Combining Data Assimilation and Machine Learning to emulate a numerical model

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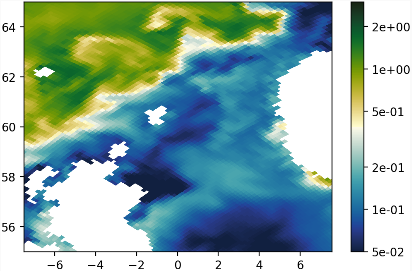
Motivation

Chloropyhll-a (Model)
July 26, 2018



TOPAZ4-ECOSMO forecast

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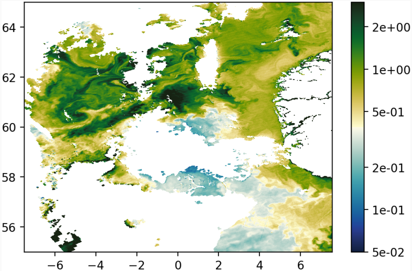

MODIS Aqua

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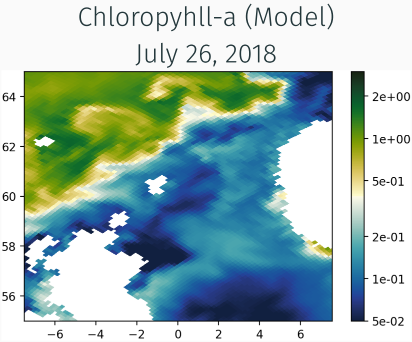

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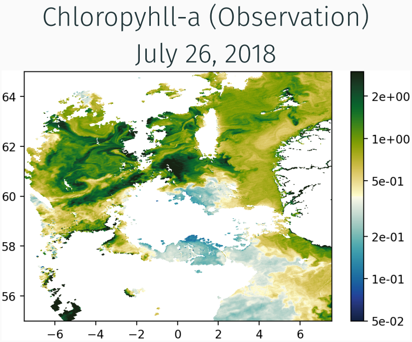

MODIS Aqua

- Unresolved process
- Unknown parameters

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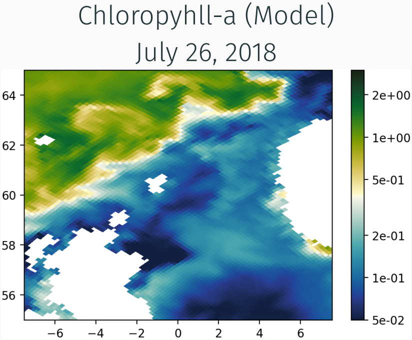

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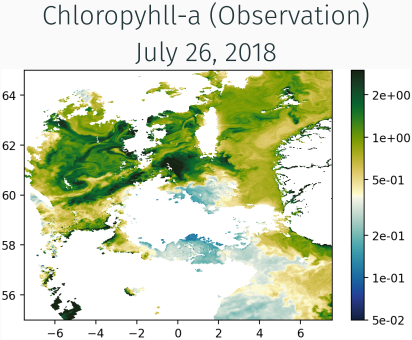

MODIS Aqua

- Sparse
- Noisy

Typology of problems and approaches

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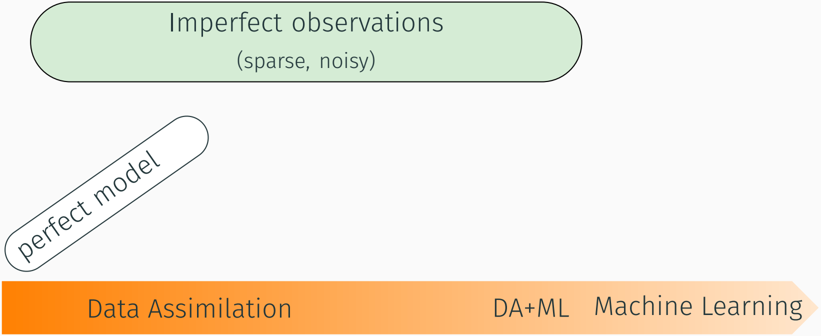

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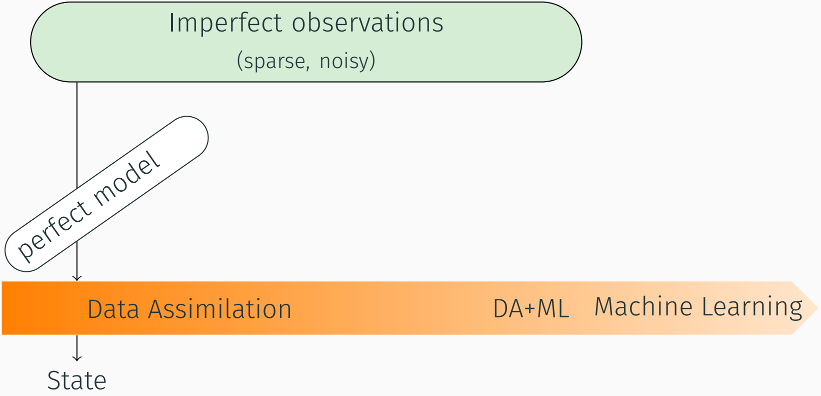

