# Machine Learning for Earth and Climate Sciences

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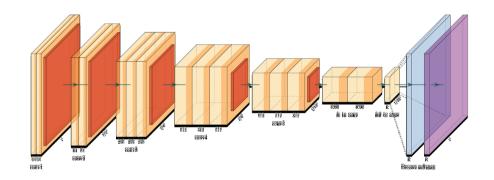


#### Earth science



# Earth observation

#### **Deep learning**



PERSPECTIVE

#### Deep learning and process understanding for data-driven Earth system science

https://doi.org/10.1038/s41586-019-0912-1

Markus Reichstein<sup>1,2#</sup>, Gustau Camps-Valls<sup>3</sup>, Bjorn Stevens<sup>4</sup>, Martin Jung<sup>1</sup>, Joachim Denzler<sup>2,5</sup>, Nuno Carvalhais<sup>1,6</sup> & Prabhat<sup>7</sup>

Reichstein, Camps-Valls et al, Nature, 2019 Camps-Valls, Tuia, Xiang, Reichstein. Wiley & Sons book, 2021 Machine learning approaches are increasingly used to extract patterns and insights from the ever-increasing stream of geospatial data, but current approaches may not be optimal when system behaviour is dominated by spatial or temporal context. Here, rather than amending classical machine learning, we argue that these contextual cues should be used as part of deep learning (an approach that is able to extract spatio-temporal features automatically) to gain further process understanding of Earth system science problems, improving the predictive ability of seasonal forecasting and modelling of long-range spatial connections across multiple timescales, for example. The next step will be a hybrid modelling approach, coupling physical process models with the versatility of data-driven machine learning. EDITED BY GUSTAU CAMPS-VALLS • DEVIS TUIA XIAO XIANG ZHU • MARKUS REICHSTEIN

