Bridging Physics and Learning: application to ocean dynamics

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AI & Ocean Science: General context

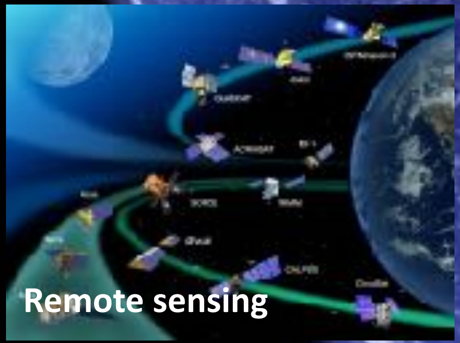
Bridging physics paradigms and deep learning

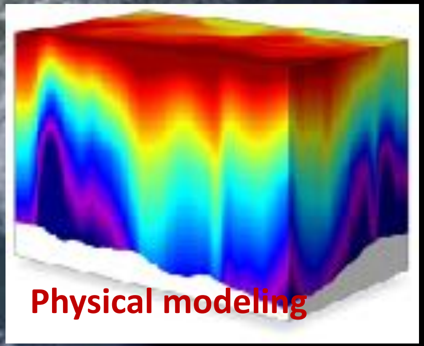
Focus on DL & Inverse Problems

Some illustrations

General question

How to solve sampling gaps and extract high-level information for ocean monitoring and surveillance ?





Context: No observation / simulation system to resolve all scales and processes simultaneously

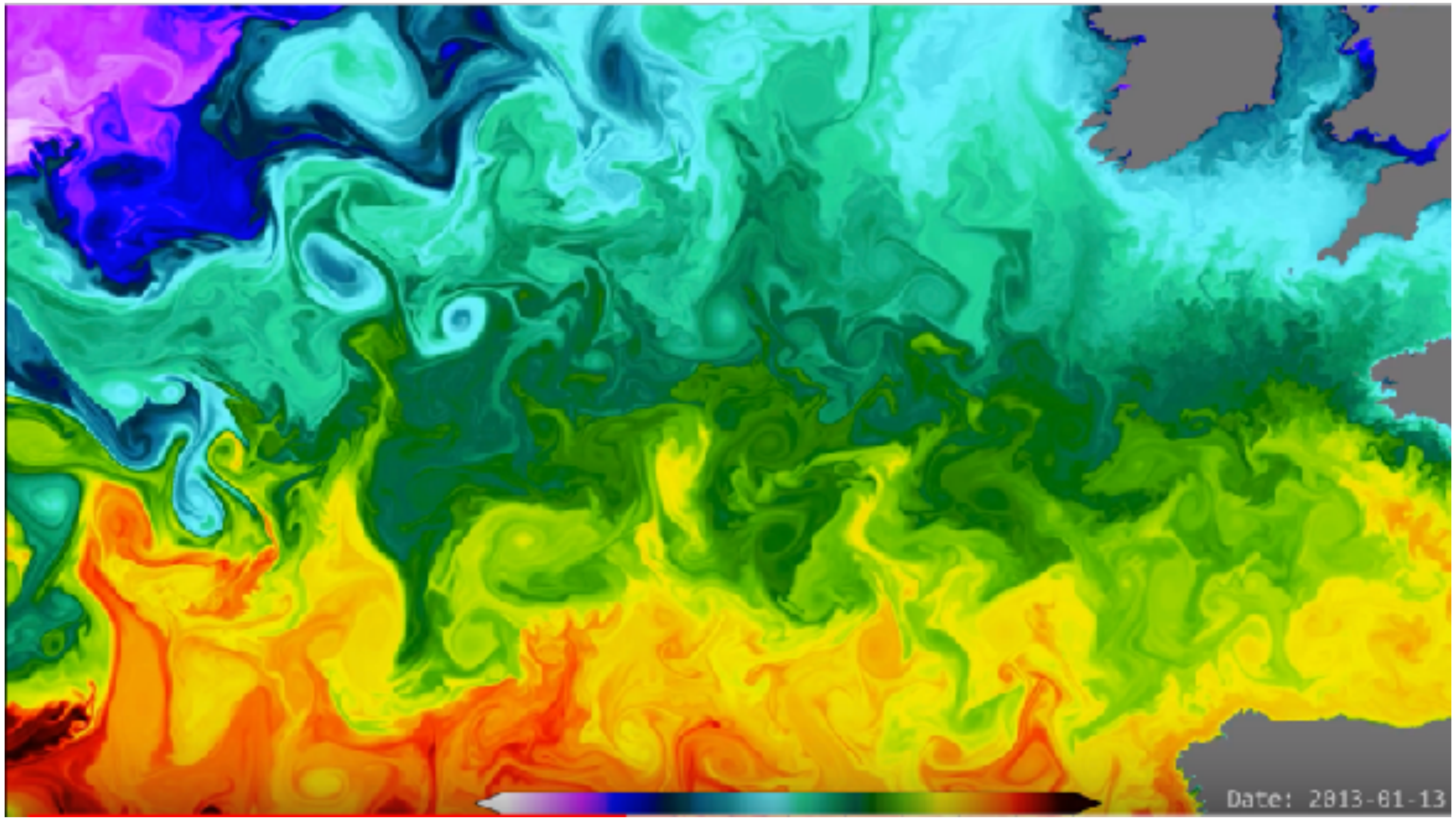
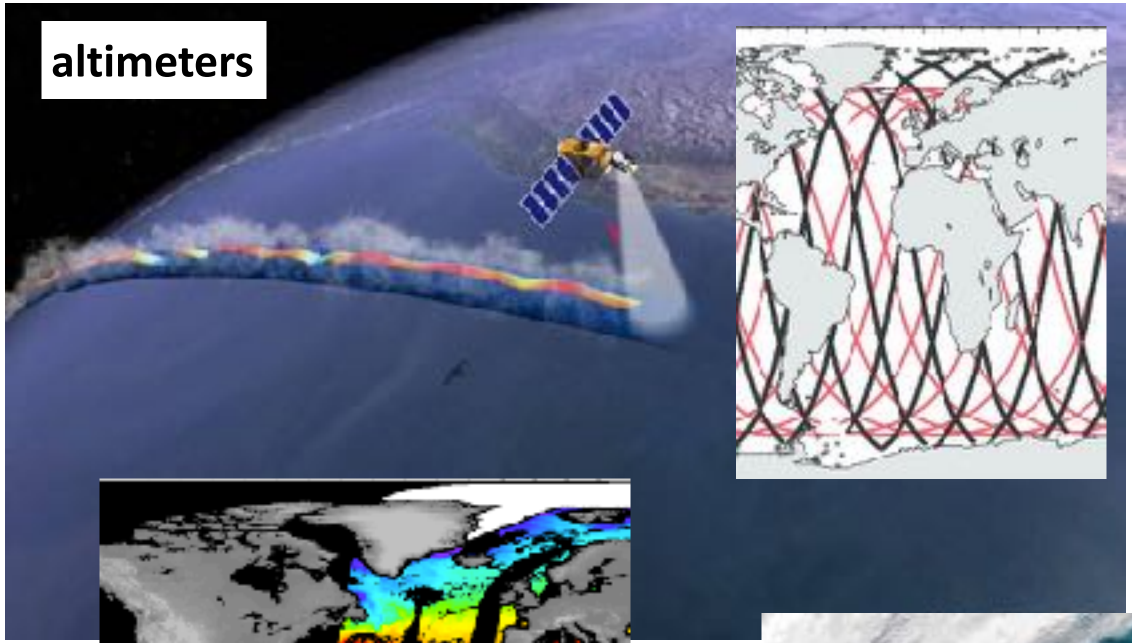
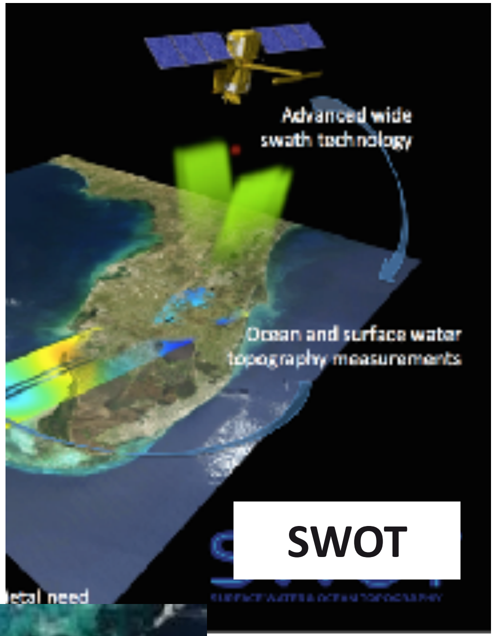
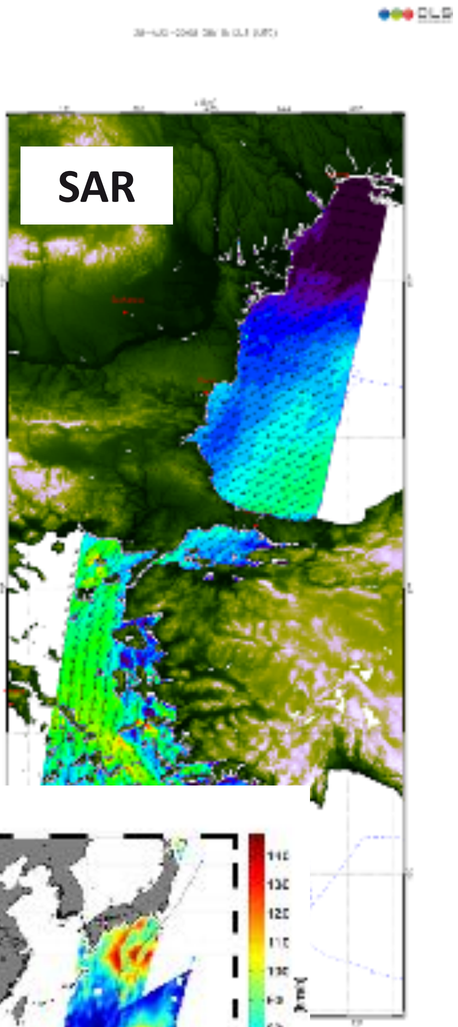
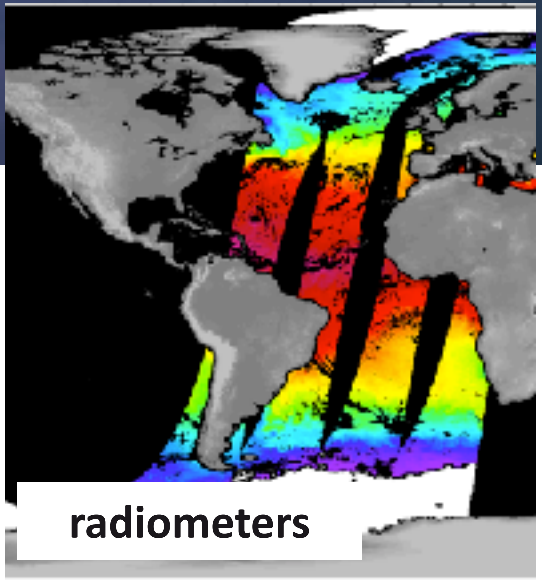


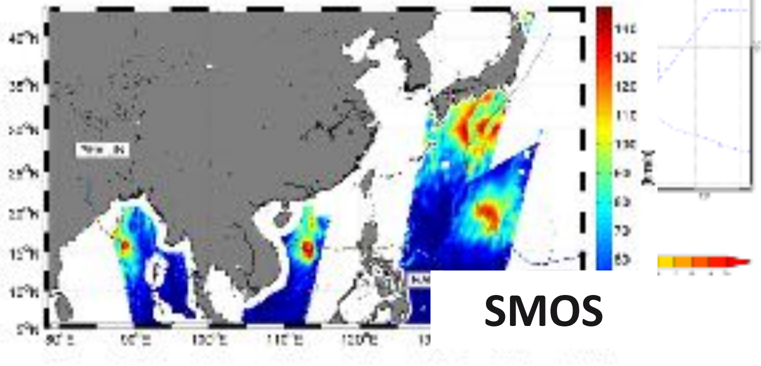
Illustration of satellite-derived sea surface observations







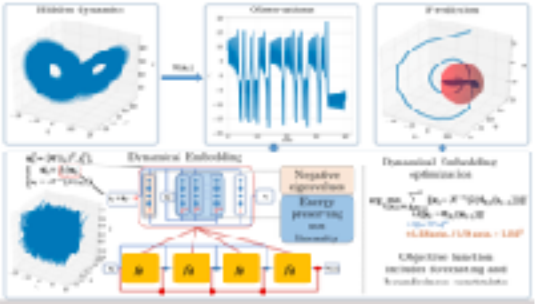




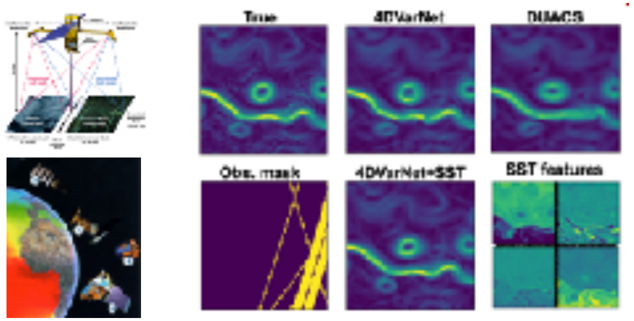
What about deep learning to solve sampling gaps and infer higher-level information ?

Topics of interest with emphasis of DL approaches

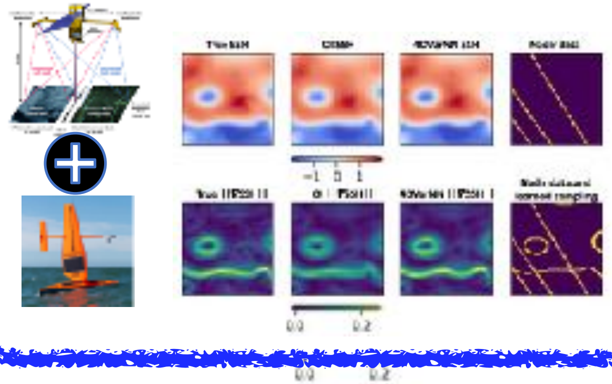
Observation-driven forecasting



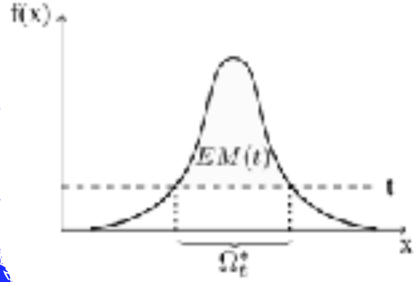
Multimodal reconstruction



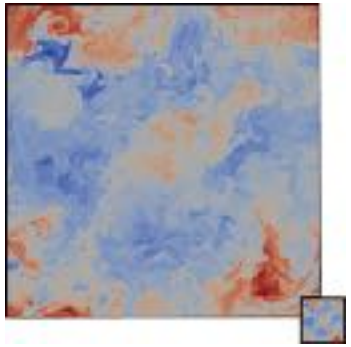
Learning where to sample ?