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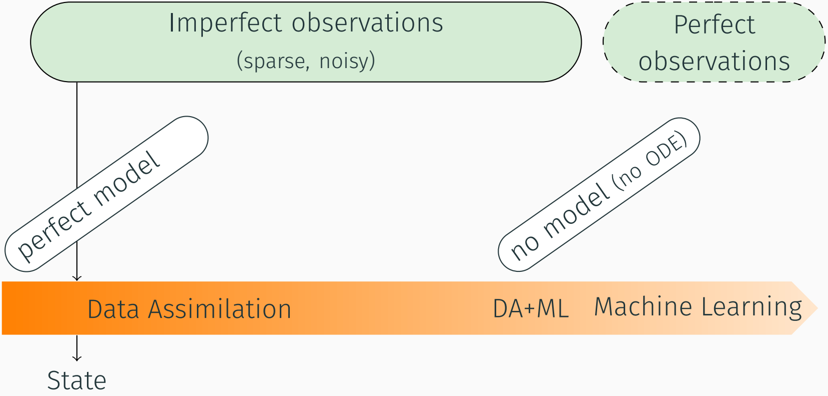

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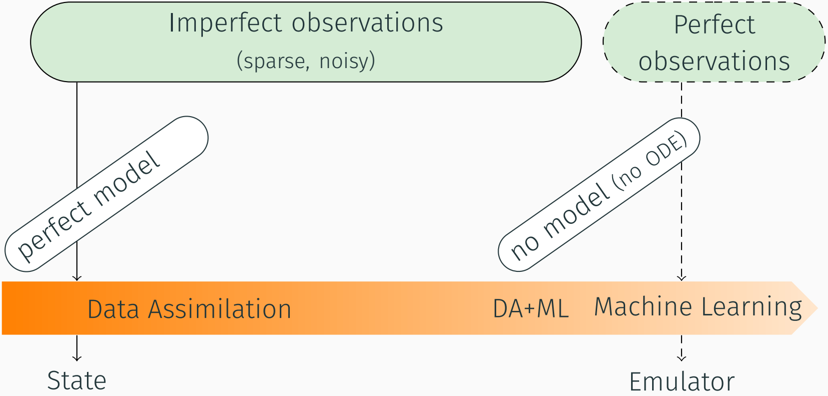

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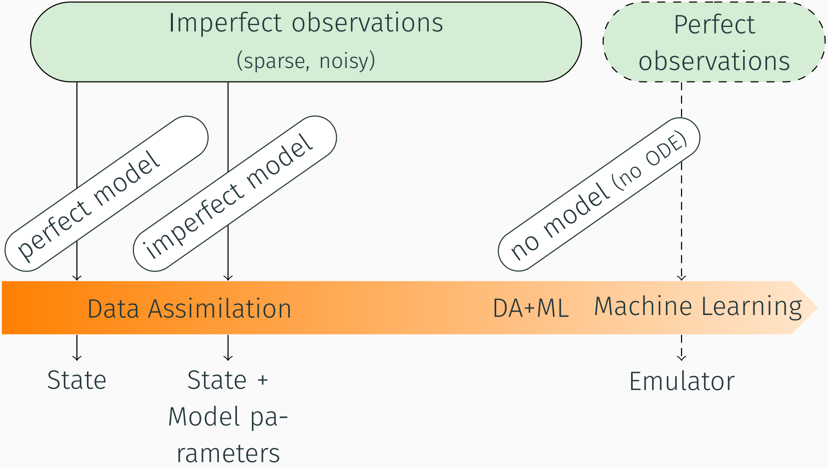

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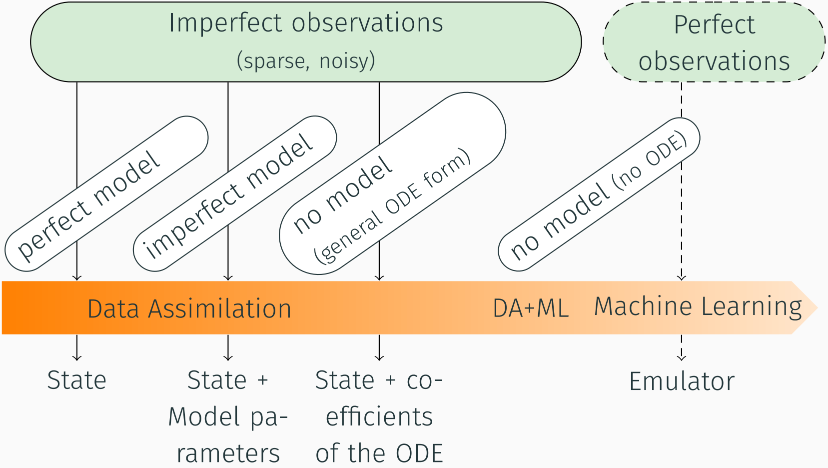

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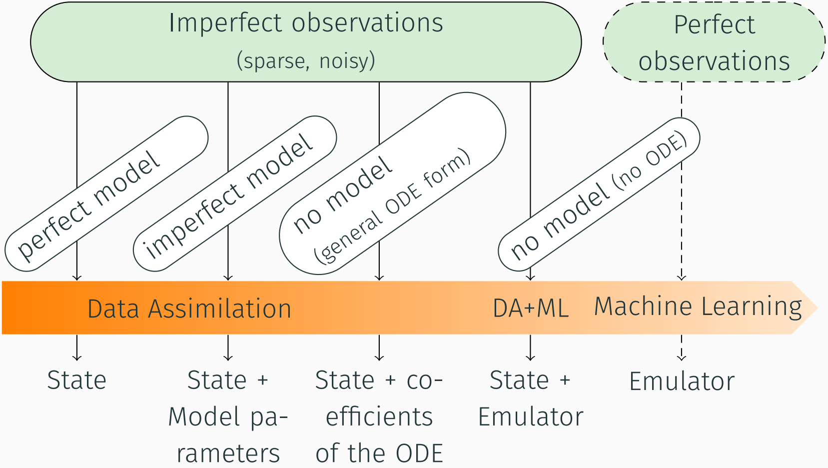