#### **DEEP LEARNING** FOR THE **EARTH SCIENCES**

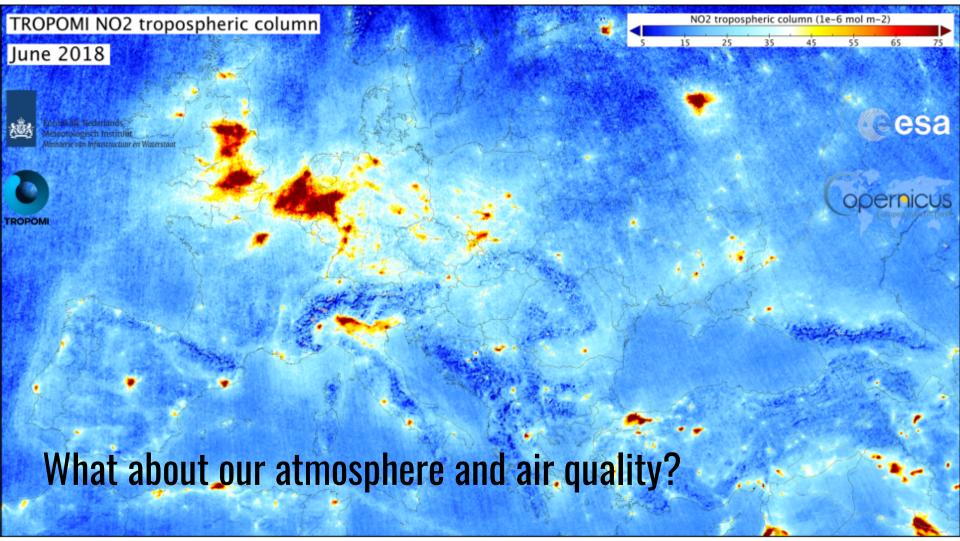
A COMPREHENSIVE APPROACH TO REMOTE SENSING, CLIMATE SCIENCE AND GEOSCIENCES

WILEY



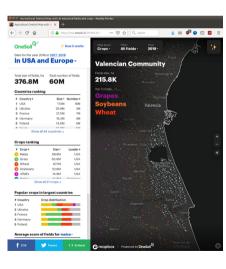
# Prediction of crop yield from space

# How is our coastline and ocean?



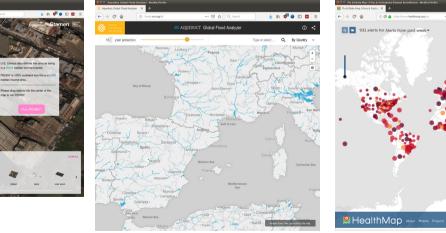
# Some machine learning applications

#### **One soil map** https://map.onesoil.ai



#### Global wealth map http://penny.digitalglobe.com

# Flood analyzer alglobe.com http://floods.wri.org



#### **Disease mapping** https://www.healthmap.org

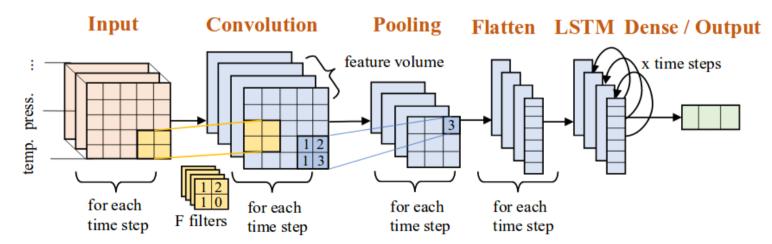


## Al opportunities



### Neural networks for spatio-temporal classification

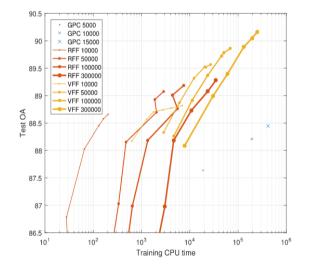
- Convolutional neural nets (CNN): hierarchical structure exploits spatial relations
- Long short-term memory (LSTM): recurrent network that accounts for memory/dynamics

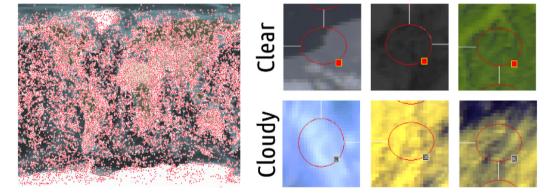


"A Deep Network Approach to Multitemporal Cloud Detection" Tuia and Camps-Valls, IEEE IGARSS 2018, http://isp.uv.es/code/landmarks.html

#### Probabilistic and scalable classifiers

- Gaussian processes as an alternative to neural nets
- GPs allow a probabilistic treatment, confidence intervals, feature ranking, deep too!
- Gaussian processes start to be scalable ...





"Remote Sensing Image Classification With Large-Scale Variational Gaussian Processes," Morales, Molina and Camps-Valls, IEEE Trans. Geosc. Rem. Sens, 2018

## **Multitask learning**

- Multiple inter-related outputs? Data from multiple sources?
- Learn to fuse heterogeneous information

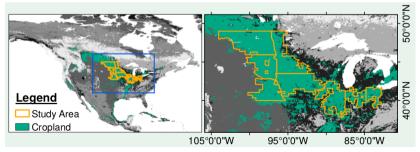


"**Multitask Remote Sensing Data Classification**" Leiva and Camps-Valls, IEEE Trans. Geosc, Rem. Sens 2015

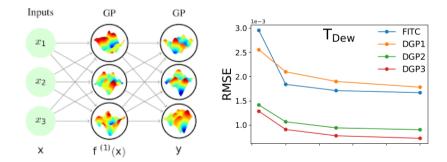
#### Spatio-temporal variable prediction

- **STA** is common place in climate informatics, neuroscience, video processing, NLP, ...
- **Current approaches:** CNN + LSTM, space-time Gaussian processes
- Novel approaches: distribution regression and variational deep GPs

 $P \mapsto \mu_k(\mathcal{P}) \to \mathcal{P} \mapsto [\mathbb{E}\phi_1(X), \dots, \mathbb{E}\phi_s(X)] \in \mathbb{R}^s \\ \langle \mu_k(\mathcal{P}), \mu_k(\mathcal{Q}) \rangle_{\mathcal{H}_k} = \mathbb{E}_{X \sim \mathcal{P}, Y \sim \mathcal{Q}} k(X, Y)$ 



"Nonlinear Distribution Regression for Remote Sensing Applications" Adsuara, Perez,Muñoz, Mateo, Piles, Camps-Valls, IEEE TGARS 2019