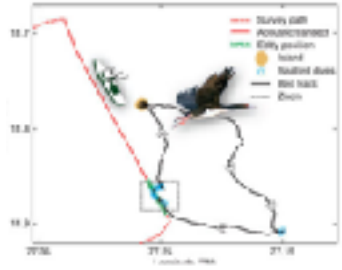
Predicting extremes



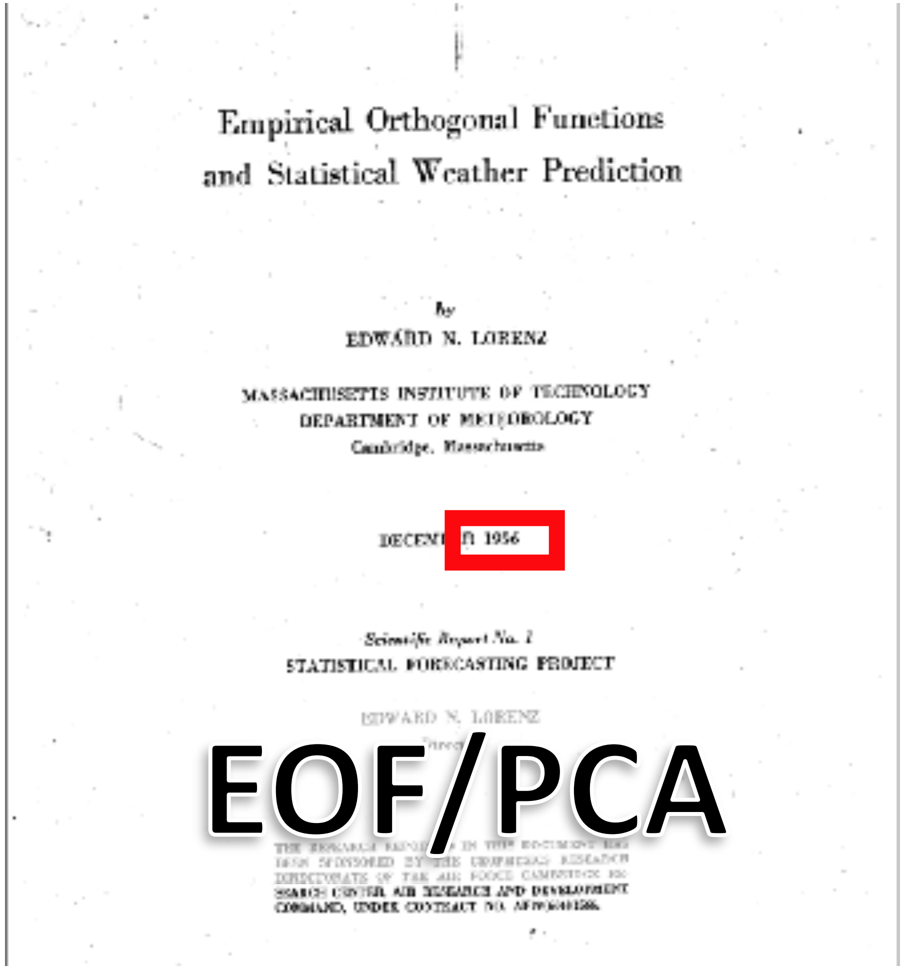
Ocean modeling



Trajectory data analysis and modeling



Learning & Geoscience: an old story ?



Empirical Orthogonal Functions
and Statistical Weather Prediction

by

EDWARD N. LORENZ

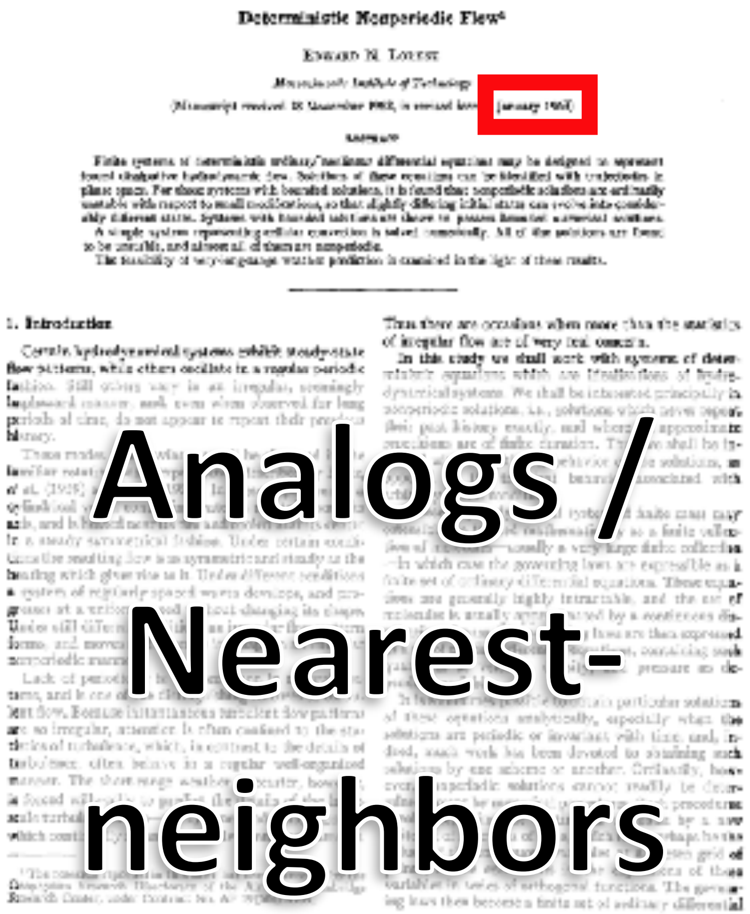
MASSACHUSETTS INSTITUTE OF TECHNOLOGY
DEPARTMENT OF METEOROLOGY
Cambridge, Massachusetts

DECEMBER 1956

Scientific Report No. 1
STATISTICAL FORECASTING PROJECT

EDWARD N. LORENZ

EOF/PCA



Deterministic Nonperiodic Flow

Edward N. Lorenz

Massachusetts Institute of Technology

January 1963

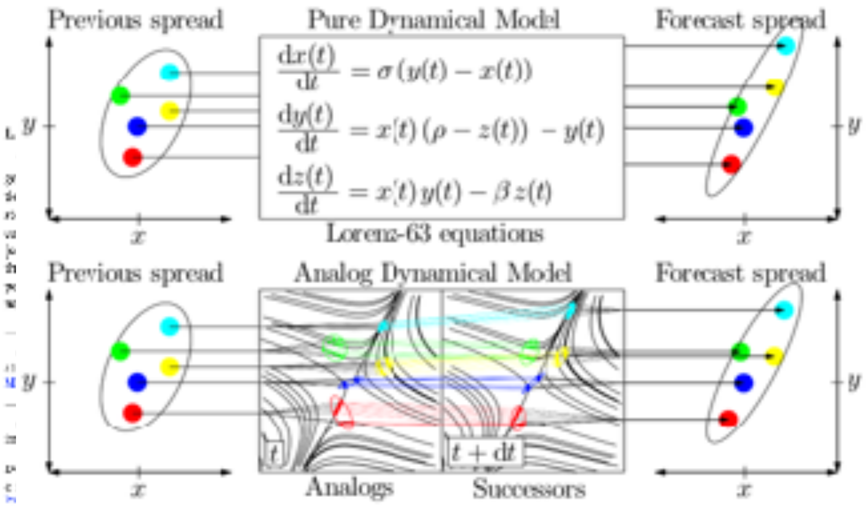
1. Introduction

Analogs / Nearest-neighbors

Learning & Geoscience: Data-driven approaches for data assimilation

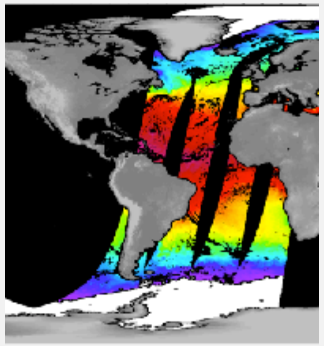
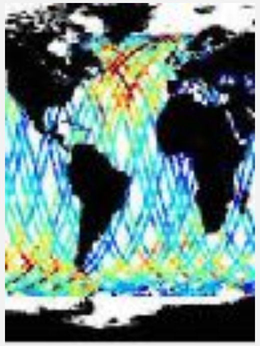
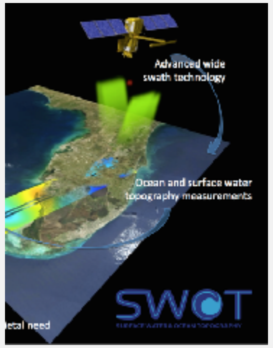

The Analog Data Assimilation

ABSTRACT



The analog data assimilation [Lguensat et al., 2017]

- Combination of analog forecasting strategies and EnKF assimilation schemes
- Extension to 2D+t geophysical dynamics

Open questions

- Bridging model-driven and data-driven paradigms
- Learning data-driven representations from real observation data

General context

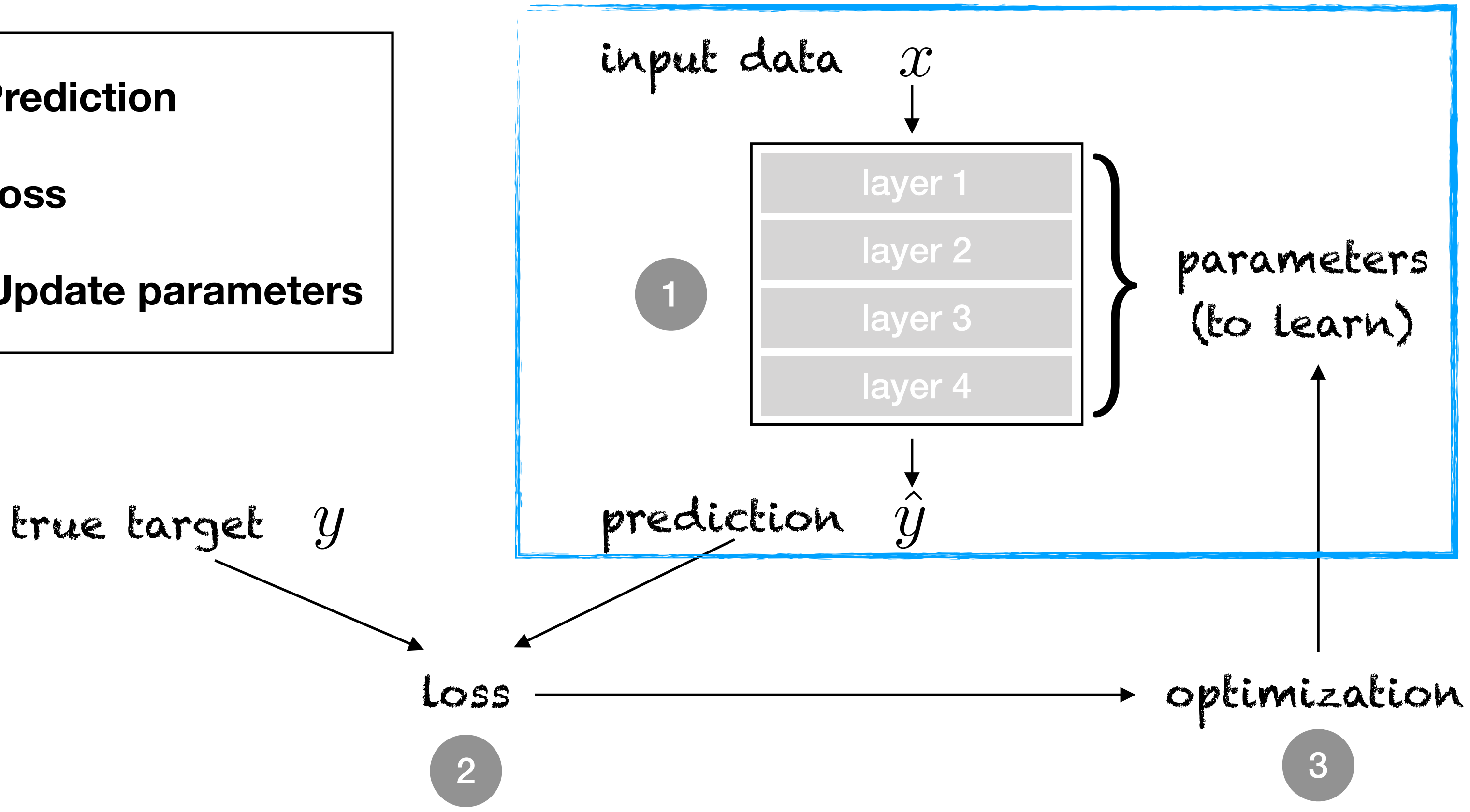
Short reminder on NNs and Automatic Differentiation

Bridging physics paradigms and deep learning

Beyond Ocean Dynamics

What’s learning (for a computer) ?

1. **Prediction**
2. **Loss**
3. **Update parameters**



What’s learning (for a computer) ?

Mathematical formulation: Learning comes to minimising some loss function given w.r.t. model parameters and training data

$$\widehat{\theta} = \arg\min_{\theta} \mathcal{L}\left(\{x_i, y_i\}_{i \in \{1,..,N\}}; f_\theta\right)$$

Key questions:

- Which parameterisation for model f ?
- Which loss function ?

Neural networks: composition idea

- **Approximation through the composition of (simple) elementary functions:**

$$f_\theta(x) = f_{\theta_N} \circ \ldots \circ f_{\theta_2} \circ f_{\theta_1}(x)$$

- **Key features:**
  - Any continuous function can be approximated as the composition of elementary functions
  - Analytical/exact computation of the derivative of f with respect to parameters and input variables
  - Direct exploitation of gradient-based optimisation schemes for learning

Neural networks: automatic differentiation

- **Given the general composition idea:**

$$f_\theta(x) = f_{\theta_N} \circ \ldots \circ f_{\theta_2} \circ f_{\theta_1}(x)$$

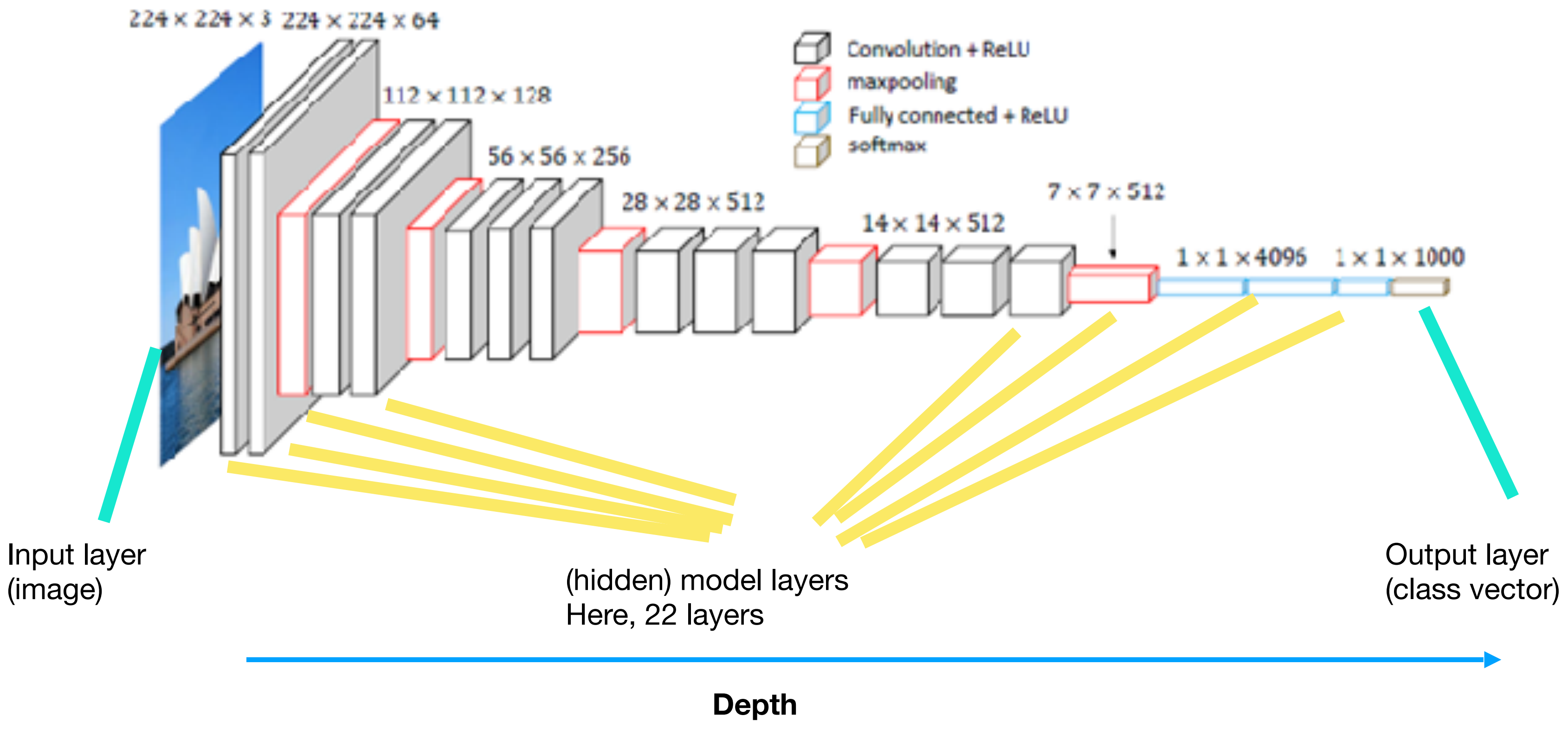
- **NNs can implement automatic differentiation knowing the symbolic differentiation for elementary functions:**
  - AD example: https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html
  - Basis of the backpropagation algorithm (similar to adjoint method)

- **Resulting gradient descent for learning model parameters:**

$$\widehat{\theta} = \arg\min_\theta \mathcal{L}\left(\{x_i, y_i\}_i; f_\theta\right) \Longrightarrow \theta^{(k+1)} = \theta^{(k+1)} + \lambda_k \nabla_\theta \mathcal{L}\left(\{x_i, y_i\}_i; f_\theta\right)$$

Deep learning models

DL models are (in general) feedforward models. VGG16 as an illustration



The more layers, the deeper…… Some models may have up to several hundreds to thousands of layers.