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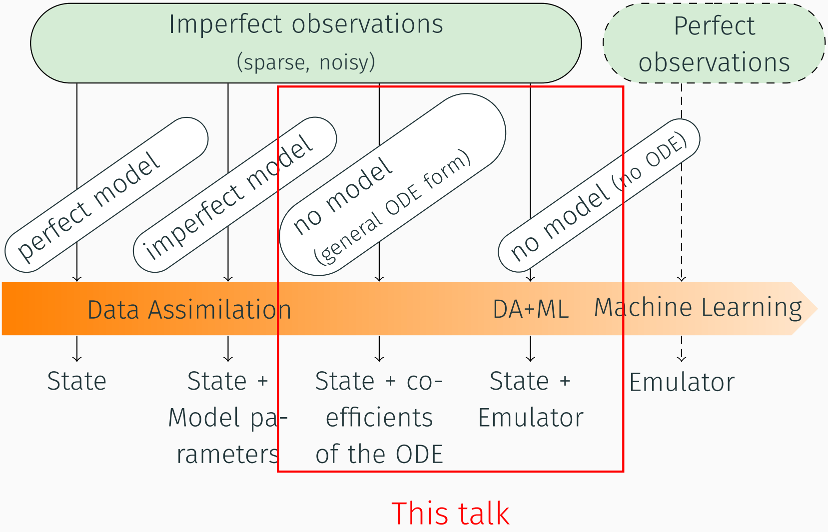

Our Objective:

Producing an accurate and reliable emulator of a numerical model given sparse and noisy observations

Specification of the problem

Data

Multidimensional time series $\mathsf{y}_k^{\mathrm{obs}}$ $(1 \leq k \leq K)$ observed from an underlying dynamical process:

$$\mathsf{y}_k^{\mathrm{obs}} = \mathcal{H}_k(\mathsf{x}_k) + \epsilon_k^{\mathrm{obs}}$$

- $\mathcal{H}_k$ is the known observation operator: $\mathbb{R}^{N_x} \to \mathbb{R}^p$
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Underlying dynamical model:

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Resolvent:

$$\mathsf{x}_{k+1} = \mathsf{x}_k + \int_{t_k}^{t_{k+1}} \phi(\mathsf{x})\,\mathrm{d}t,$$

Two complementary goals

1. Inferring the ODE using **only** DA algorithm [Bocquet et al., 2019]:

$$\frac{\mathrm{d}\mathsf{x}}{\mathrm{d}t} = \phi_{\mathsf{A}}(\mathsf{x}), \qquad \phi_{\mathsf{A}}(\mathsf{x}) = \mathsf{A}\mathsf{r}(\mathsf{x}),$$

where $\mathsf{r}(\mathsf{x}) \in \mathbb{R}^{N_p}$ is specified and $\mathsf{A} \in \mathbb{R}^{N_x \times N_p}$ is to be determined.

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2. Emulation of the resolvent **combining** DA and ML [Brajard et al., 2019]:

$$\mathsf{x}_{k+1} = \mathcal{G}_{\mathsf{W}}(\mathsf{x}_k) + \epsilon_k^{\mathrm{m}},$$

   where $\mathcal{G}_{\mathsf{W}}$ is a neural network parametrized by W and ϵ_k^{m} is a stochastic noise.

First goal: Inferring the ODE using DA

First goal: ODE representation for the surrogate model

Ordinary differential equations (ODEs) representation of the surrogate dynamics

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where

- $\mathsf{A} \in \mathbb{R}^{N_x \times N_p}$ is a matrix of coefficients to be determined.
- $\mathsf{r}(\mathsf{x})$ is a vector of nonlinear regressors of size N_p. For instance, for one-dimensional spatial systems and up to bilinear order:

$$\mathsf{r}(\mathsf{x}) = \left[1, \{x_n\}_{0 \le n < N_x}, \{x_n x_m\}_{0 \le n \le m < N_x}\right].$$

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$N_p = \binom{N_x+1}{2} = \frac{1}{2}(N_x + 1)(N_x + 2).$

$\longrightarrow$ Intractable in high-dimension! Typically, $N_x = \mathcal{O}(10^{6-9})$.

Reducing the number of regressors

Locality

Physical locality of the physics: all multivariate monomials in the ODEs have variables x_n that belong to a stencil, i.e. a local arrangement of grid points around a given node.

In 1D and with a stencil of size $2L+1$, the size of the dense $\mathbf{A}$ is

$$N_x \times N_\mathrm{a} \quad \text{where} \quad N_\mathrm{a} = \sum_{l=L+1}^{2L+2} l = \frac{3}{2}(L+1)(L+2).$$

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Homogeneity

Moreover, we can additionally assume translational invariance. In that case $\mathbf{A}$ becomes a vector of size N_{a}.

Bayesian analysis of the problem

Bayesian view on state and model estimation:

$$p(\mathsf{A}, \mathbf{x}_{0:K} | \mathbf{y}_{0:K}) = \frac{p(\mathbf{y}_{0:K} | \mathbf{x}_{0:K}, \mathsf{A}) p(\mathbf{x}_{0:K} | \mathsf{A}) p(\mathsf{A})}{p(\mathbf{y}_{0:K})}.$$

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Data assimilation cost function assuming Gaussian error statistics and Markovian dynamics:

$$\mathcal{J}(\mathbf{A}, \mathbf{x}_{0:K}) = \frac{1}{2} \sum_{k=0}^{K} \|\mathbf{y}_k - \mathbf{H}_k(\mathbf{x}_k)\|^2_{\mathbf{R}_k^{-1}} + \frac{1}{2} \sum_{k=1}^{K} \|\mathbf{x}_k - \mathbf{F}_{\mathbf{A}}(\mathbf{x}_{k-1})\|^2_{\mathbf{Q}_k^{-1}} - \ln p(\mathbf{x}_0, \mathbf{A}),$$

where $\mathbf{F}_{\mathbf{A}}$ is the resolvent of the model between t_k and $t_k + \Delta_t$.