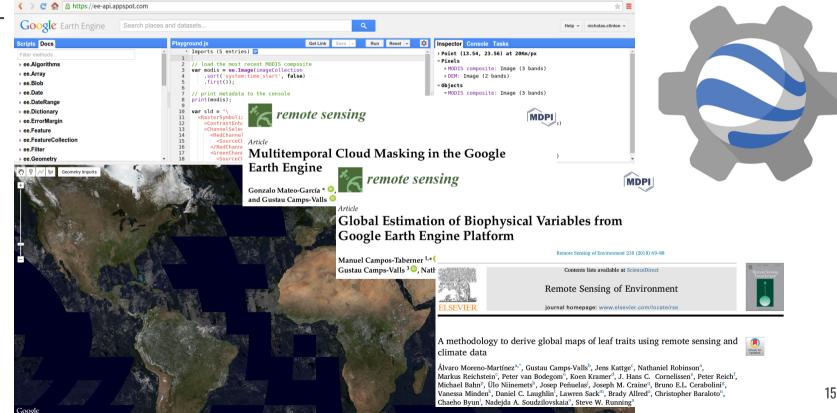


"A Survey on Gaussian Processes for Earth Observation Data Analysis" Camps-Valls et al. IEEE Geoscience and Remote Sensing Magazine 2016

**"Deep Gaussian Processes for Retrieval of bio-geo-physical parameters",** Svendsen, Ruescas and Camps-Valls, IEEE Trans. Geosc. Rem. Sens, 2019

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# **Google Earth Engine**



#### Potential risks and challenges



# ML in Earth science rocks... <u>only</u> when some things happen!

- Strong spatial and temporal correlations
- Big data accessible
- Cheap computing resources available
- Fast scalable ML models available
- No expert knowledge needed
- High prediction accuracy is enough
- Understanding the system is not that relevant

### Machine/deep learning challenges

- **Do Models respect Physics Laws? Physics-aware ML**
- What did the ML model learn? Explainable AI (XAI)
- **Do they get cause-effect relations? Causal discovery and inference**



The New Hork Times

Opinion

#### **Eight (No, Nine!) Problems With Big Data**

By Gary Marcus and Ernest Davis

<b>nature</b> International weekly journal of science											
Home	News & Comment	Research	Careers & Jobs	Current Issue	Archive	Audio &					
Archive	Volume 538	Issue 7623	News Feature	Article							

#### NATURE | NEWS FEATURE

#### Can we open the black box of AI?

Artificial intelligence is everywhere. But before scientists trust it, they first need t understand how machines learn.

#### Davide Castelvecchi



XΛ	
AA	

Methods	HSI	ANN	Mechansim		
CAM with global average pooling [41], [90]	×	√			
+ Grad-CAM [42] generalizes CAM, utilizing gradient	$\checkmark$	$\checkmark$			
+ Guided Grad-CAM and Feature Occlusion [67]	×	$\checkmark$			
+ Respond CAM 43	×	$\checkmark$			
+ Multi-layer CAM 91	×	$\checkmark$			
LRP (Layer-wise Relevance Propagation) [13], [52]	×	N.A.			
+ Image classifications. PASCAL VOC 2009 etc [44]	×	$\checkmark$			
+ Audio classification. AudioMNIST [46]	×	$\checkmark$	Decomposition		
+ LRP on DeepLight. fMRI data from Human Connectome Project [47]	×	$\checkmark$			
+ LRP on CNN and on BoW(bag of words)/SVM [48]	×	$\checkmark$		s	
+ LRP on compressed domain action recognition algorithm [49]	×	×		E.	
+ LRP on video deep learning, selective relevance method [51]	×	✓		Saliency	
+ BiLRP 50	×	$\checkmark$		19	
DeepLIFT [56]	×	$\checkmark$			2
Prediction Difference Analysis 57	×	$\checkmark$			
Slot Activation Vectors [40]	×	✓			p
PRM (Peak Response Mapping) 58	×	$\checkmark$			
LIME (Local Interpretable Model-agnostic Explanations) [14]		√			
+ MUSE with LIME [84]	$\checkmark$	$\checkmark$	Sensitivity		
+ Guidelinebased Additive eXplanation optimizes complexity, similar to LIME [92]	✓	✓	Sensitivity		Pic Pic
# Also listed elsewhere: [55], [68], [70], [93]	N.A.	N.A.			ta
Others. Also listed elsewhere: 94	N.A.	N.A.			Perceptive Interpretability
+ Direct output labels. Training NN via multiple instance learning [64]	×	$\checkmark$	Others		2
+ Image corruption and testing Region of Interest statistically [65]	×	$\checkmark$	Others		
+ Attention map with autofocus convolutional layer [66]	×	✓			
DeconvNet [71]	×	~			1
Inverting representation with natural image prior [72]	×	$\checkmark$	Inversion		
Inversion using CNN [73]	×	✓	Inversion		
Guided backpropagation [74], [90]	×	✓		S	
Activation maximization/optimization [37]	×	√		Signal	
+ Activation maximization on DBN (Deep Belief Network) [75]	×	$\checkmark$		<u>a</u>	
+ Activation maximization, multifaceted feature visualization [76]	×	$\checkmark$	Optimization		
Visualization via regularized optimization [77]	×	$\checkmark$			
Semantic dictionary [38]	×	$\checkmark$			
Decision trees	N.A.	N.A.			1
Propositional logic, rule-based [81]		×	Verbal		
Sparse decision list [82] Decision sets, rule sets [83], [84]		×			
		×			
Encoder-generator framework 85	×	$\checkmark$			
Filter Attribute Probability Density Function [86]	×	×			
MUSE (Model Understanding through Subspace Explanations) [84]	$\checkmark$	$\checkmark$			

