

§ f is approximated using a catalog of the partial system

$$\dot{\mathbf{x}} = \tilde{f}(\mathbf{x})$$

State-space model (with augmented state) :

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \boldsymbol{\eta}$$

 $\mathbf{y} = h(\mathbf{x}) + \boldsymbol{\epsilon}$

- $\mathbf{x} = [\mathbf{x}, \boldsymbol{\theta}] \rightarrow$ augmented state
- heta
 ightarrow unknown parameters
- f
 ightarrow dynamical model for x and $oldsymbol{ heta}$
- see [Ruiz et al., 2013] for more details

Example of the Lorenz system:

- $\mathbf{x} = [x_1, x_2, x_3, \sigma, \rho, \beta]$
- f corresponds to the system of 3 ODEs to predict [x₁, x₂, x₃]
- f also corresponds to random walks for $[\sigma, \rho, \beta]$



Example of Lotka-Volterra:

- $\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, \alpha, \beta, \gamma, \delta]$
- f corresponds to the system of 2 ODEs to predict $[x_1, x_2]$
- $\bullet~f$ also corresponds to random walks for $[\alpha,\beta,\gamma,\delta]$



Example of Lotka-Volterra:

- x₁ and x₂ are observed
- $\alpha,~\beta,~\gamma,~{\rm and}~\delta$ are initialized using random values





State-space model (with emulated model) :

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \boldsymbol{\eta}$$

 $\mathbf{y} = h(\mathbf{x}) + \boldsymbol{\epsilon}$

- $f = \tilde{f} \rightarrow$ emulated dynamical model
- $\tilde{f} \rightarrow$ build using a **full catalog** and **regression methods**

More details about the Analog Data Assimilation (AnDA):

f is learned using a catalog of analogs and successors
 forecasts from *f* are compared to observations



Source: [Tandeo et al., 2015] and [Lguensat et al., 2017]

Example of the Lorenz system:

- \tilde{f} is build using a catalog of $\mathbf{x} = [x_1, x_2, x_3]$
- x₂ is observed, but never x₁ nor x₃



Example of the Hare-Lynx database:

- \tilde{f} is build using a catalog of $\mathbf{x} = [Hare, Lynx]$ until 1907
- after 1907, Lynx are observed, but never Hares





State-space model (with emulated model + augmented state) :

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \boldsymbol{\eta}$$

 $\mathbf{y} = h(\mathbf{x}) + \boldsymbol{\epsilon}$

- $f = \tilde{f} \rightarrow$ emulated dynamical model
- $\tilde{f} \rightarrow$ build using a partial database and regression methods
- $\bullet \ x = [x,z] \rightarrow augmented state with latent variables <math display="inline">z$

Schematic representation of the proposed iterative algorithm:



 \Rightarrow starting from a **Gaussian white noise**, the latent variable automatically adjusts over **iterations**

Example of the Lorenz system:

- $\mathbf{x} = [x_2, x_3, z_1]$
- x_2 and x_3 are observed, but never x_1

Example of the Hare-Lynx database:

- $\mathbf{x} = [Lynx, z]$
- Lynx are observed, but never Hares

Conclusions (presented here):

- a dynamical model *f* can be **improved or learned**
- using observations and appropriate tools (DA and ML)

Important remarks (not presented here):

- estimation of model and observation errors is crucial (see [Tandeo et al., 2020] for a review)
- using optimization algorithms
 - (e.g., descent gradient or Expectation-Maximization)

ありがとうございます (arigatō gozaimasu)!

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Figure: Nice places to visit near Brest, France: Crozon (left), Huelgoat (middle), Monts d'Arrée (right).

Bibliography I



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