$\longrightarrow$ Allows to handle partial and noisy observations.

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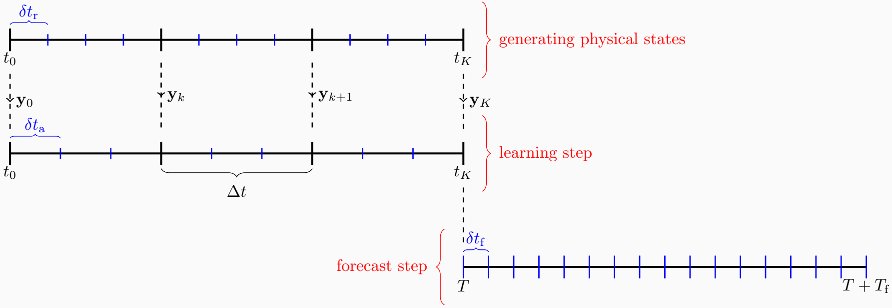
Typical machine learning cost function with $\mathbf{H}_k = \mathbf{I}_k$ in the limit $\mathbf{R}_k \longrightarrow \mathbf{0}$:

$$\mathcal{J}(\mathbf{A}) \approx \frac{1}{2}\sum_{k=1}^{K} \|\mathbf{y}_k - \mathbf{F}_{\mathbf{A}}(\mathbf{y}_{k-1})\|^2_{\mathbf{Q}_k^{-1}} - \ln p(\mathbf{y}_0, \mathbf{A}).$$

Experiment setup



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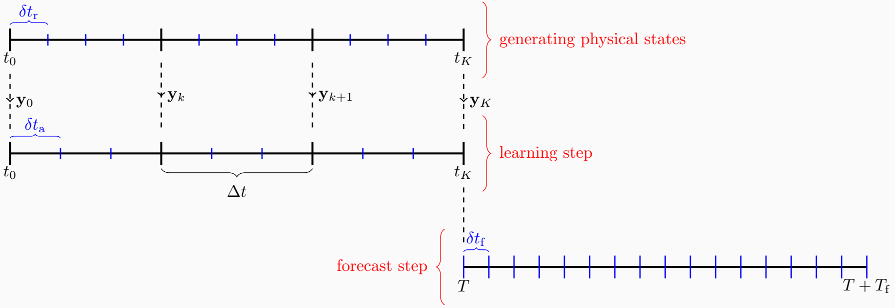


Illustration using a Lorenz 96 model:

- Size of the state $N_x = 40$
- Integration scheme: 4th order RK (RK4)
- Integration time step: $\delta t_r = \Delta t = 0.05$
- integration length: $K = 50$

Case studies

Model	scheme	time step	Observation noise
Identifiable	RK4	$\delta t_a = \Delta t = 0.05$	0
Non identifiable	RK2	$\delta t_a = 0.05/N_c$	0
Identifiable	RK4	$\delta t_a = \Delta t = 0.05$	$\sigma_y > 0$

Identifiable model:

- The true model $\phi(\mathsf{x})$ is included in the candidates $\phi_\mathsf{A}(\mathsf{x})$,
- The integration scheme and the step time used for generating the observations is the same as the one used for the surrogate model.

Case 1: Identifiable model and perfect observations

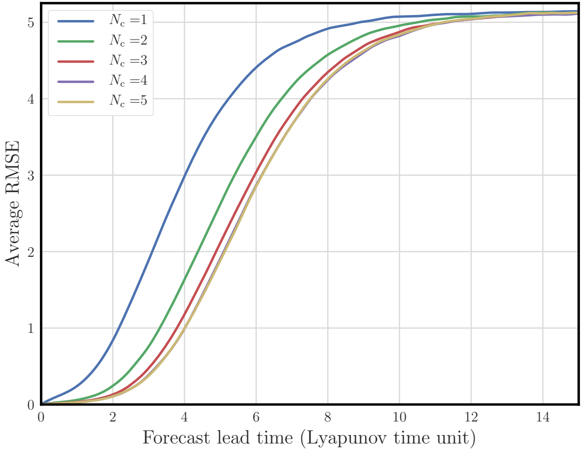
Comparison of the ODE coefficients

$\|\mathsf{A}_{\mathrm{a}} - \mathsf{A}_{\mathrm{r}}\|_{\infty} \sim 10^{-13}$,
where A_{r} are the coefficients of the reference equation (truth) and A_{a} are the coefficients of the surrogate ODE.

Almost perfect reconstruction to the machine precision.

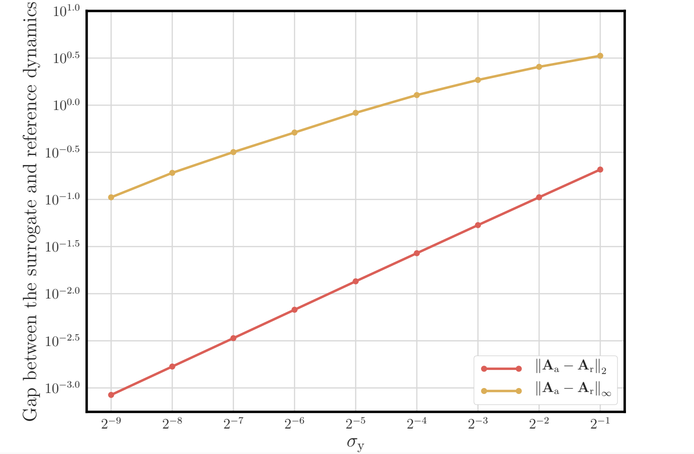
Case 2: Non-identifiable model and perfect observations

Surrogate model based on an RK2 scheme, $\delta t_a = \Delta t / N_c$.
Analysis of the modelling depth as a function of N_c.