General context

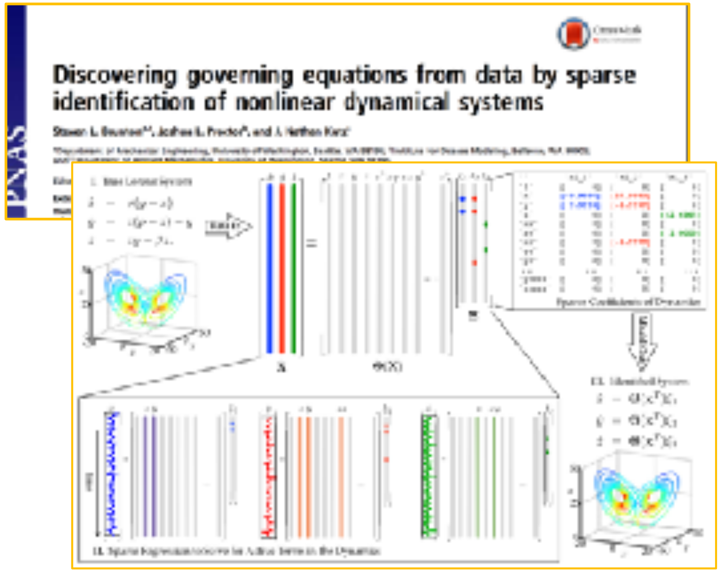
Introduction to deep learning and NNs

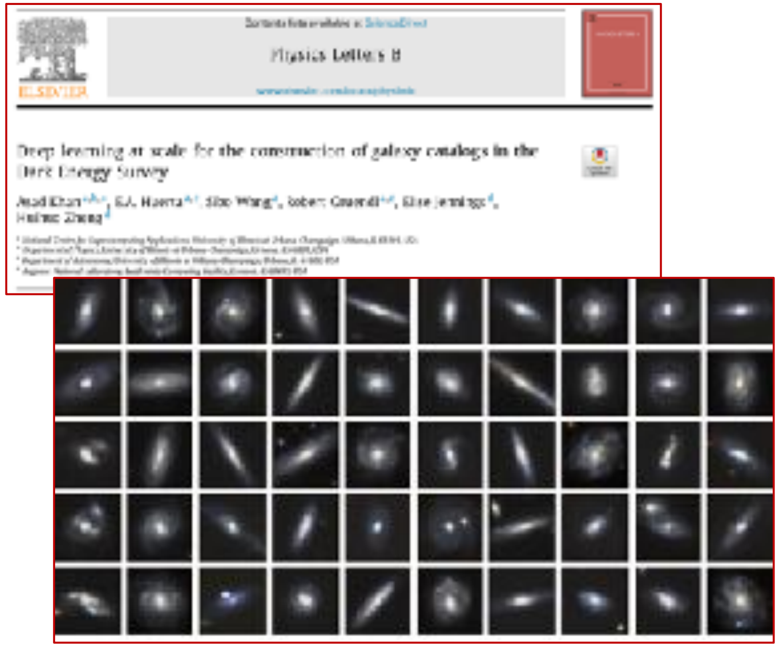
Bridging physics paradigms and deep learning

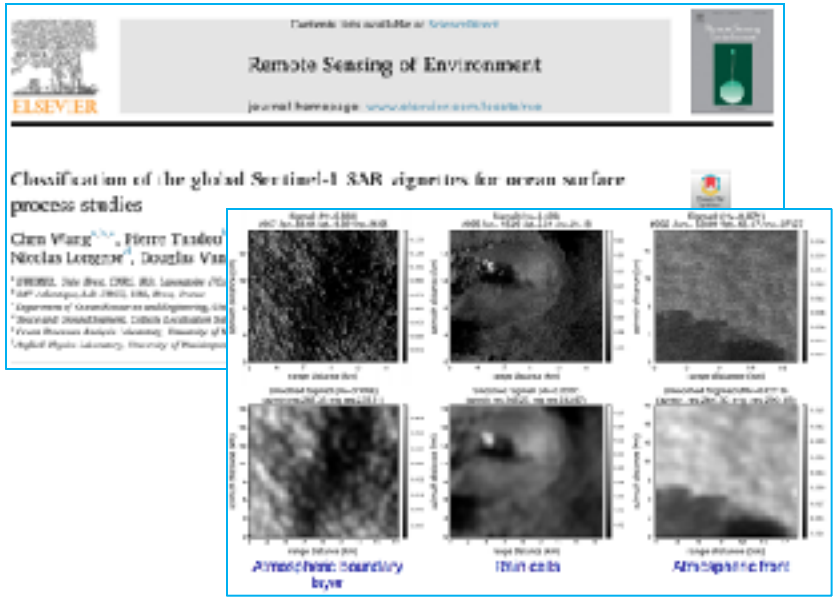
Beyond Ocean Dynamics

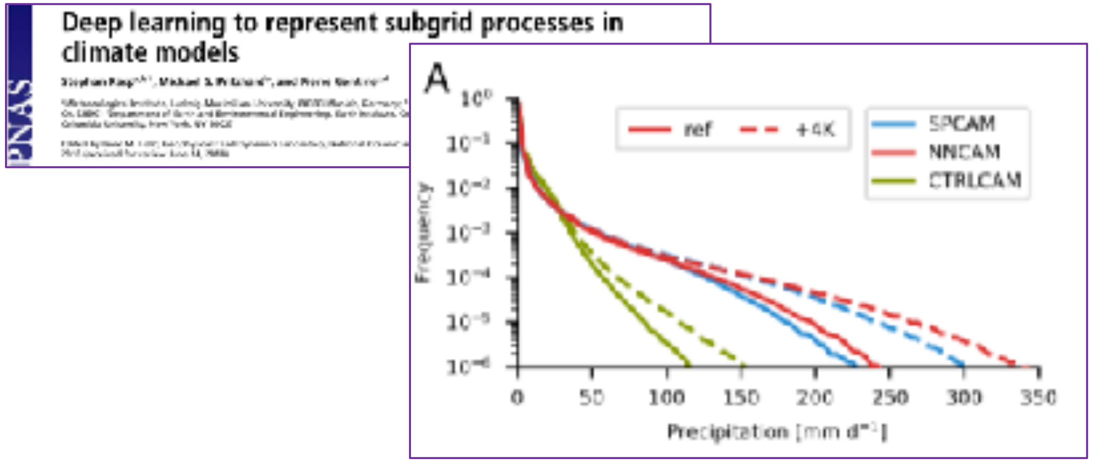
Deep Learning applied to physics

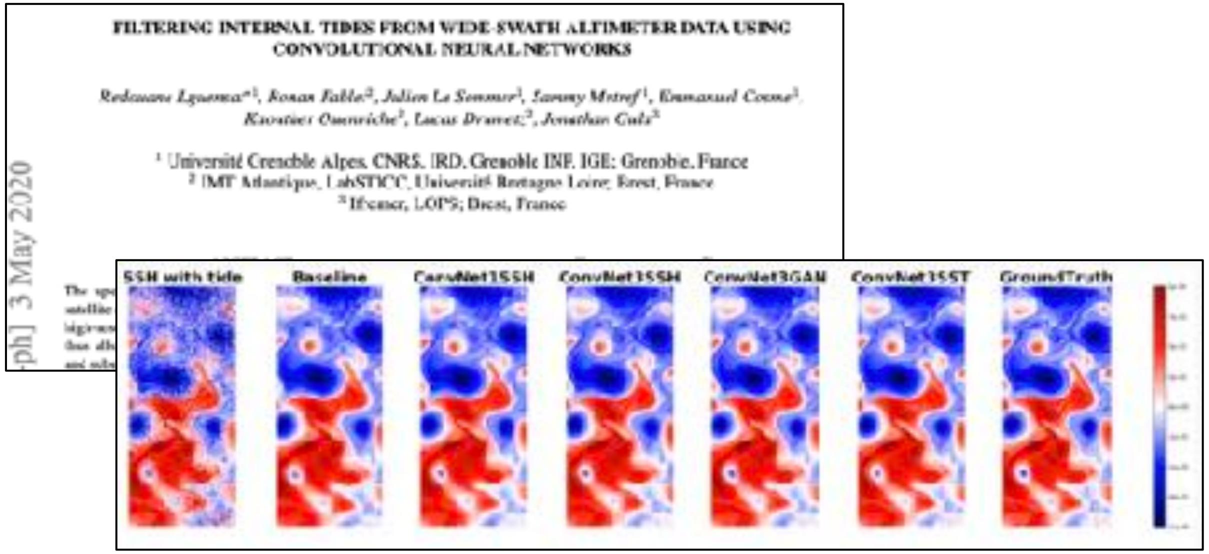
Direct applications of DL schemes to physics-related issues





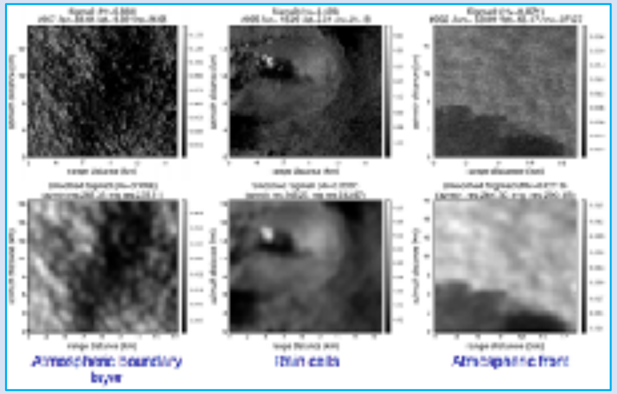




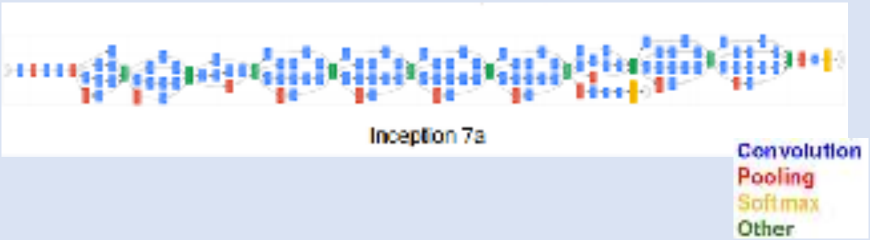


How to (directly) apply DL to physics-related issues ?

1 Build a groundtruthed dataset



2 Design or choose an architecture



Many architectures available online (VGG, ResNet, U-Net,….)

3 Choose a DL framework

TensorFlow

Keras

PYTORCH

4 Learn the model

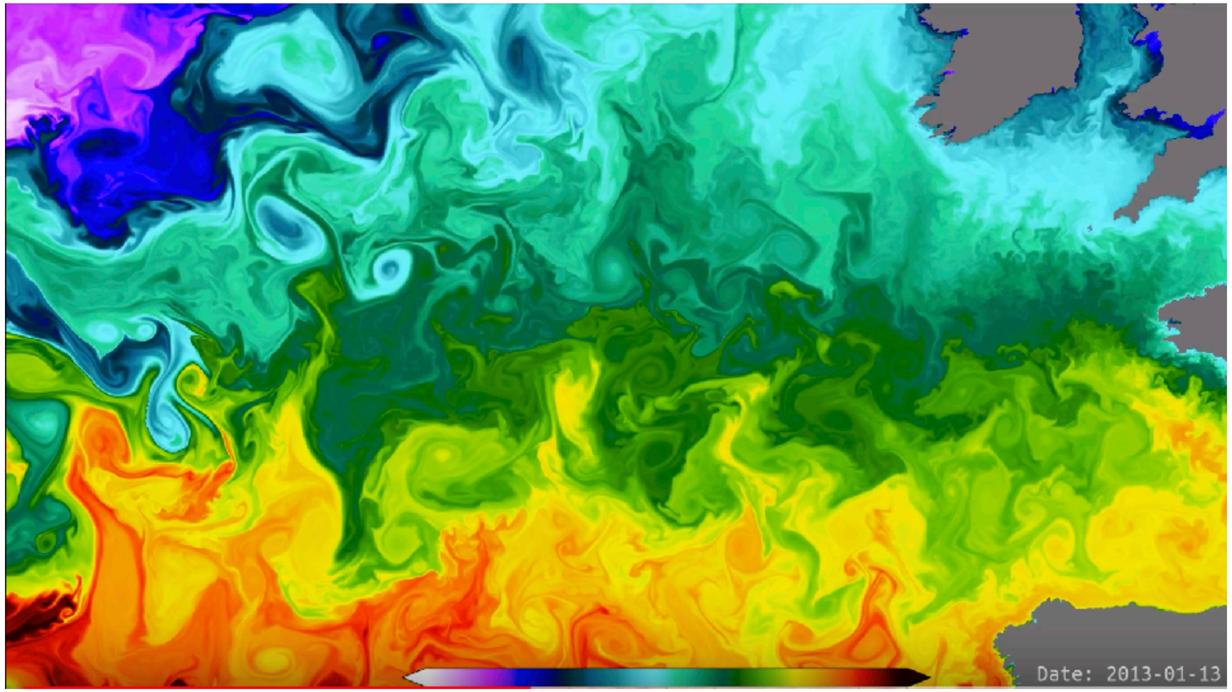
Select a training loss

Optimize model parameters using optimizers embedded in DL frameworks

A toy example using Tensorflow-Keras: https://www.tensorflow.org/tutorials/keras/classification

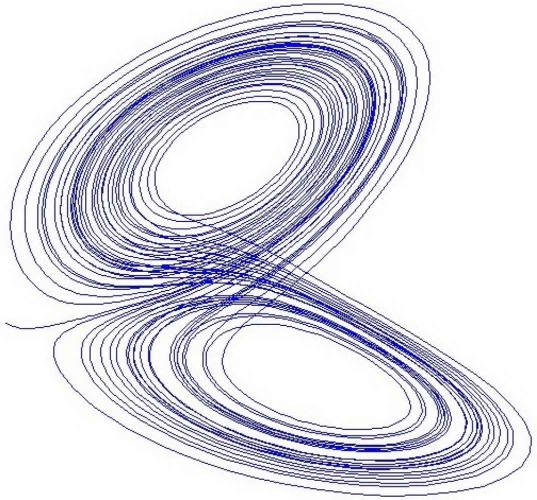
How to exploit physics prior in deep learning schemes?