"A Survey on Explainable Artificial Intelligence(XAI): towards Medical **XAI**", Tjoa 2019 "Advancing Deep Learning For Earth Sciences: From Hybrid Modeling To Interpretability", Camps-Valls, G. and

Reichstein, M. and Zhu, Z. and Tuia, D. IEEE IGARSS (2020)

### **Physics-aware ML**

Data-model blendingJoint Gaussian processesDistribution regression

Surrogate modeling Gaussian processes Bayesian optimization

Learning to parameterize Variational inference Monte Carlo, Gibbs **Learning physics** Sparse regression Latent force models

#### PERSPECTIVE

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Machine learning approaches are increasingly used to extract patterns and insights from the ever-increasing stream of geospatial data, but current approaches may not be optimal when system behaviour is dominated by spatial or temporal context. Here, rather than amending classical machine learning, we argue that these contextual cues should be used as part of deep learning (an approach that is able to extract spatio-temporal features automatically) to gain further process understanding of Earth system science problems, improving the predictive ability of seasonal forecasting and modelling of long-range spatial connections across multiple timescales, for example. The next step will be a hybrid modelling approach, coupling physical process models with the versatility of data-driven machine learning.

"Deep learning and process understanding for data-driven Earth System Science", Reichstein, Camps-Valls et al. Nature, 2019.

"Living in the Physics - Machine Learning Interplay for Earth Observation"

Camps-Valls et al. AAAI Fall Series 2020 Symposium on Physics-guided AI for Accelerating Scientific Discovery, 2020. arxiv.org/abs/2010.09031

# **Causality**

PERSPECTIVE

COMMUNICATIONS

https://doi.org/10.1038/s41467-019-10105-3

#### Inferring causation from time series in Earth system sciences

OPEN

Jakob Runge <sup>1,2</sup>, Sebastian Bathiany<sup>3,4</sup>, Erik Bollt<sup>5</sup>, Gustau Camps-Valls<sup>6</sup>, Dim Coumou<sup>7,8</sup>, Ethan Devle<sup>9</sup>, Clark Glymour<sup>10</sup>, Marlene Kretschmer<sup>8</sup>, Miguel D. Mahecha <sup>11</sup>, Jordi Muñoz-Marí<sup>6</sup>, Egbert H. van Nes<sup>4</sup>, Jonas Peters<sup>12</sup>, Rick Quax<sup>13,14</sup>, Markus Reichstein<sup>11</sup>, Marten Scheffer<sup>4</sup>, Bernhard Schölkopf<sup>15</sup>, Peter Spirtes<sup>10</sup>, George Sugihara<sup>9</sup>, Jie Sun <sup>5,16</sup>, Kun Zhang<sup>10</sup> & Jakob Zscheischler () 17,18,19

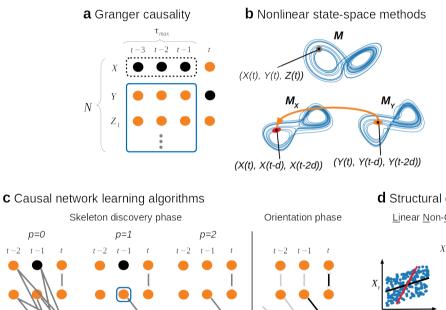
IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING

#### Causal Inference in Geoscience and Remote Sensing From Observational Data

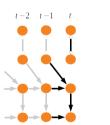
Adrián Pérez-Suay<sup>®</sup>, Member, IEEE, and Gustau Camps-Valls<sup>®</sup>, Fellow, IEEE

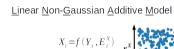
this is of special relevance to better understand the earth's system and the complex interactions between the governing processes.