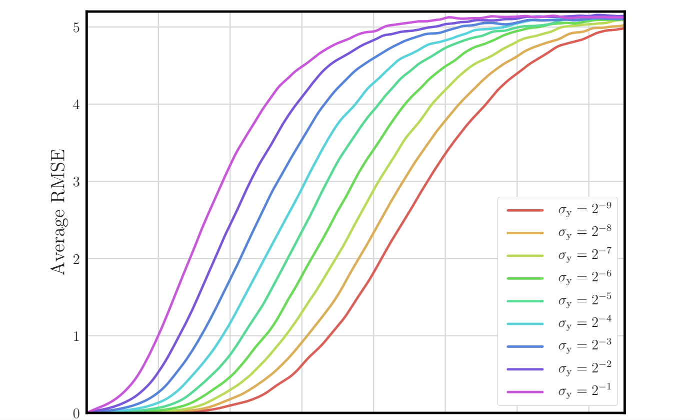
Case 3: Identifiable model and imperfect observations

ODE coefficients



Case 3: Identifiable model and imperfect observations

Forecast skill



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Dynamical system	Residual deep neural network
Parametrized forecasting model	Layer of a neural network
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Adjoint modelling	Backpropagation
Locality assumption	Convolutional layers

Second goal: Emulating a model by combining DA and ML

General remarks

What is Data Assimilation good at?

Given a numerical model, some observations and assumptions on uncertainties:

- Estimate the state of a system in an objective way,
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- Retrieve some hidden relationships in the dataset.

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Idea

Combining both approaches to develop accurate emulator of numerical models.

Proposed algorithm

- Observations: $\mathsf{y}_k^{\mathrm{obs}} = \mathcal{H}_k(\mathsf{x}_k) + \epsilon_k^{\mathrm{obs}}$
- The neural net: $\mathsf{x}_{k+1} = \mathcal{G}_{\mathsf{W}}(\mathsf{x}_k) + \epsilon_k^{\mathrm{m}} = \mathsf{x}_k + \int_{t_k}^{t_{k+1}} \phi(\mathsf{x})\,\mathrm{d}t$

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Initialization: W

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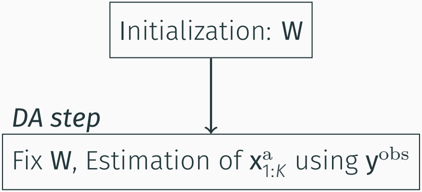

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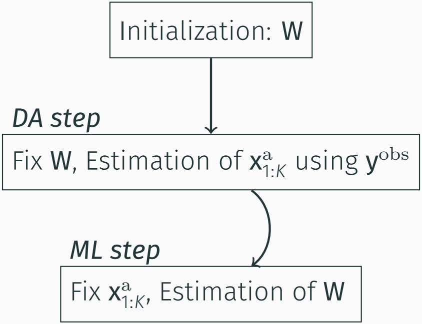

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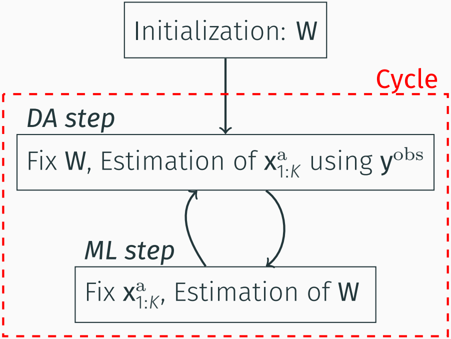

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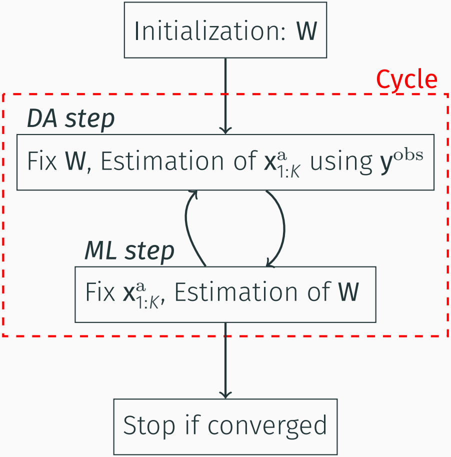