How to model Geophysical Dynamics?



$$\frac{dx(t)}{dt} = \sigma\,(y(t) - x(t))$$
$$\frac{dy(t)}{dt} = x(t)\,(\rho - z(t)) - y(t)$$
$$\frac{dz(t)}{dt} = x(t)\,y(t) - \beta\,z(t)$$

Lorenz-63 equations



What are chaotic dynamics?

https://github.com/CIA-Oceanix/DLGD2021/blob/main/lecture-5-inverse-problems/notebookPyTorch_InvProb_ModelBased_L63_Students.ipynb

Bridging physics & AI: a broader picture

Physical model

$$\frac{\partial u}{\partial t} + \langle \nabla u, v \rangle = \kappa \Delta u$$

Representation learning

Trainable representation

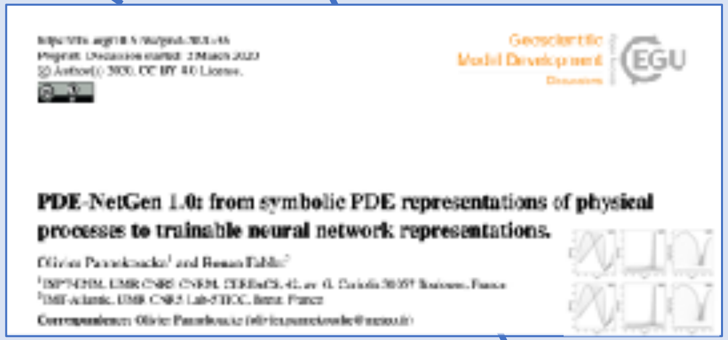
Making the most of AI and Physics Theory

- Model-Driven/Theory-Guided & Data-Constrained schemes
- Data-Driven & Physics-Aware schemes (eg, Ouala et al., 2019)

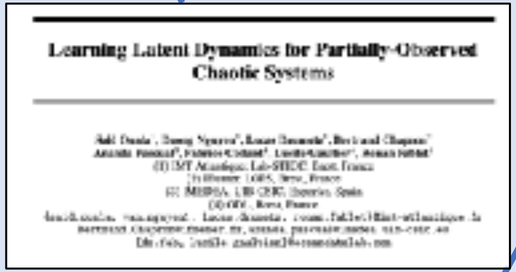
Bridging Physics & AI: a broader picture

Model-driven

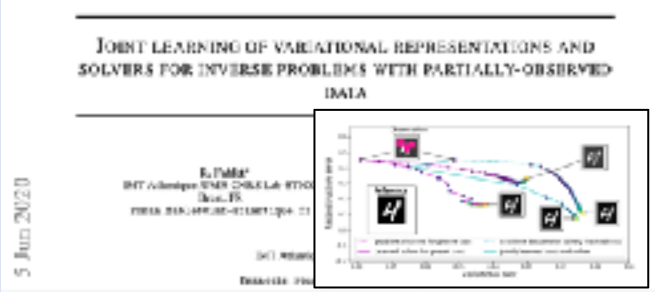
ODEs/PDEs
Variational models
State-space models
Data Assimilation
….



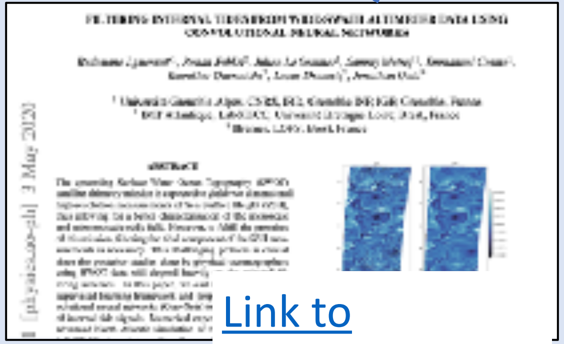
PDE-NetGen 1.0: from symbolic PDE representations of physical processes to trainable neural network representations.



Learning Latent Dynamics for Partially-Observed Chaotic Systems



Joint learning of variational representations and solvers for inverse problems with partially-observed data



Link to animation

Data-driven

Analog methods
Kernel methods
Neural Networks
…..

Physics-informed & Data-constrained

Data-driven & Physics-aware

Bridging physics & AI: Expected breakthroughs

Physical model

$$\frac{\partial u}{\partial t} + \langle \nabla u, v \rangle = \kappa \Delta u$$

Representation learning

Data-driven representation

Making the most of AI and Physics Theory

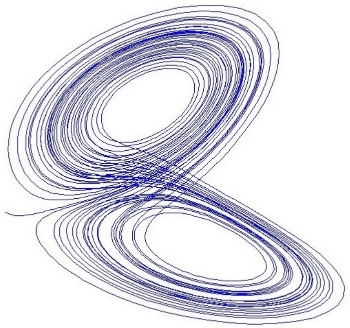
- **Model-Driven/Theory-Guided & Data-Constrained schemes**
- Data-Driven & Physically-Sound schemes (eg, Ouala et al., 2019)

How to embed physics-driven priors in DL models ?

An illustration through neural ODE for Lorenz-63 dynamics (Fablet et al., 2018)

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \sigma\left(y(t) - x(t)\right)$$
$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = x(t)\left(\rho - z(t)\right) - y(t)$$
$$\frac{\mathrm{d}z(t)}{\mathrm{d}t} = x(t)\,y(t) - \beta\, z(t)$$

Lorenz-63 equations

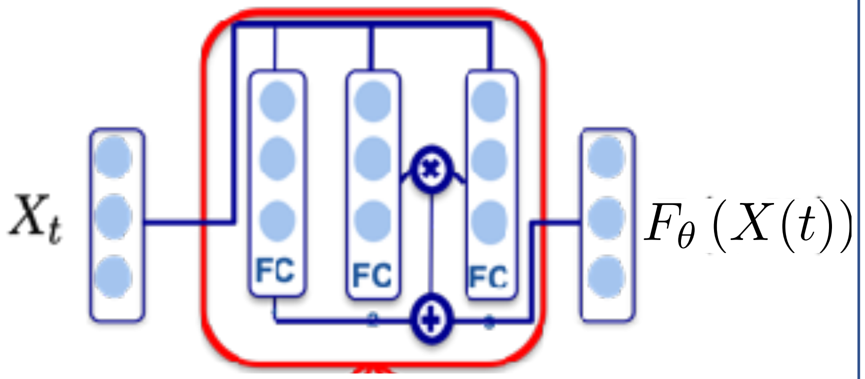


Associated Euler integration scheme

$$d_t X(t) = F_\theta\left(X(t)\right)$$

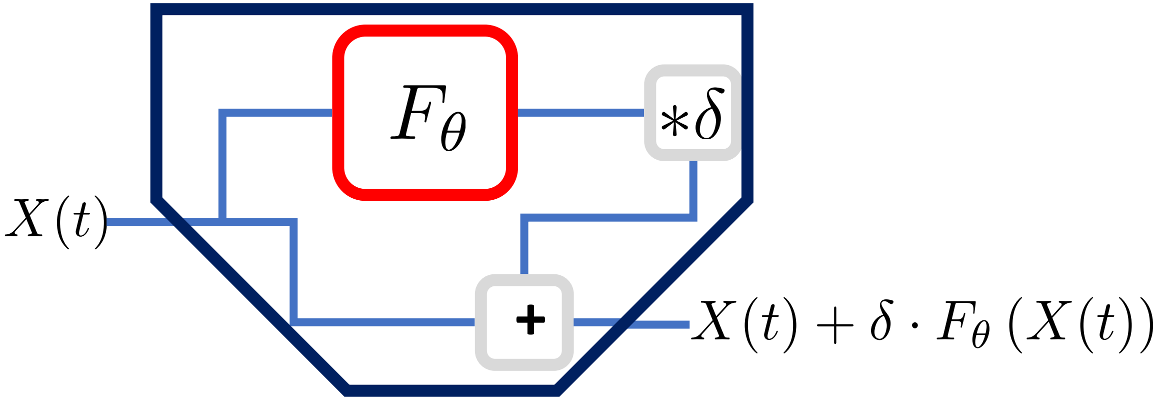
$$X(t+\delta) = X(t) + \delta \cdot F_\theta\left(X(t)\right)$$

NN architecture for differential operator



Bilinear architecture

NN architecture for integration scheme



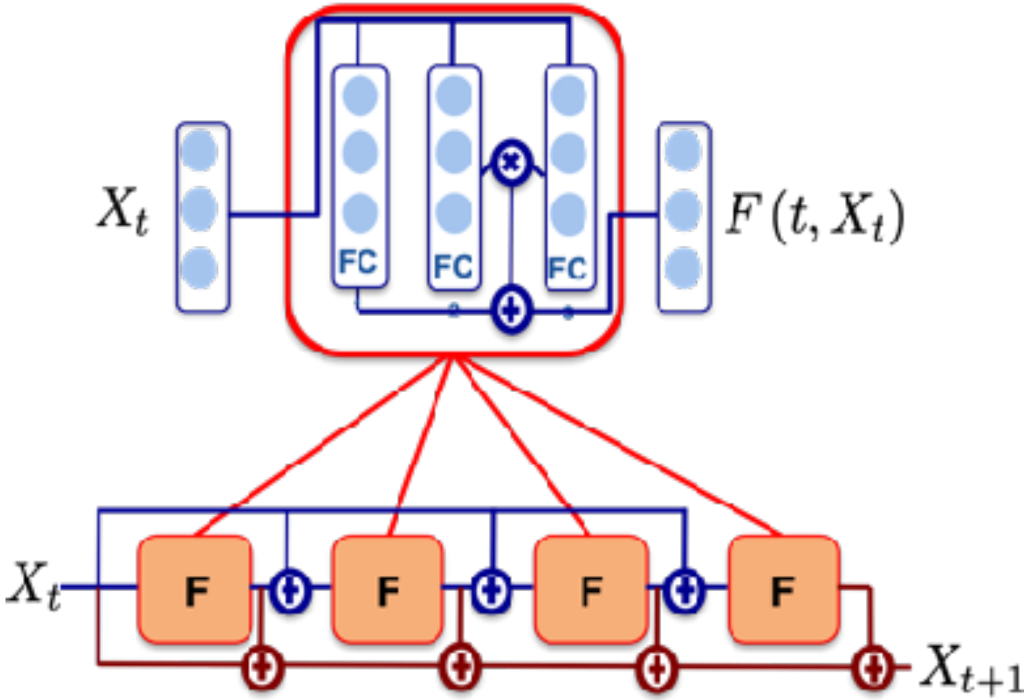
ResNet architecture (Residual Network)

How to embed physics-driven priors in DL models ?

An illustration through neural ODE for Lorenz-63 dynamics (Fablet et al., 2018)

$$\begin{aligned}
\frac{dx(t)}{dt} &= \sigma\left(y(t) - x(t)\right) \\
\frac{dy(t)}{dt} &= x(t)\left(\rho - z(t)\right) - y(t) \\
\frac{dz(t)}{dt} &= x(t)\,y(t) - \beta\, z(t)
\end{aligned}$$

Lorenz-63 equations



Generalization to higher-order integration schemes (eg, RK4)

$$d_t X(t) = F_\theta\left(X(t)\right)$$

$$X(t+\delta) = X(t) + \sum_i \beta_i k_i$$

with $k_i = F_\theta\left(X(t) + \delta \alpha_i k_{i-1}\right)$

NB: Same number of trainable model parameters as the Euler-based architecture

How to embed physics-driven priors in DL models ?

An illustration through L63 dynamics: numerical experiments (Fablet et al., 2018)

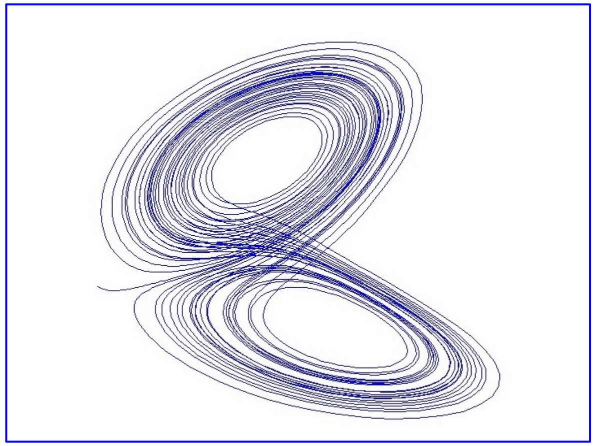
Forecasting experiments

Noise-free training data

Forecasting time step	t_0+h	t_0+4h	t_0+8h
Analog forecasting	$<10^{-6}$	0.002	0.005
Sparse regression	$<10^{-6}$	0.002	0.006
MLP	$<10^{-6}$	0.018	0.044
Bi-NN(4)	***$<10^{-6}$***	***$<10^{-6}$***	***$<10^{-6}$***

Noisy training data (σ=0.5)

Forecasting time step	t_0+h	t_0+4h	t_0+8h
Analog forecasting	$<10^{-6}$	2.01	2.2
Bi-NN(4)	**$<10^{-6}$**	***0.054***	***0.14***



Assimilation experiment

(1 obs. every 8 time steps)

Noise standard deviation in training data	0	0.25	1
True model	*0.50*	-	-
Analog forecasting	0.65	1.17	1.81
Bi-NN(4)	***0.60***	***0.75***	***0.86***

NN Generator from Symbolic PDEs (Pannekoucke et al., 2020)

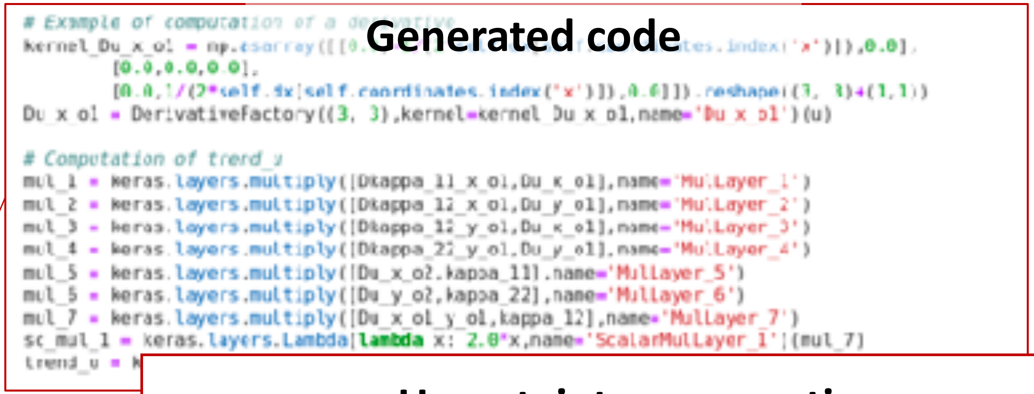
$$\partial_t u + u\partial_x u = \kappa\partial_x^2 u$$

Symbolic calculus (Simpy)

PDE-GenNet (keras)

$$\begin{pmatrix} \mu_u(t) \\ \Sigma_u(t) \end{pmatrix} \longrightarrow \textit{ResNet} \longrightarrow \begin{pmatrix} \mu_u(t+1) \\ \Sigma_u(t+1) \end{pmatrix}$$

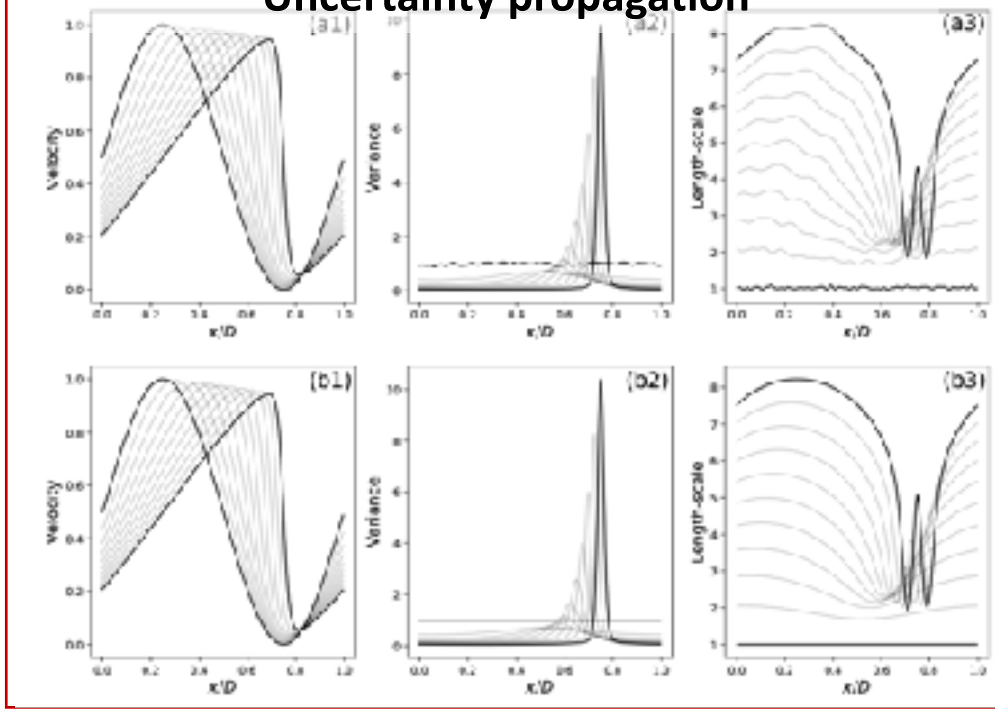
Generated code



```
# Example of computation of a derivative
kernel_Du_x_o1 = np.asarray([[0. ... index('x')]),0.0],
        [0.0,0.0,0.0],
        [0.0,1/(2*self.dx[self.coordinates.index('x')]),0.0]]).reshape((3, 3)+(1,1))
Du_x_o1 = DerivativeFactory((3, 3),kernel=kernel_Du_x_o1,name='Du_x_o1')(u)

# Computation of trend_u
mul_1 = keras.layers.multiply([Dkappa_11_x_o1,Du_x_o1],name='MulLayer_1')
mul_2 = keras.layers.multiply([Dkappa_12_x_o1,Du_y_o1],name='MulLayer_2')
mul_3 = keras.layers.multiply([Dkappa_12_y_o1,Du_x_o1],name='MulLayer_3')
mul_4 = keras.layers.multiply([Dkappa_22_y_o1,Du_y_o1],name='MulLayer_4')
mul_5 = keras.layers.multiply([Du_x_o2,kappa_11],name='MulLayer_5')
mul_5 = keras.layers.multiply([Du_y_o2,kappa_22],name='MulLayer_6')
mul_7 = keras.layers.multiply([Du_x_o1_y_o1,kappa_12],name='MulLayer_7')
sc_mul_1 = keras.layers.Lambda(lambda x: 2.0*x,name='ScalarMulLayer_1')(mul_7)
trend_u = k
```