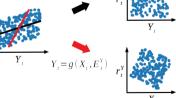
Abstract-Establishing causal relations between random vari- with societal, economical, and environmental challenges, such ables from observational data is perhaps the most important as climate change [2], [3]. There is an urgent need for tools challenge in today's science. In remote sensing and geosciences, that help us to observe and study the earth system. Nowadays, machine learning and signal processing play a crucial role in



#### **d** Structural causal models







"Inferring causation from time series with perspectives in Earth system sciences", Runge, Bathiany, Bollt, Camps-Valls, et al. Nat Comm., 2019 "Causal Inference in Geoscience and Remote Sensing from Observational Data," Pérez-Suay and Camps-Valls, IEEE Trans. Geosc. Rem. Sens, 2018 "CauseMe: An online system for benchmarking causal inference methods," Muñoz-Marí, Mateo, Runge, Camps-Valls. In preparation (2019), CauseMe: http://causeme.uv.es

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#### **ELLIS, ELISE and AIDA**



## ELLIS.eu



- ELLIS: European Laboratory for Learning and Intelligent Systems
- Distributed center of excellence in Al
- ELLIS goals and mandates:
  - Coordinates research, fosters collaborations with industry and users, promotes technology adoption, support PhD fellowships & postdoc visits/stays, organize focused workshops
- ELLIS legacy:
  - place Europe in the global map of top Al research and transfer to industry
  - Make Europe an international talent magnet, incubator of innovation, and ecosystem
- Largely multidisciplinary & organized in Research Programs:
  - Robotics, robustness, health, language processing, earth, etc.

#### https://ellis.eu

# **ELLIS.eu & ELISE-AI**



elise European Network of Al Excellence Centres

- ELLIS is Largely multidisciplinary & organized in Research Programs:
  - Robotics, robustness, health, language processing, etc.
- "Machine learning for Earth and climate sciences" (Dir.: Gustau Camps & Markus Reichstein)
  - **<u>Goal</u>**: Model & understand the Earth with Machine Learning and Process Understanding
    - Spatio-temporal anomaly and extreme events detection, anticipation and attribution
    - Data-driven dynamic modelling and forecasting
    - Hybrid modeling: linking physics and machine learning models
    - Causal inference, Learning and explaining feature representations
    - Earth and Climate model emulation, generative modelling and data-model fusion
  - 20 ELLIS Fellow members, regular meetings/workshops, exchange students, teaching material
- Universitat de València is a core center in the ICT-48 project ELISE

#### https://www.elise-ai.eu/

# **AIDA - AI Doctoral Academy**



- All ICT-48 networks (Al4Media, ELISE, HumanE-Al NET, TAILOR) + VISION consortium joined forces
- New joint instrument to support world-level AI education and research programme
- AIDA offers:
  - access to resources, knowledge & expertise for the latest developments and trends on Al research and innovation
  - operate as an umbrella organisation for AI PhD and Postdoc studies
  - support a new generation of alumni
  - enhance networking and collaboration among talented researchers
  - provide access to workshops/conferences, short courses, mobilities, training/job opportunities

#### https://www.i-aida.org/

## Conclusions

#### Take-home message

- Al is a paradigm shift
  - Excel in classification, (change) detection, parameter retrieval
  - Automate & understand processes
- Challenges: interpretability + causal relations + physics consistency
- Future:
  - User-centric AI + trustworthiness + accountability
  - Holistic & interdisciplinary education

**"Towards a Collective Agenda on AI for Earth Science Data Analysis"** Tuia, Roscher, Wegner, Jacobs, Zhu, and Camps-Valls, G. IEEE Geoscience and Remote Sensing Magazine 2021, arxiv.org/abs/2104.05107 **"Living in the Physics - Machine Learning Interplay for Earth Observation"** Camps-Valls et al. AAAI Fall Series 2020 Symposium on Physics-guided AI for Accelerating Scientific Discovery, 2020. arxiv.org/abs/2010.09031