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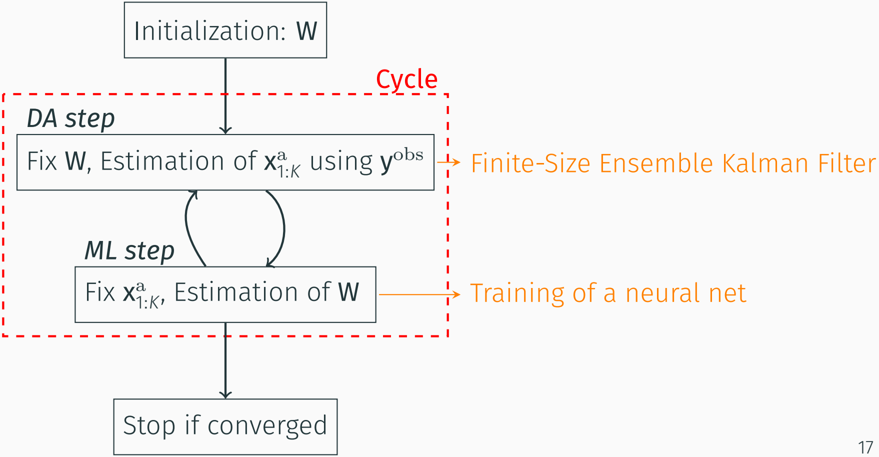
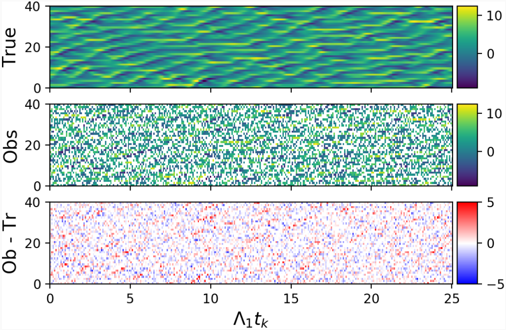


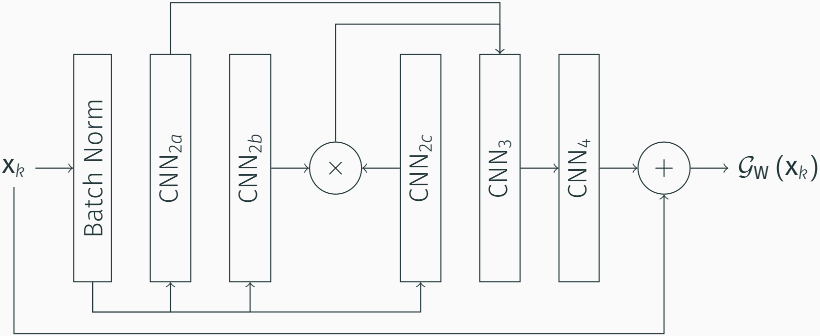
Numerical experiment: Lorenz 96 model

A simulation is performed over $K = 40,000$ time steps: $\mathsf{x}_{0:K}^{\mathrm{ref}}$
$\mathsf{y}_k^{\mathrm{obs}} = \mathcal{H}_t(\mathsf{x}_k^{\mathrm{ref}}) + \epsilon_k^{\mathrm{obs}}; \mathsf{y}_t^{\mathrm{obs}} \in \mathbb{R}^p$



- $\mathcal{H}_k$ is defined at each time step by randomly sample p=20 observations (50% of the state space).
- $\epsilon_k^{\mathrm{obs}}$ is generated using a Gaussian law of mean 0 and standard deviation 1.

Neural Network setup



Layer	number of unit	filter size	number of weights
1 (batchnorm)			2
2 (bilinear)	24×3	5	144×3
3 (convolutive)	37	5	8917
4 (linear)	1	1	38

Residual bi-linear convolutive neural network (9391 weights),

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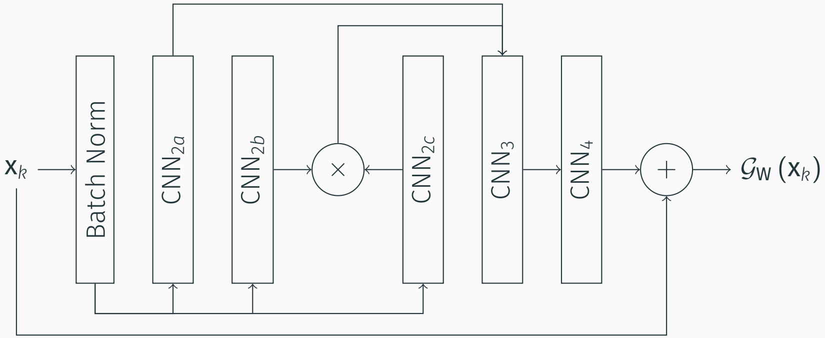

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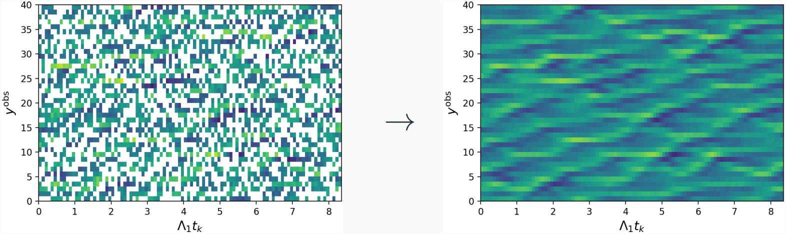
Residual bi-linear convolutive neural network (9391 weights), compared with $N_\mathrm{a} = 18$ in case of ODE parametrization.

Evaluation

- Interpolating the observations:



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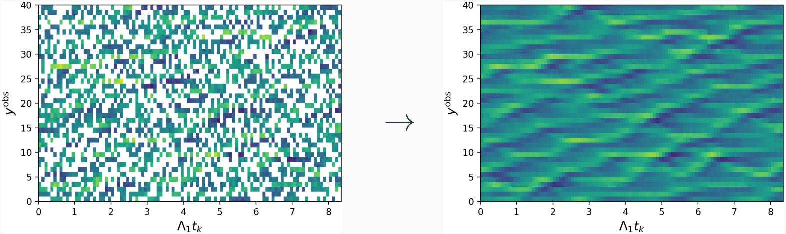