Uncertainty propagation



Bridging physics & AI: Expected breakthroughs

Representation learning

Physical model

$$\frac{\partial u}{\partial t} + \langle \nabla u, v \rangle = \kappa \Delta u$$

Data-driven representation

Making the most of AI and Physics Theory

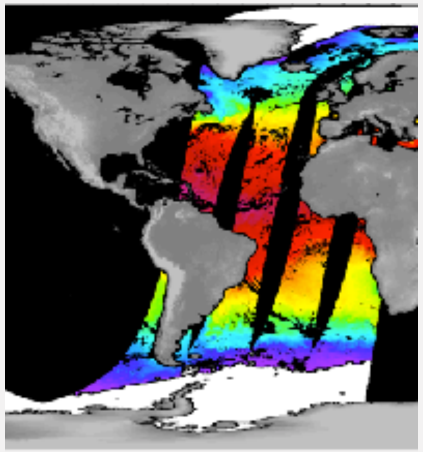
- **Model-Driven/Theory-Guided & Data-Constrained schemes**
- **Data-Driven & Physically-Sound schemes (eg, Ouala et al., 2019)**

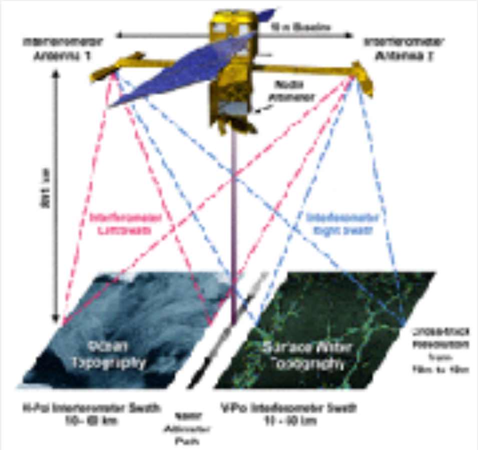
Focus on Inverse Problems and Deep Learning

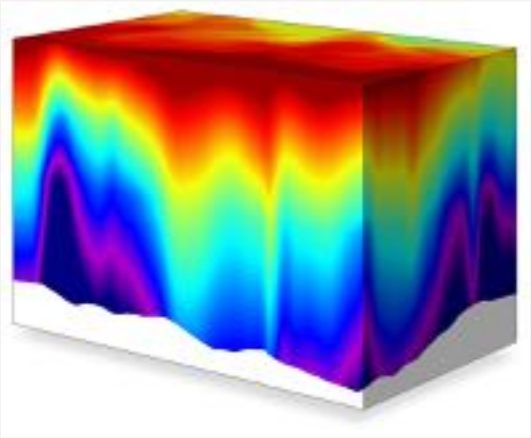
Deep learning for irregularly-sampled and partially-observed systems

Dealing with partially-observed and irregularly-sampled ocean dynamics

Can we learn directly from observation data ?







Generic issue:

Joint identification and inversion

Dynamical model

$$X_t \rightarrow \boxed{\partial_t X = F(X, \xi, t, \theta)} \rightarrow X_{t+1}$$

+

Observation model

$$Y_t = H(X, \zeta, t, \phi)$$

Fablet et al. **4DVarNet: Trainable Data Assimilation for Sea Surface dynamics**
https://cia-oceanix.github.io/

Method

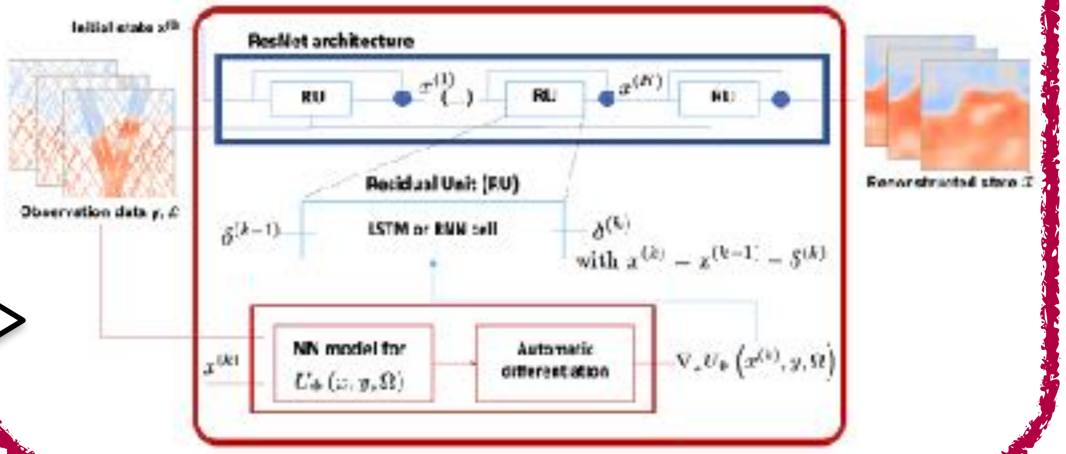
From a Variational DA formulation

$$\hat{x} = \arg\min_{x} \|x - y\|^2 + \lambda \|x - \phi(x)\|^2$$

Trainable variational model

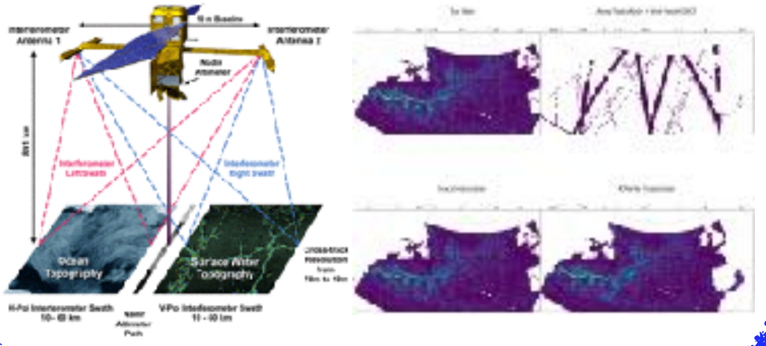
Trainable gradient-based solver

Associated end-to-end scheme

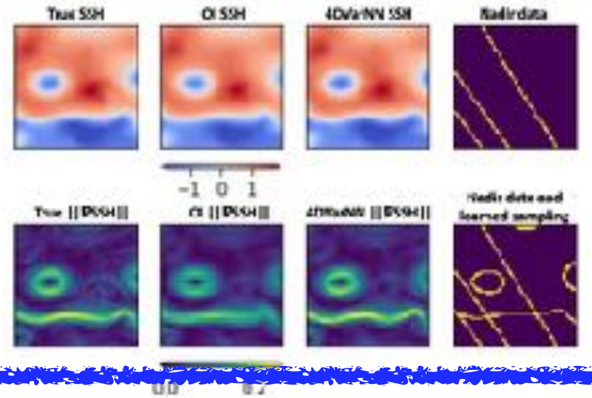


Applications

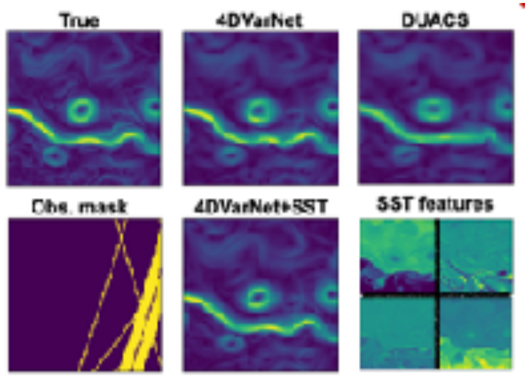
Interpolation & Forecasting



Learning where to sample ?



Multimodal learning



Trainable observation operators

Learning where to sample ?

Learning what to measure ?

4DVarNet models with trainable observation models

$$\hat{x} = \arg\min_x \|x - y\|^2 + \lambda \|x - \phi(x)\|^2$$

Sparse sampling operator

$$\|H(z) * (x - y)\|^2$$

$$\text{s.t. } \forall z, \ \|H(z)\|_1 < \epsilon$$

Multimodal observation

$$\|x - y\|^2$$

$$+$$

$$\alpha \|G * x - F * z\|^2$$

Trainable observation operators

4DVarNet models with trainable observation models

Spase sampling operator

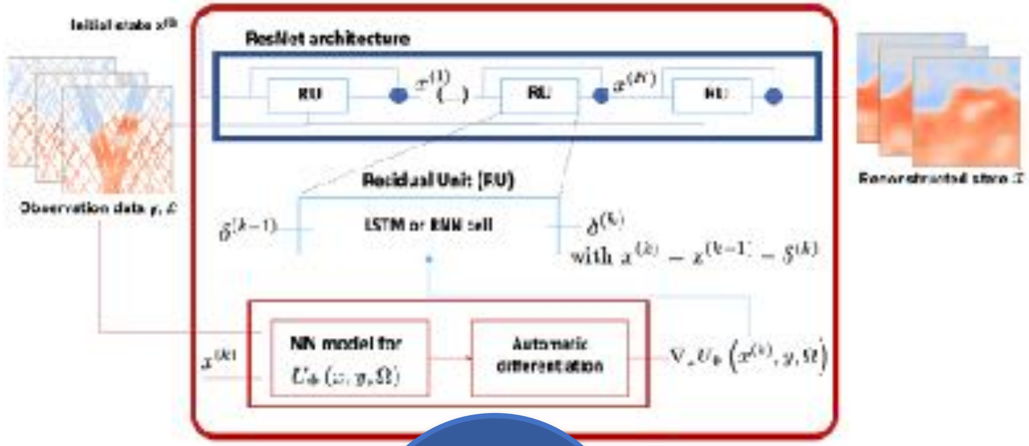
$$\|H(z) * (x - y)\|^2$$

$$\text{s.t. } \forall z,\ \|H(z)\|_1 < \epsilon$$

Multimodal observation

$$\|x - y\|^2$$
$$+$$
$$\alpha\|G * x - F * z\|^2$$

End-to-end 4DVarNet



Supervised training loss

(under sparsity constraint for the optimal sampling case)

Multimodal data assimilation

SSH-SST case-study

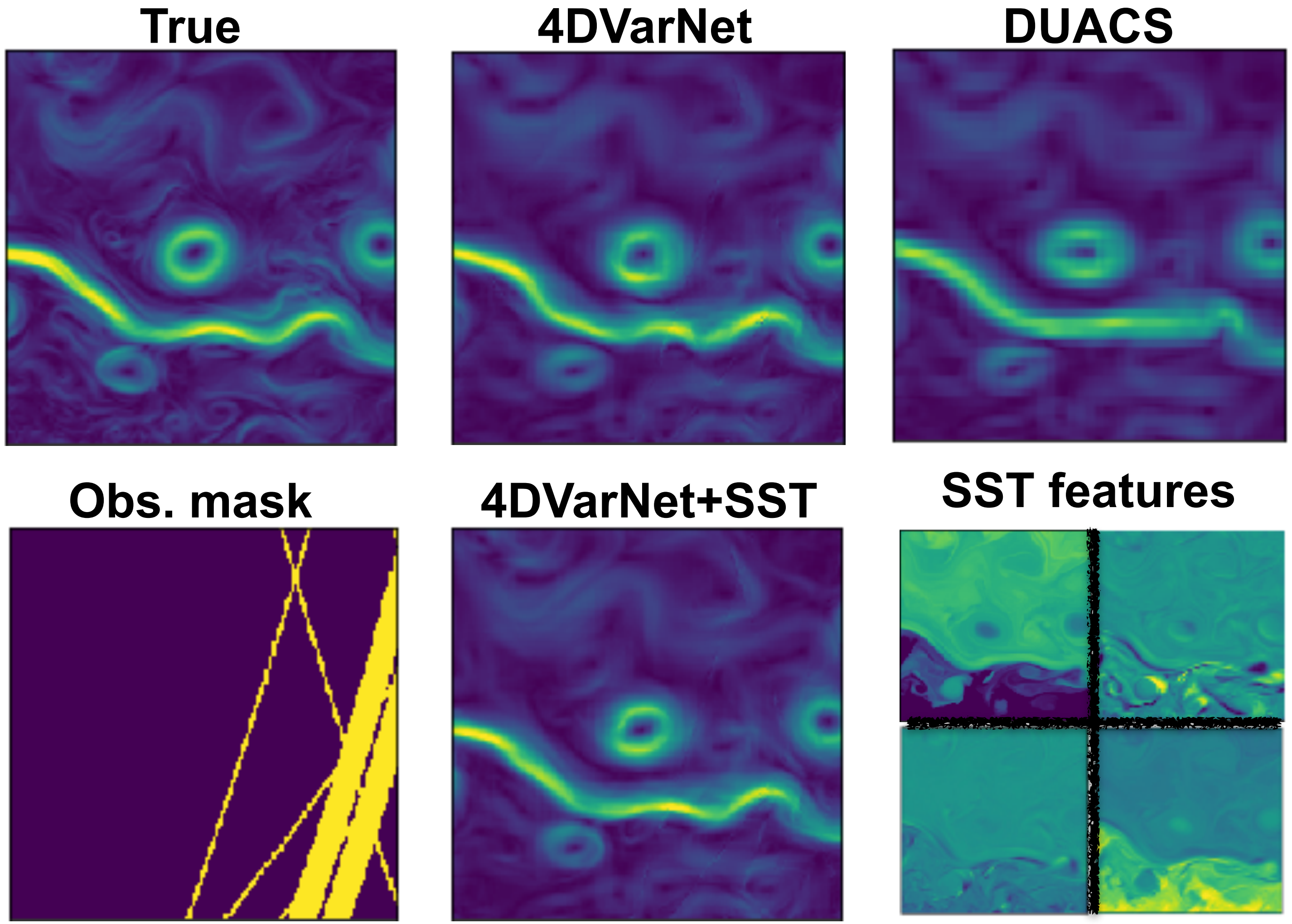
OSSE with NATL60 data

4-nadir-altimeter + SWOT + DUACS baseline

Gulf Stream area (10°x10°)

63% vs. 53% gain in SSH MSE w.r.t. DUACS with/ without SST (Winter period)