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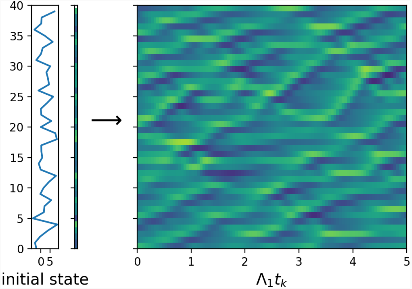
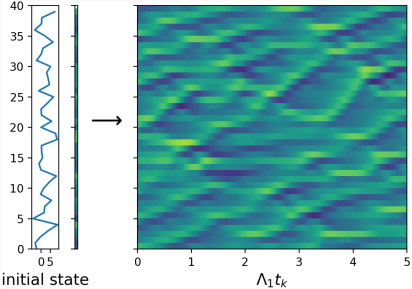
- Forecasting skill



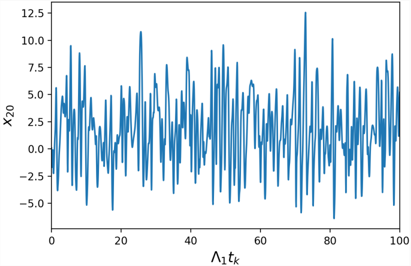
Evaluation

- Interpolating the observations:
  Score: RMSE-a (Root-mean square error of the analysis)
- Forecasting skill
  Score: RMSE-f (Root-mean square error of the forecast as a function of leading time)



Evaluation

- Interpolating the observations:
  Score: RMSE-a (Root-mean square error of the analysis)
- Forecasting skill
  Score: RMSE-f (Root-mean square error of the forecast as a function of leading time)
- Reproducing the long-term dynamics



Evaluation

- Interpolating the observations:
  Score: RMSE-a (Root-mean square error of the analysis)
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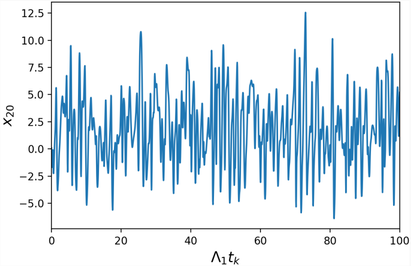
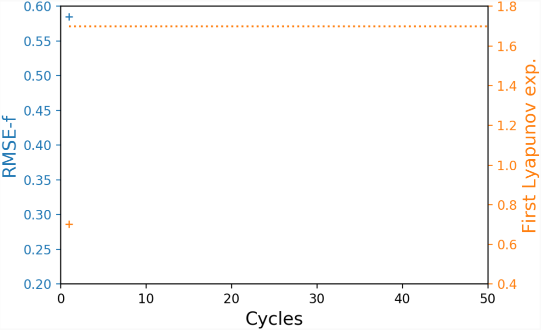
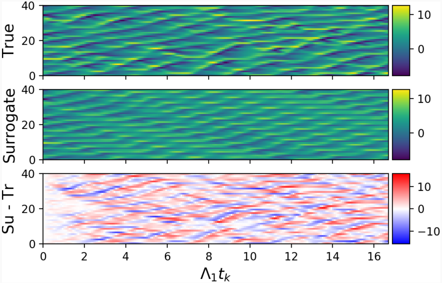
  Score: Lyapunov exponents and PSD (Power Spectral Density) compared with the true model.