50% vs. 13% gain in SSH MSE w.r.t. DUACS using nadir altimeter data only



Optimal sampling

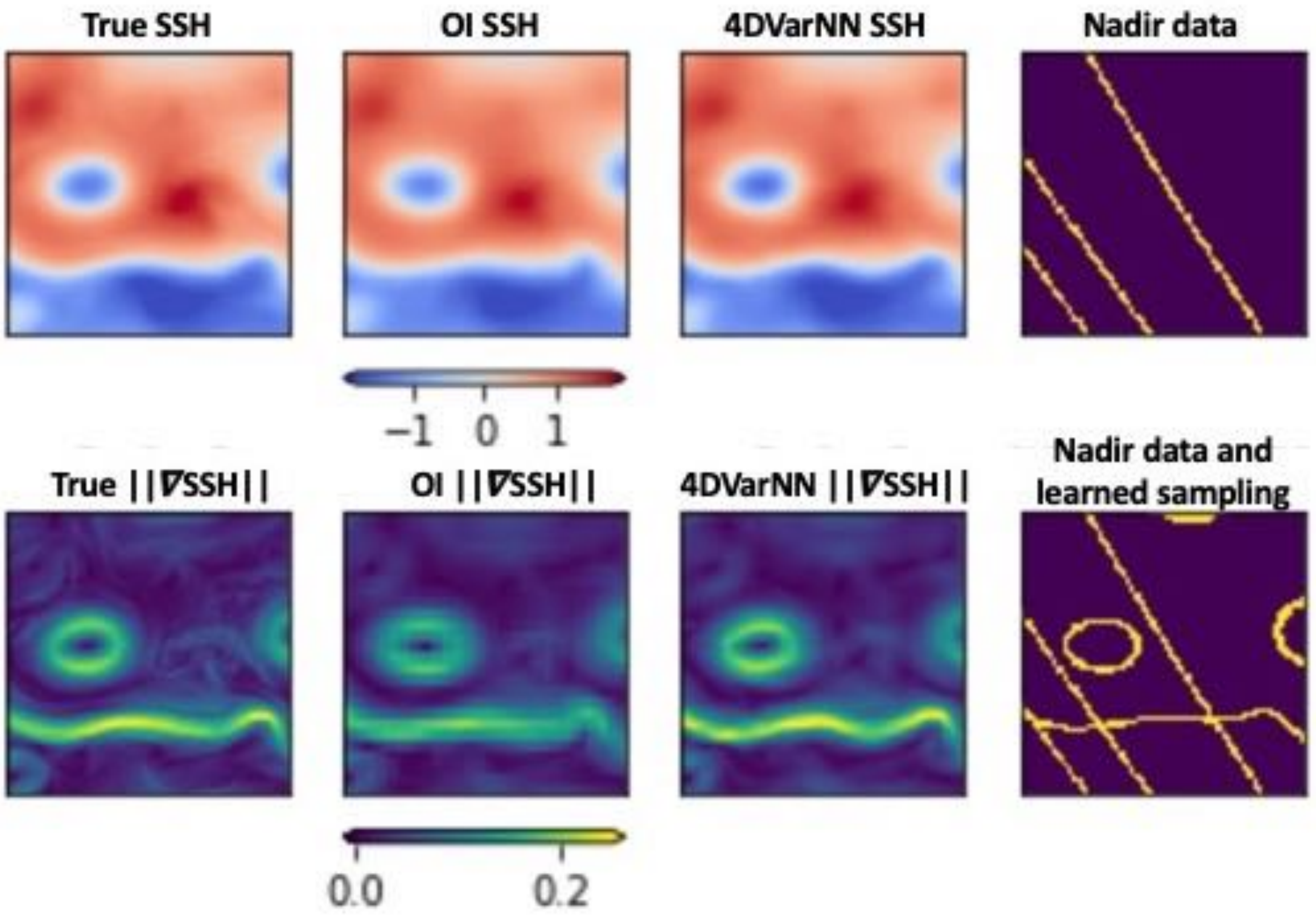
SSH case-study

OSSE with NATL60 data

4-nadir-altimeter + DUACS baseline

Gulf Stream area (10°x10°)

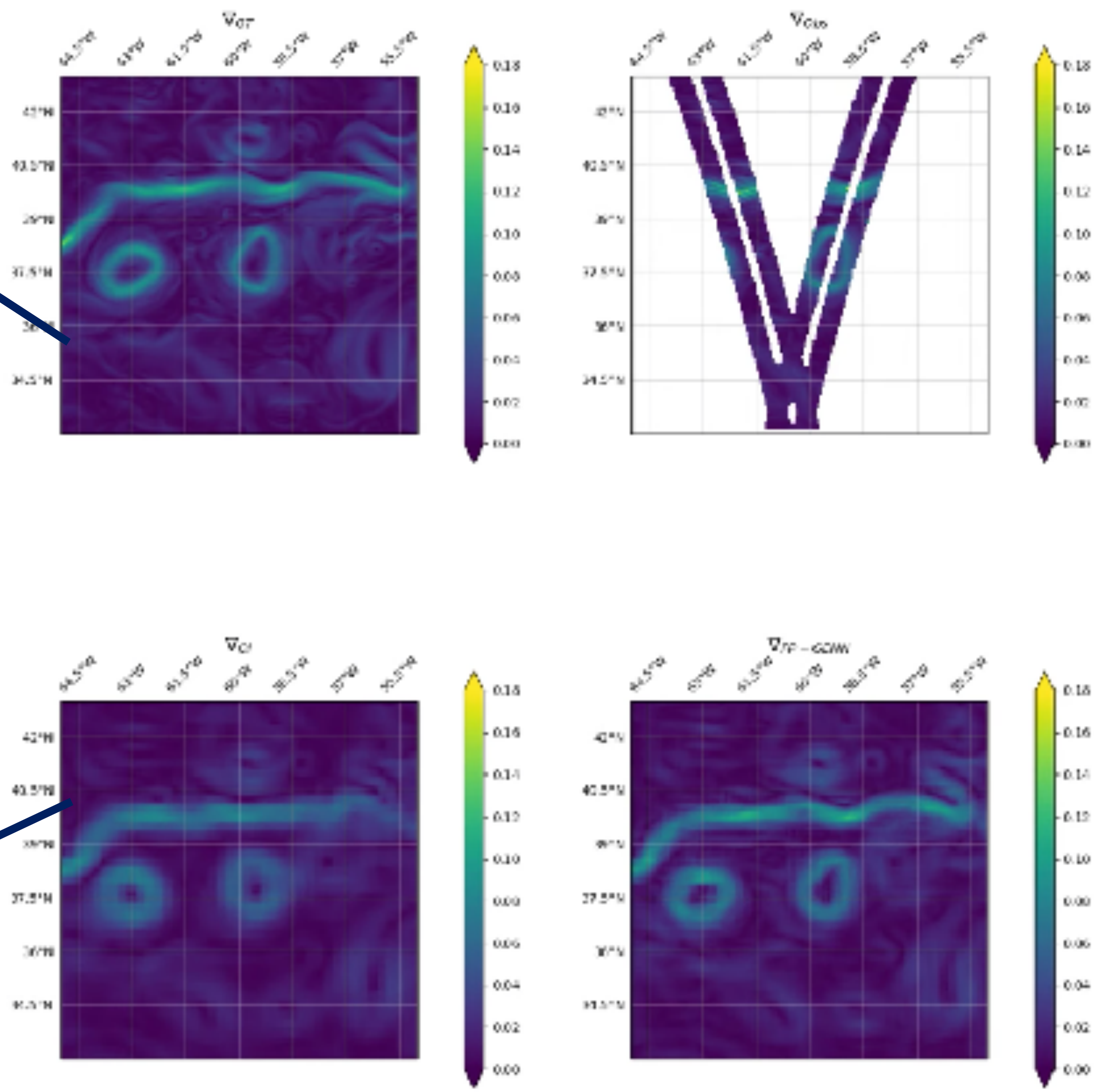
Mean relative gain of 60% in the reconstruction of the SSH using the learned sampling (~6% of the pixels vs. 1.3% for nadir altimeters)



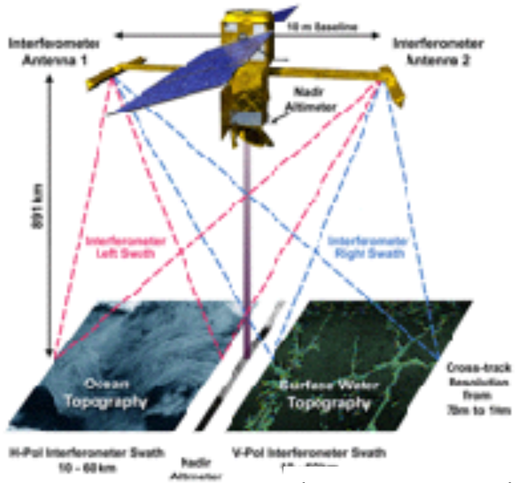
An application for upcoming SWOT mission

Groundtruth

State-of-the-art operational processing



Proposed NN framework (Fablet et al., 2019)



(From Perez et al., 2018)

End-to-end learning for inverse problems (Fablet etal., 2020)

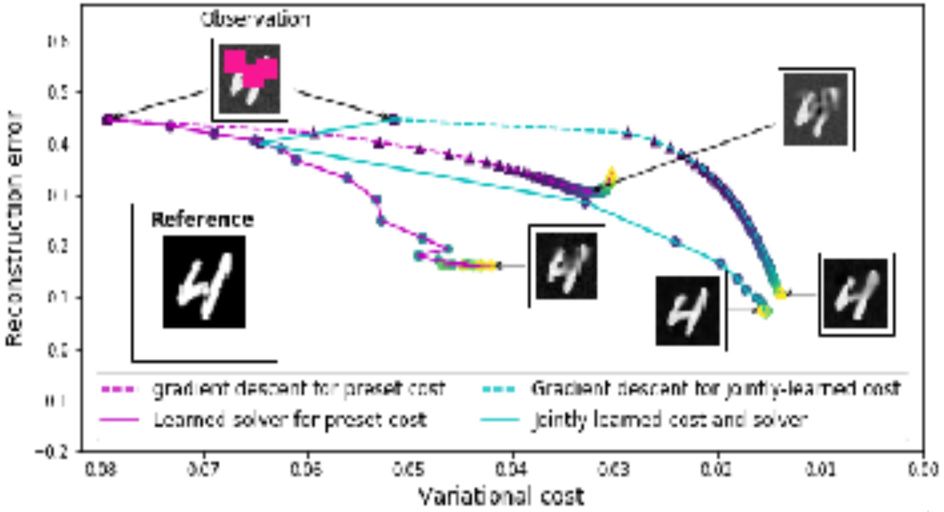
Key messages

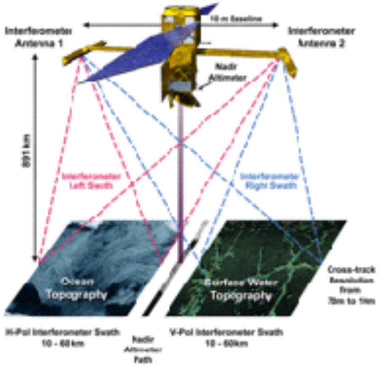
- **We can bridge DNN and variational models to solve inverse problems**

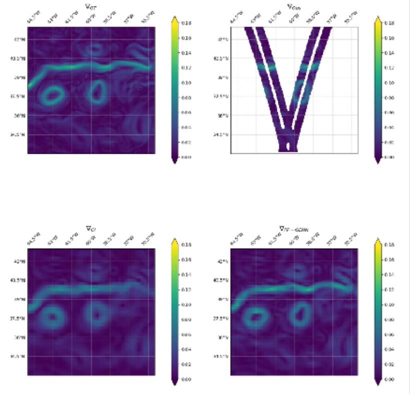
- **Learning both variational priors and solvers using groundtruthed (simulation) or observation-only data**

- **The best model may not be the TRUE one for inverse problems**

- **Generic formulation/architecture beyond space-time dynamics**





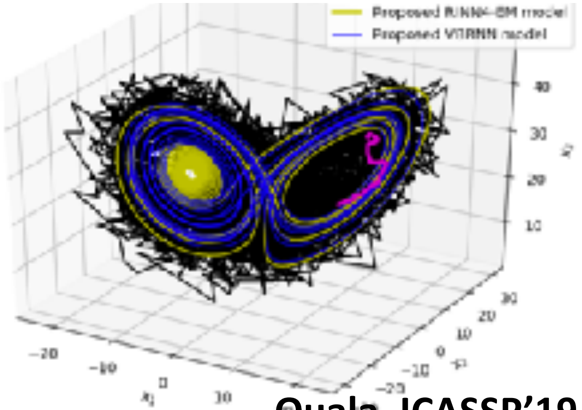


Preprint: https://arxiv.org/abs/2006.03653

Code: https://github.com/CIA-Oceanix

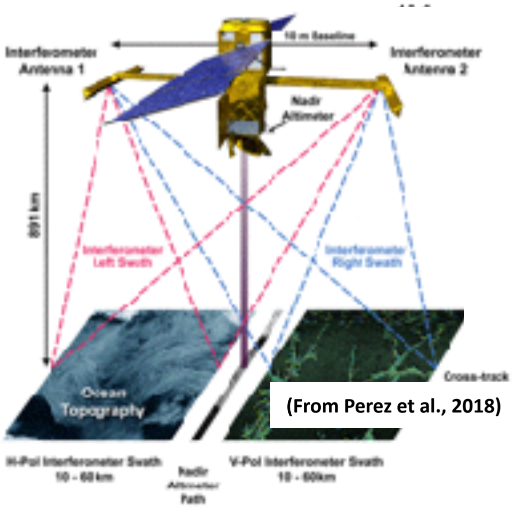
End-to-end learning from real observation data ?

Scarce time sampling

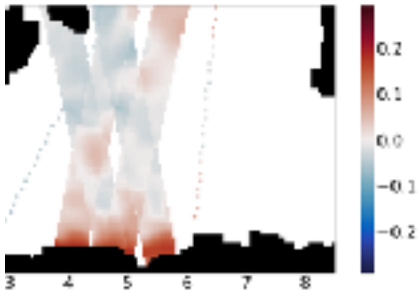


Ouala, ICASSP'19

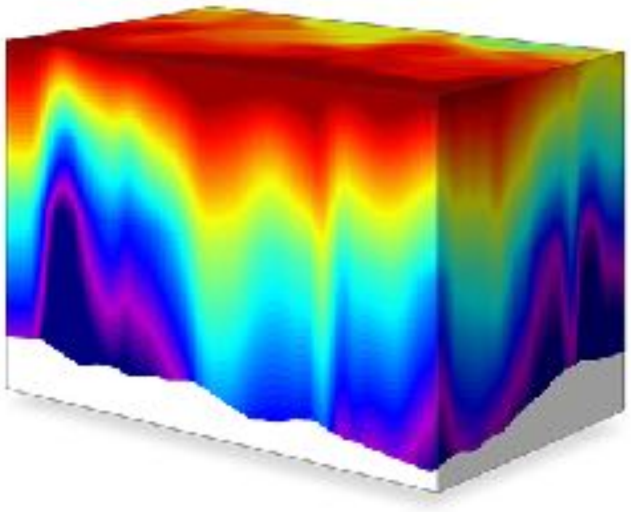
Noisy and irregular sampling



(From Perez et al., 2018)



Nguyen, ICASSP'20

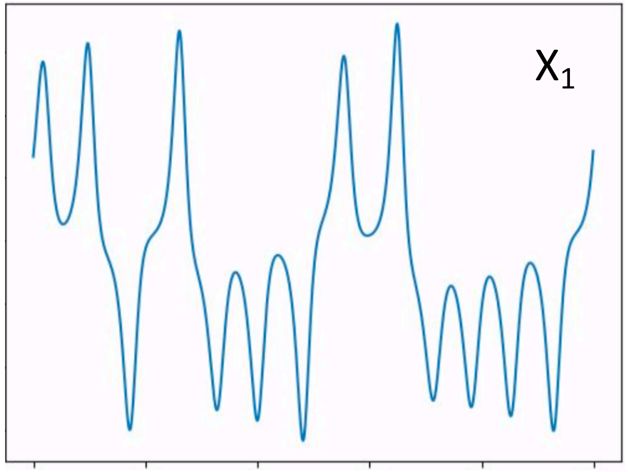


Partially-observed system

Ouala, preprint 2019

Neural ODE for partially-observed systems [Ouala et al., 2020]

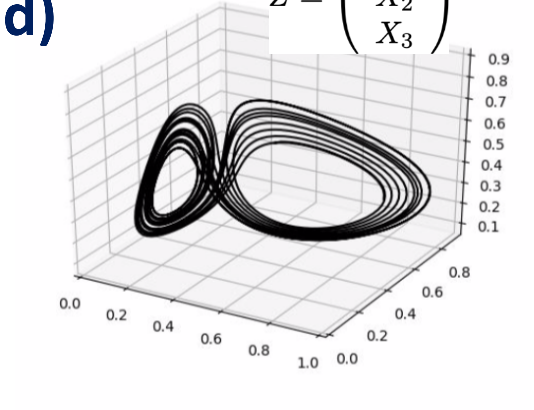
Illustration for L63 assuming only the first components is observed



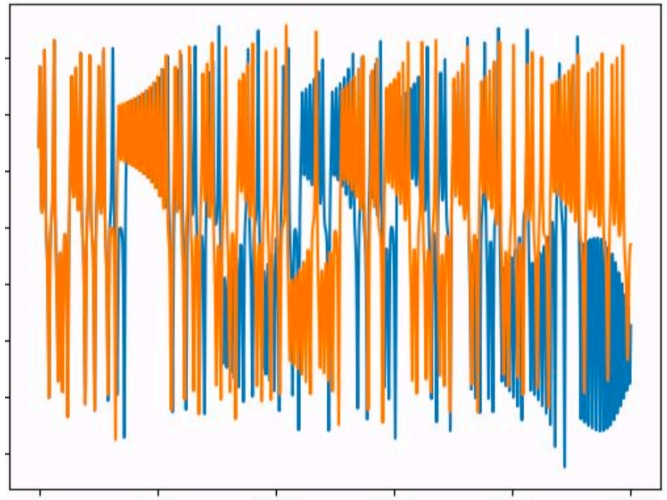
Learning Latent (unobserved) dynamics

$$d_t Z_t = \Phi_\theta(Z_t)$$

$$Z = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$



Objectives: acccurate short-term forecast and realistic « long-term » patterns for X_1



Approach: trainable variational formulation with latent dynamics

Neural ODE for partially-observed systems [Ouala et al., 2019]

Problem statement: **end-to-end learning of the latent (augmented) space and of the associated dynamics**

$$X_t = \begin{pmatrix} x_t \\ z_t \end{pmatrix}$$

Observed variables

Unknown variables

Dynamical model in the latent space

$$\partial_t X_t = f_\theta \left(X_t \right)$$

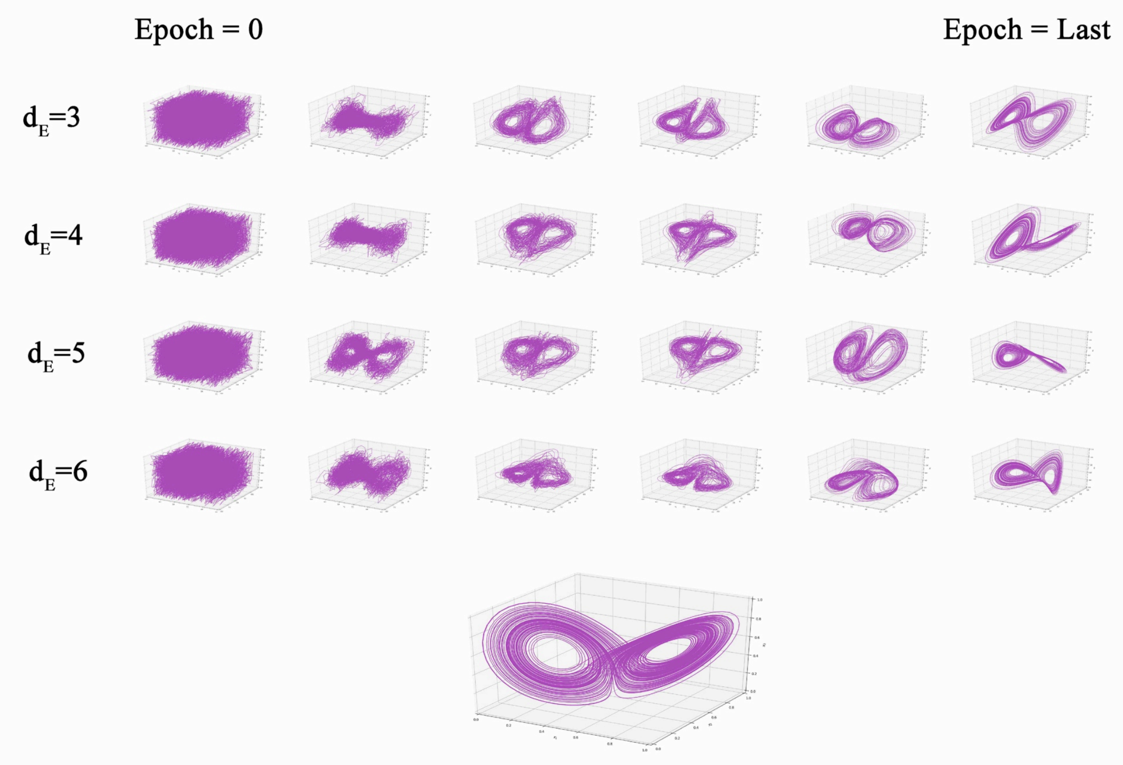
Goals:

1. **Learn model parameters θ from observed time series**
2. **Forecast future observed states given previous ones**

Proposed approach: WC 4DVar formulation with an unknown dynamical model

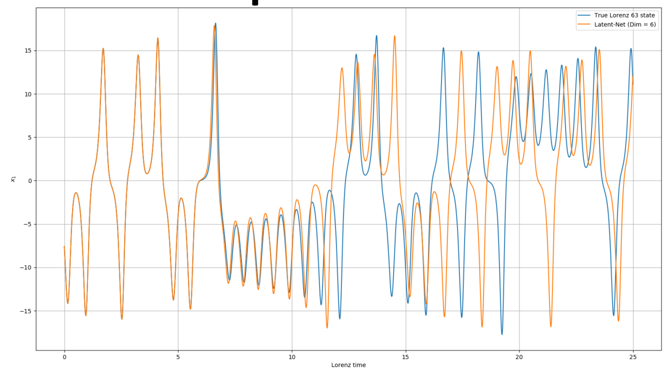
Neural ODE for partially-observed systems [Ouala et al., 2020]

Illustration on Lorenz-63 dynamics

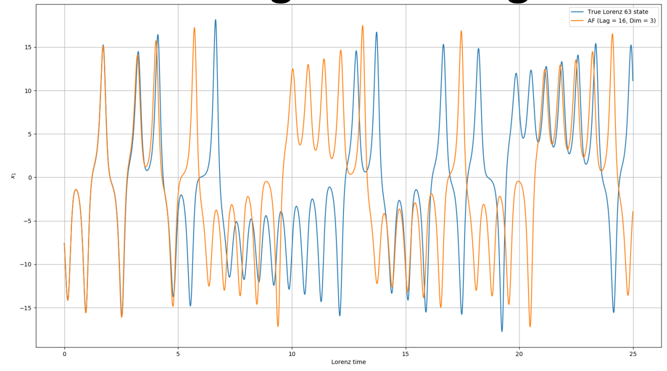


Lorenz 63 attractor

Proposed model



Analog Forecasting



Summary

- ***NNs as numerical schemes for ODE/PDE/energy-based representations of geophysical flows***

- ***Embedding geophysical priors in NN representations*** (e.g., Lguensat et al., 2019; Ouala et al., 2019)

- ***End-to-end architecture for jointly learning a representation (**eg, ODE**) and a solver*** (e.g., Fablet et al., 2020)

- ***Towards stochastic representations embedded in NN architectures*** (e.g., Pannekoucke et al., 2020, Nguyen etal., 2020)

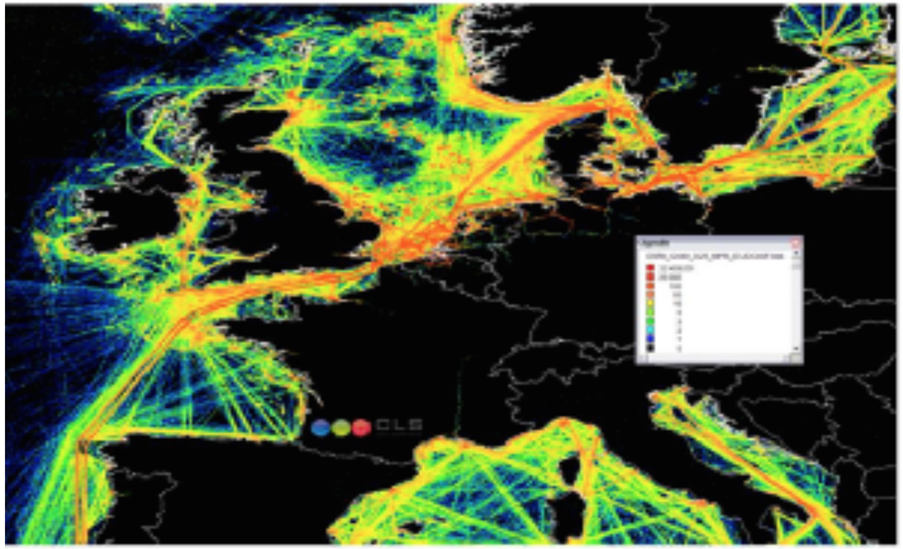
Beyond Ocean Dynamics

Learning stochastic hidden dynamics

Learning stochastic hidden dynamics [Nguyen et al., 2018]

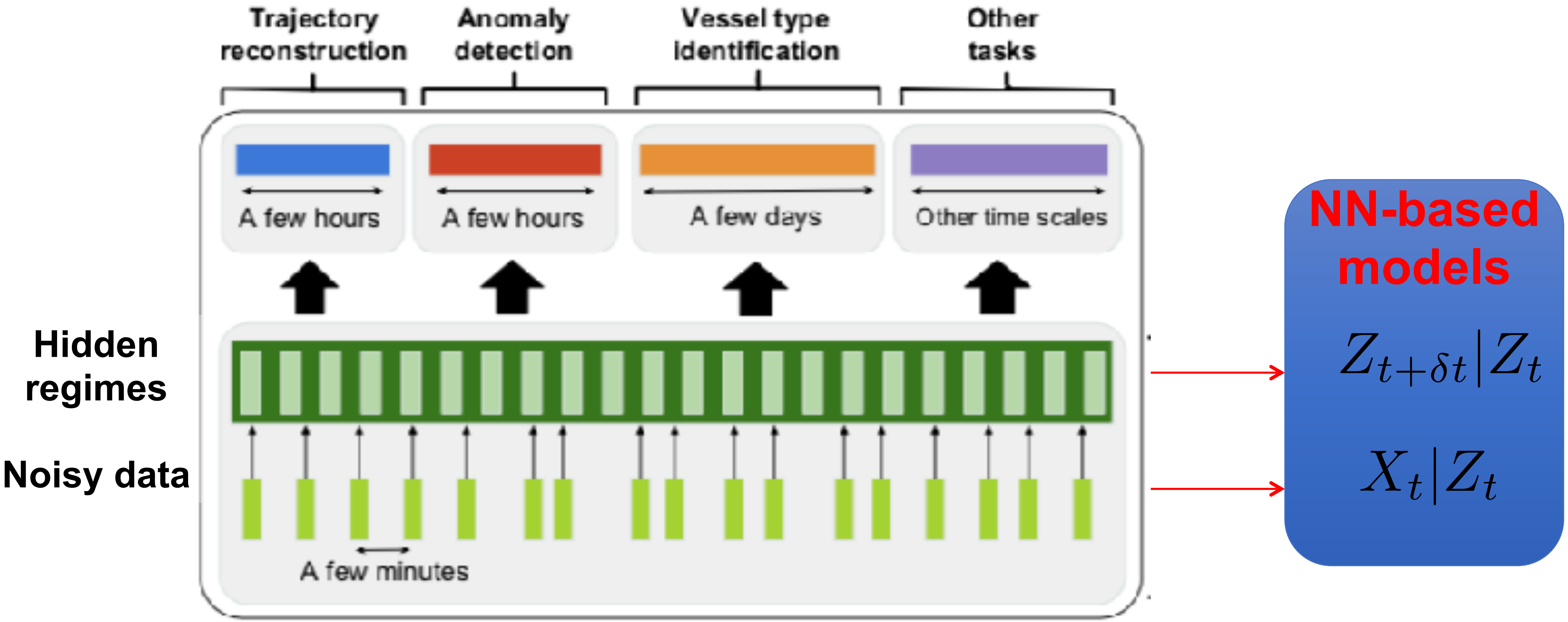
The example of AIS Vessel trajectory data

- Millions of AIS positions daily
- Noisy data: irregular sampling, corrupted data



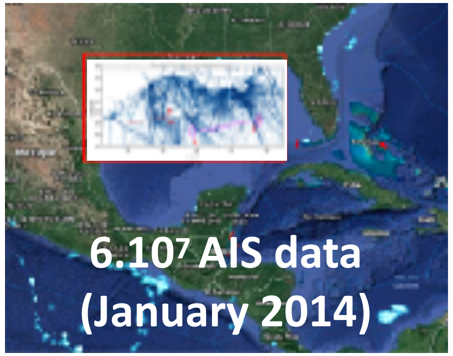
How can we learn from AIS data streams ?

Learning stochastic hidden dynamics [Nguyen et al., 2018]



Model training from noisy AIS streams using variational Bayesian approximation

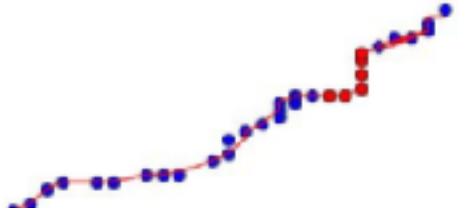
Learning stochastic hidden dynamics [Nguyen et al., 2018]

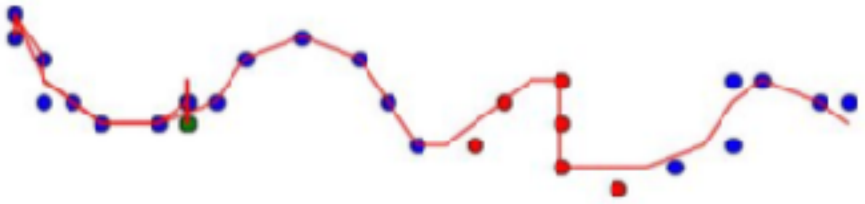


Vessel type recognition

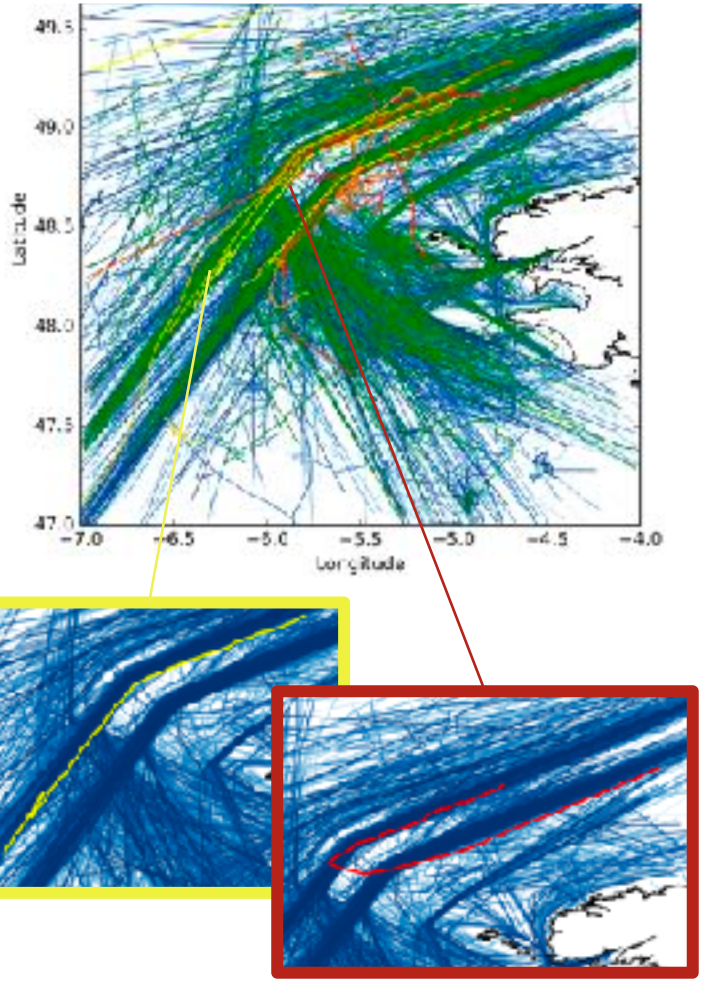
~88% of correct recognition

Trajectory reconstruction





Abnormal behaviour detection



Seabird movement simulation [Roy et al., 2021]