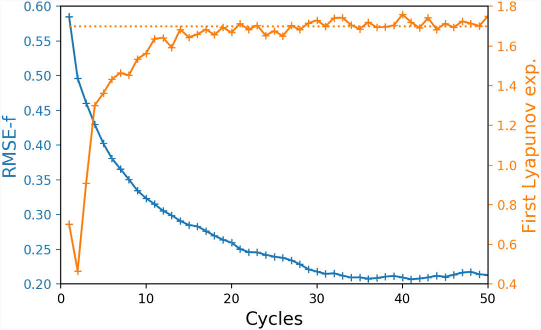


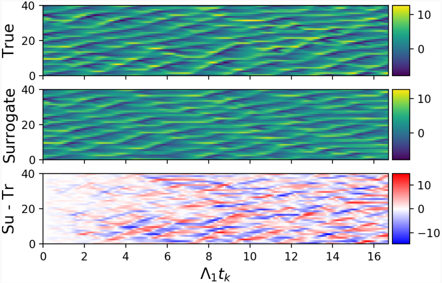
Convergence of the algorithm



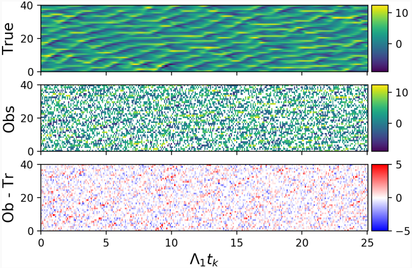


Convergence of the algorithm



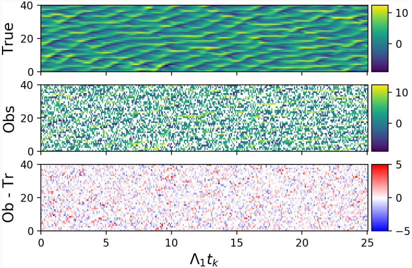


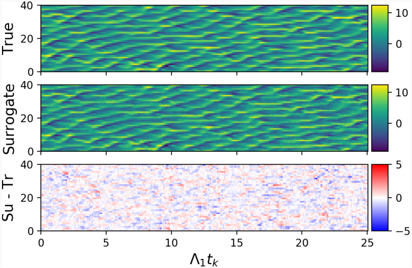
Interpolation



RMSE (obs)= 1

Interpolation

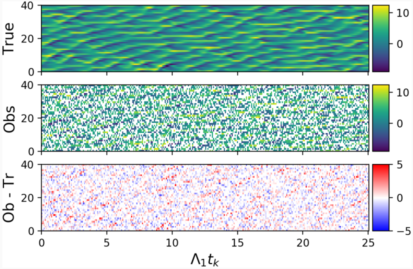




RMSE (obs)= 1

RMSE-a= 0.8

Method	RMSE-a
DA with surrogate model	0.80



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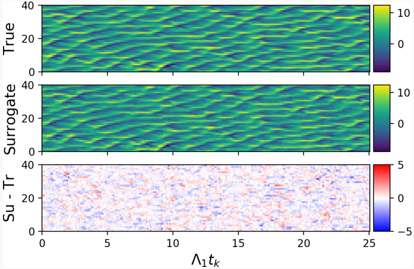
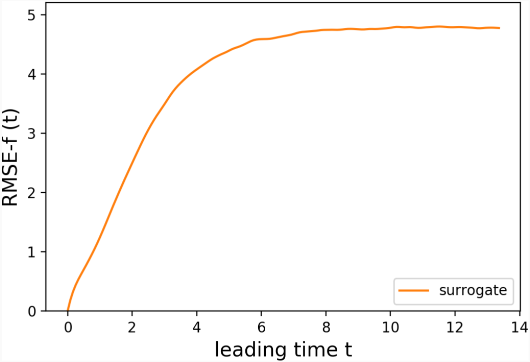


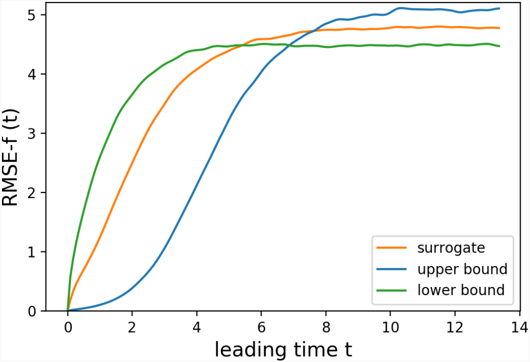
RMSE-a= 0.8

	Method	RMSE-a
Lower bound	Quadratic interpolation	2.32
	DA with surrogate model	0.80
Upper bound	DA with true model	0.34

Forecast skill



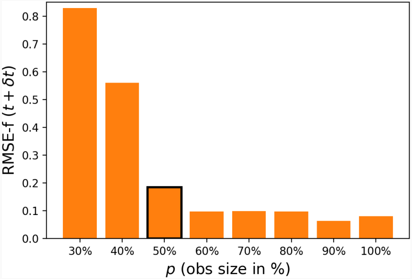
Forecast skill



- **Lower bound**: Neural Net trained with observation interpolated using quadratic interpolation (no data assimilation).
- **Upper bound**: Neural Net trained with "perfect" observations (complete, no noise).

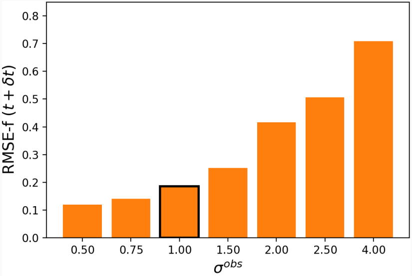
Sensitivity to noise and density of observations

Sensititvity to the density of observations



RMSE-f$(t_0 + \delta t)$
observation noise: $\sigma^{obs} = 1$

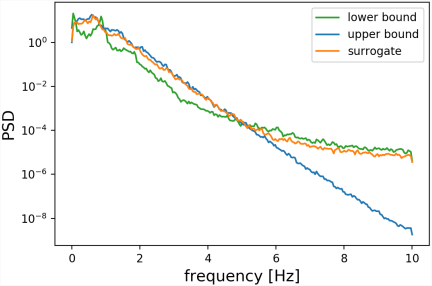
Sensititvity to the noise of observations



RMSE-f$(t_0 + \delta t)$
density of observations: 50%

Reconstruction of the long-term dynamics

Power spectral density



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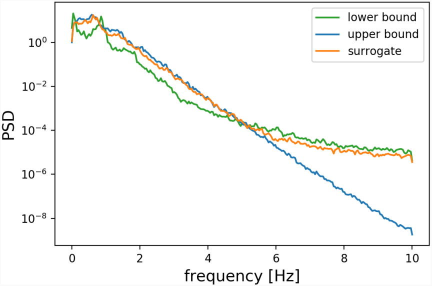
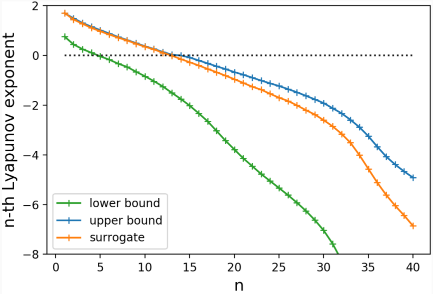
Reconstruction of the long-term dynamics

Power spectral density



Lyapunov exponents



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Conclusion

Emulate an numerical model given sparse and noisy observations

- Bayesian data assimilation for state and model estimation:
  - equivalent to a machine learning approach,
  - makes use of locality and homogeneity to reduce the dimension of the model parameters.

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Properties of the neural net surrogate model

- **Interpolation of the observations**: denoising of the observations and interpolation
- **Predictability skills**: sensitive to model noise, and to observation density below 50%
- **Replication of the long-term dynamics properties**

Marc Bocquet, Julien Brajard, Alberto Carrassi, and Laurent Bertino.
Data assimilation as a deep learning tool to infer ODE representations of dynamical models.
Nonlinear Processes in Geophysics Discussions, pages 1–29, 2019.
URL: `https://doi.org/10.5194/npg-2019-7`, `doi:10.5194/npg-2019-7`.

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