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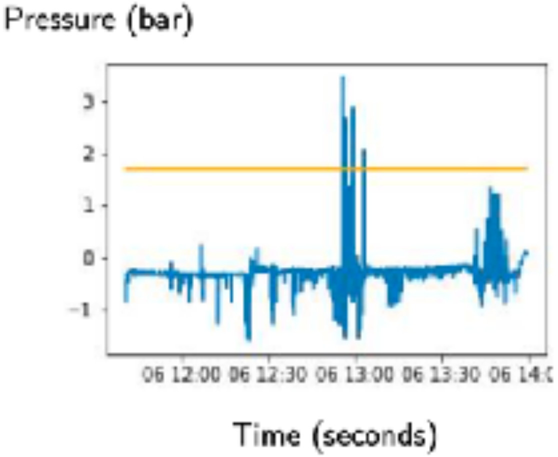
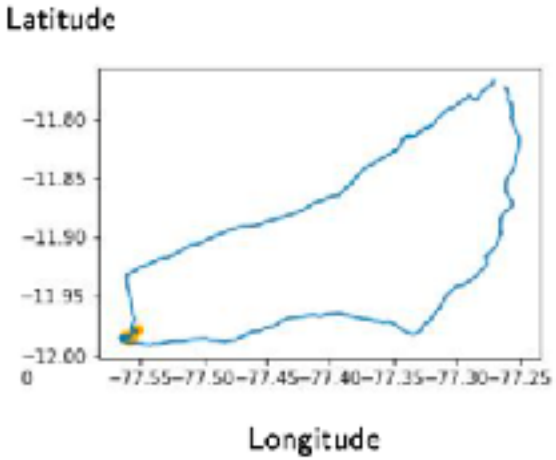
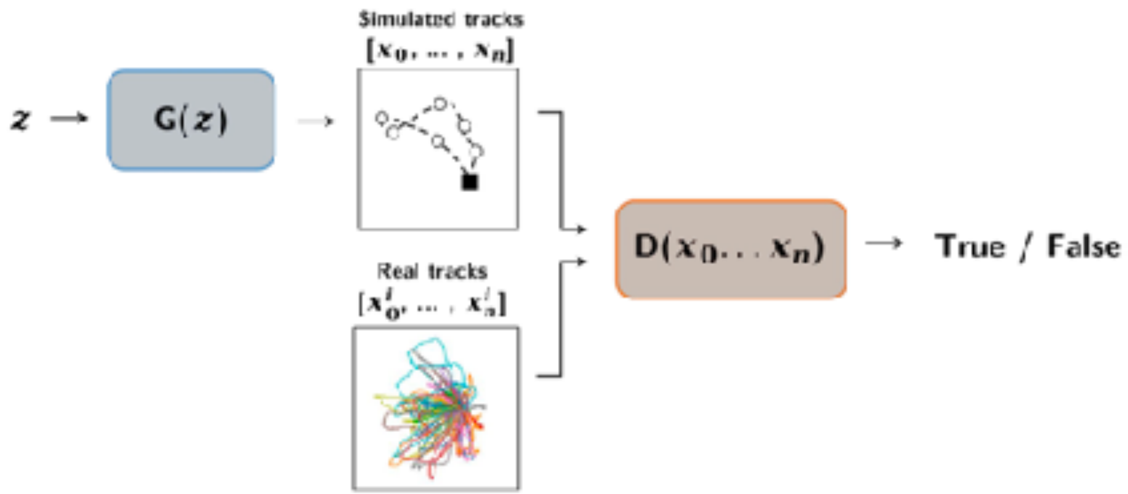




Can we learn probabilistic models to simulate seabird trajectories ?

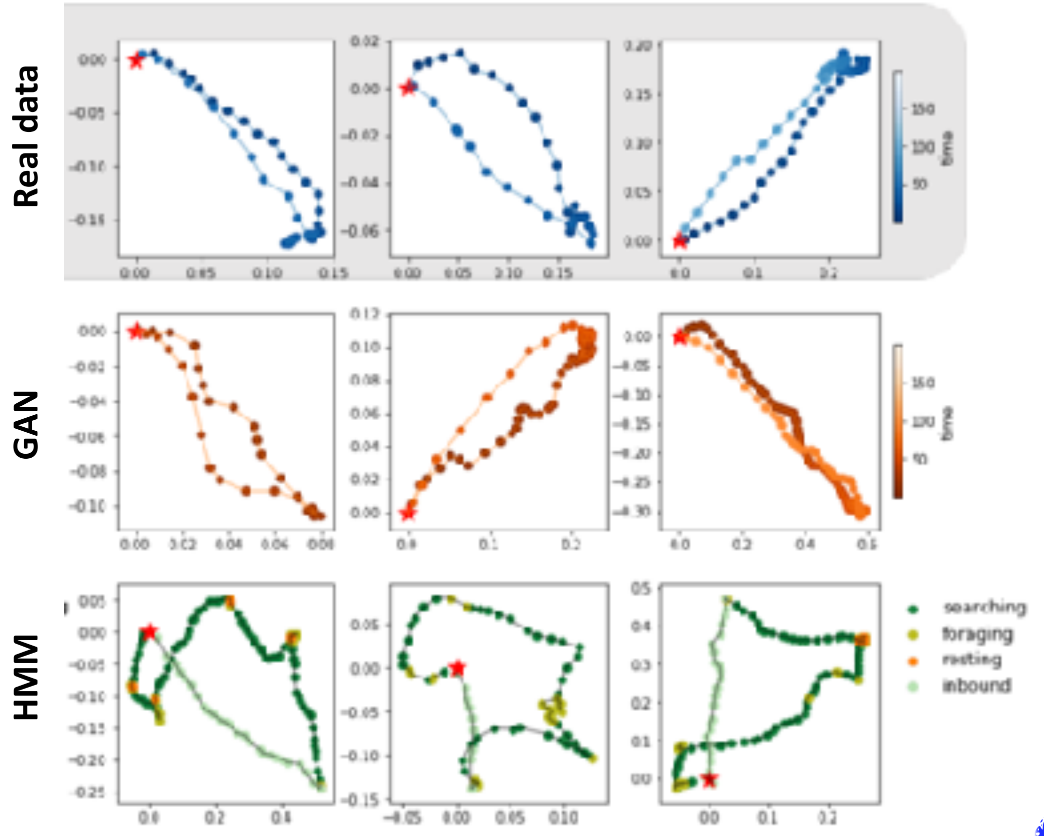
Seabird movement simulation [Roy et al., 2021]

GAN framework



Different architectures for the generator and discriminator (eg, sequential vs. Non-sequential)

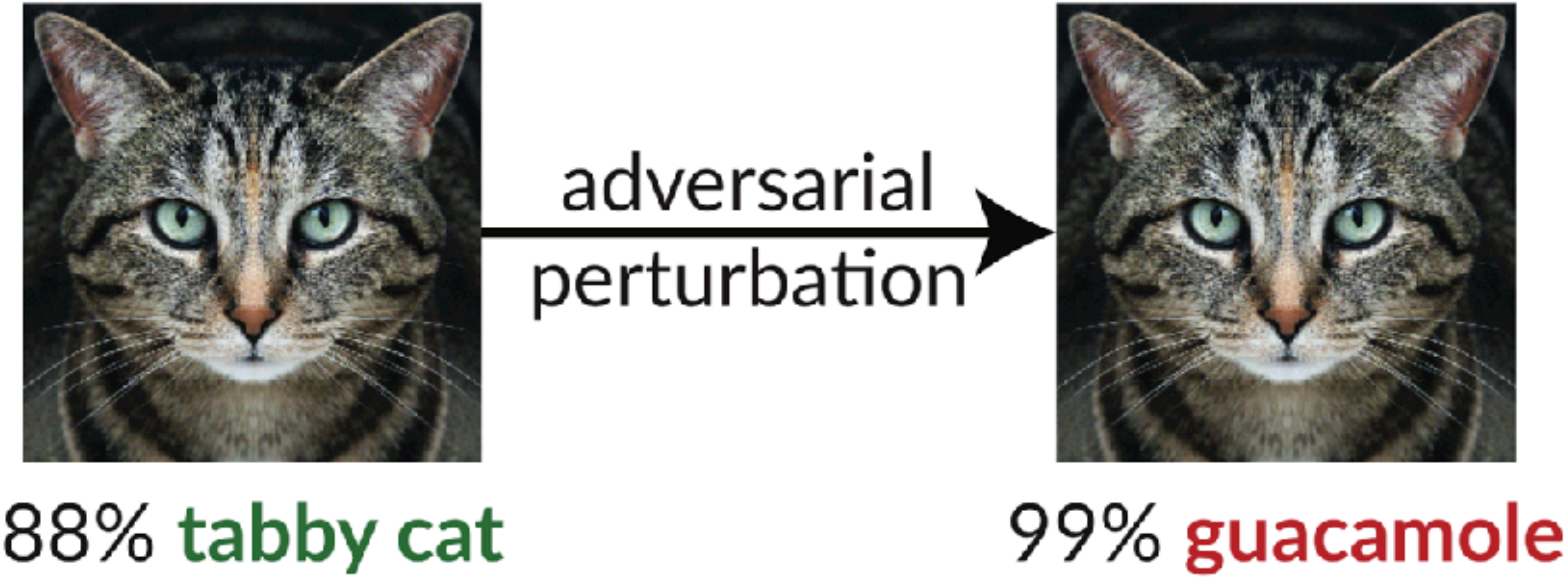
Better fit than HMM-based models



Beyond Ocean Dynamics

Dynamical System Theory for Deep Learning

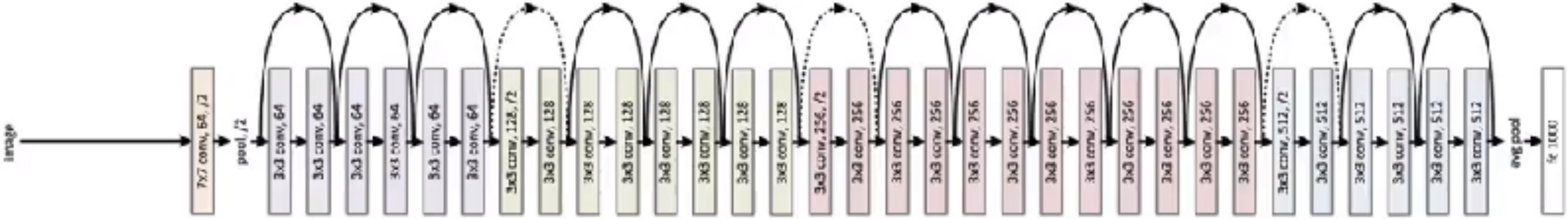
Understanding DL models ?



Szegedy et al., 2015

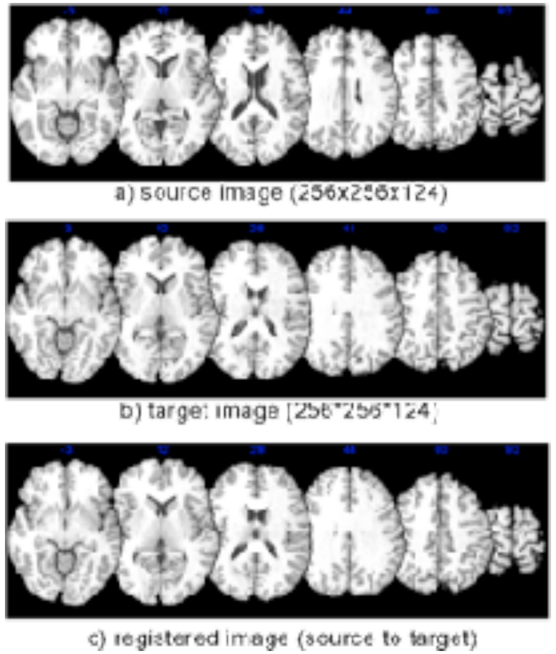
Understanding ResNets [Rousseau et al., 2019]

ResNet [He et al., 2015] regarded as space registration machines



- **Image registration examples**

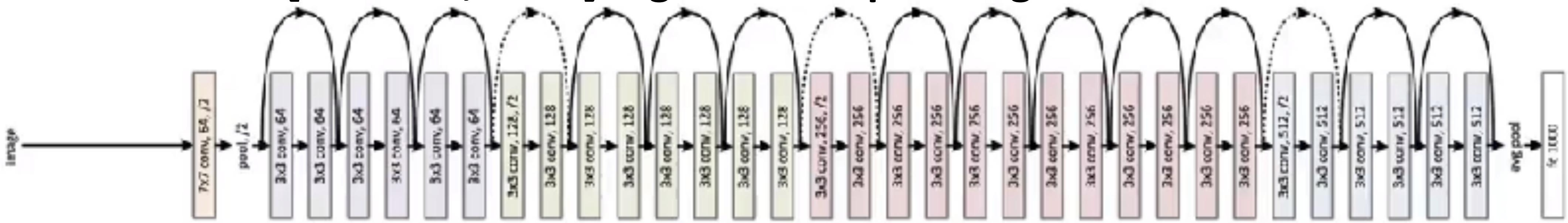
[Matlab tutorial]



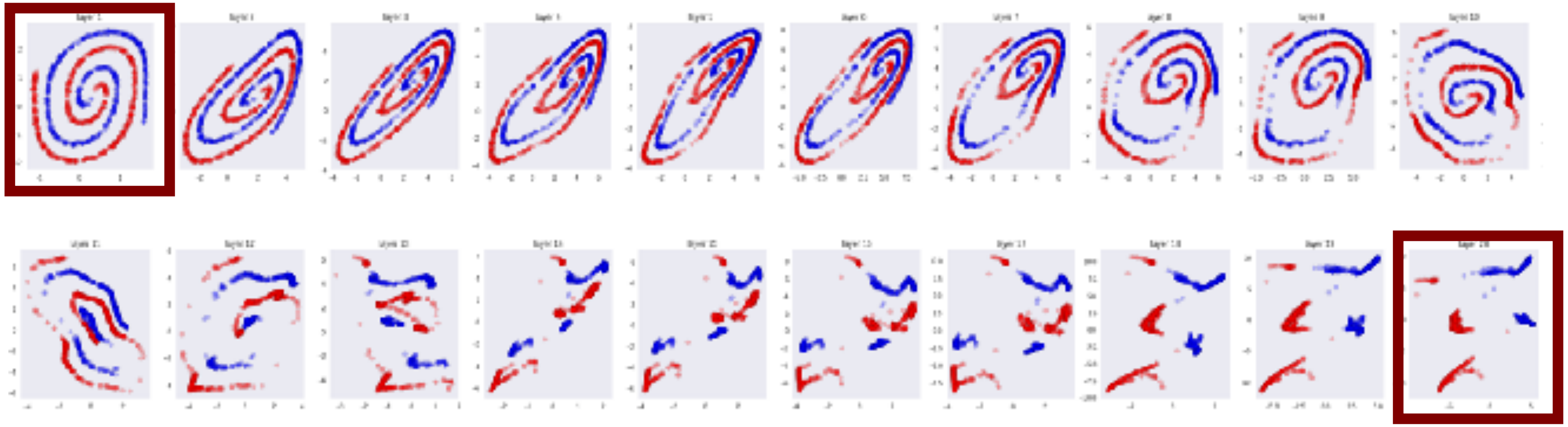
[Dramms tutorial]

Understanding ResNets [Rousseau et al., 2019]

ResNet [He et al., 2015] regarded as space registration machines



Original feature space



Registered space to make feasible a linear separation between classes

Thank you.

AI Chair OceaniX 2020-2024

Physics-informed AI for Observation-Driven Ocean AnalytiX

PI: R. Fablet, Prof. IMT Atlantique, Brest
Web: https://cia-oceanix.github.io/

Internship, PhD and postdoc opportunities

References

General Deep Learning references

- Deep Learning Book. Goodfellow et al. Online version ***http://www.deeplearningbook.org/***
- Deep Learning with Pytorch. Stevens et al. ***https://pytorch.org/assets/deep-learning/Deep-Learning-with-PyTorch.pdf***
- Physics-based deep learning. Huerey et al.

References from our team

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- Application to mapping, forecasting and optimal sampling: https://hal.archives-ouvertes.fr/hal-03189218
- AIS data streams and maritime traffic surveillance, https://hal.archives-ouvertes.fr/hal-02388260v4
- Seabird trajectory simulation, https://www.biorxiv.org/content/10.1101/2021.04.19.438554v1.full