Advances in Machine Learning for Earth Observation

Gustau Camps-Valls Image Processing Lab (IPL) Universitat de València











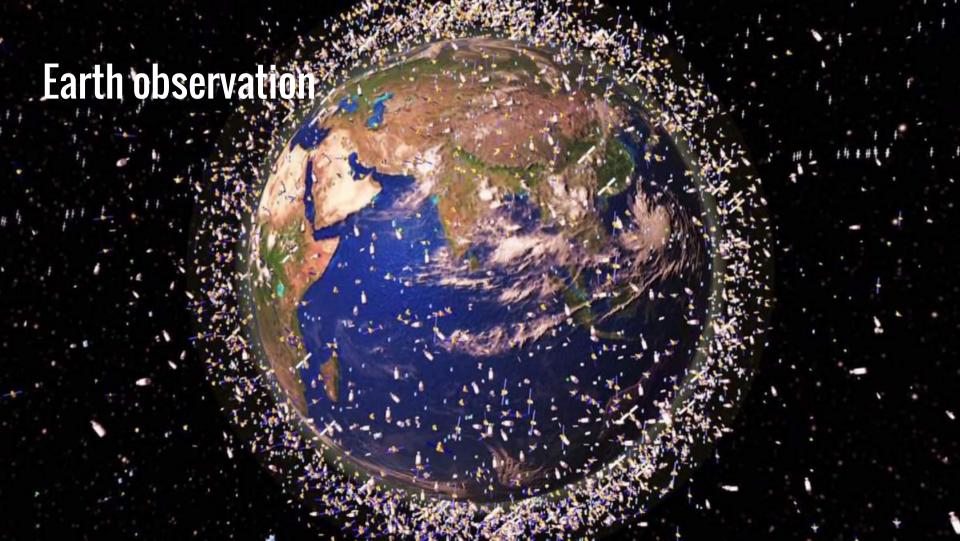


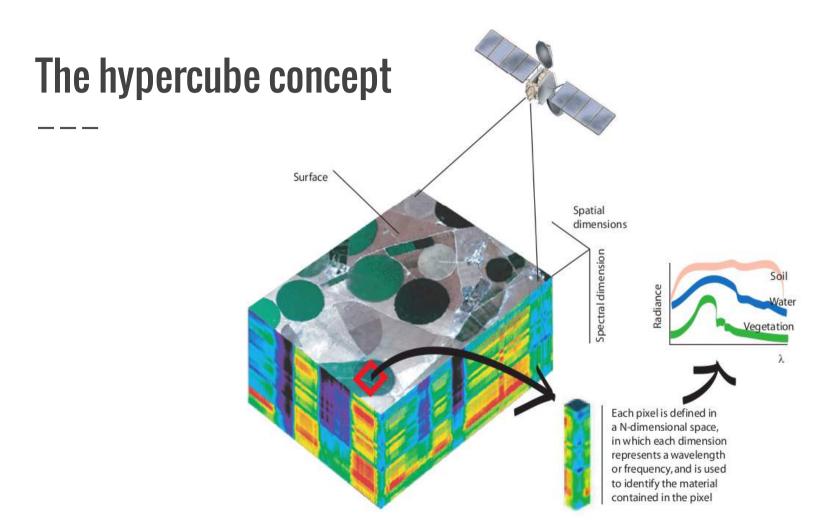
Earth observation



Earth observation

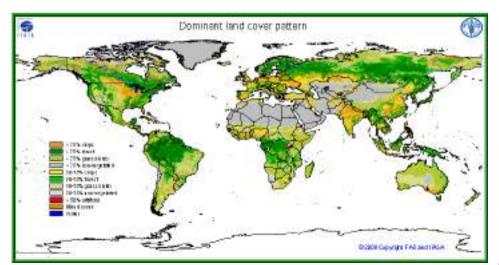
"Earth observation (EO) is the gathering of information about planet Earth's physical, chemical and biological systems via remote sensing technologies supplemented by earth surveying techniques, encompassing the collection, analysis and presentation of data"

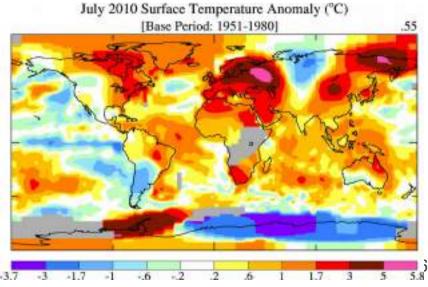




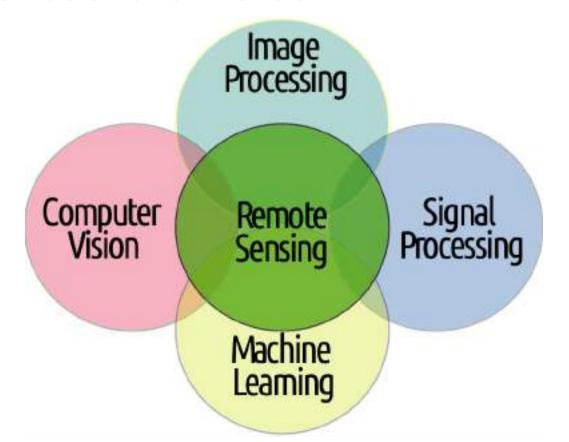
Earth observation applications

- Identify objects, classify the land cover and detecting changes
- Estimate the content of bio-geo-physical and bio-chemical prameters





Earth observation and friends



Earth observation meets machine learning

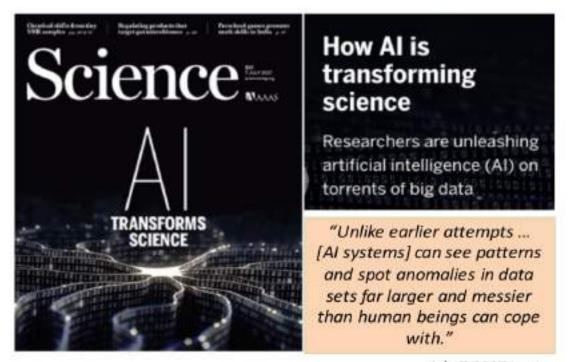


Machine learning

F(X) = y

- X: observations, independent covariates
- Y: target, dependent variable
- F: machine learning model (nonlinear, nonparametric, flexible, learned from data)

Al promises to transform scientific discovery ...







... yet only when some things happen!

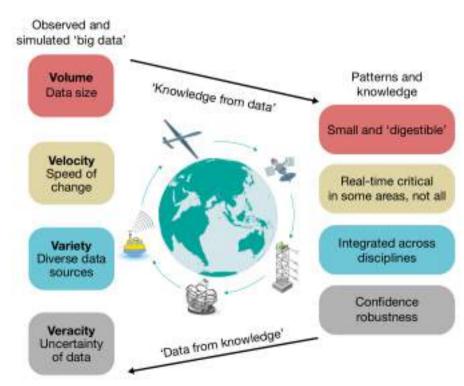
- Strong spatial and temporal correlations
- Big data accessible
- Cheap computing resources available
- Fast scalable ML models available
- No expert knowledge needed
- High prediction accuracy is enough

Challenges in Earth system science



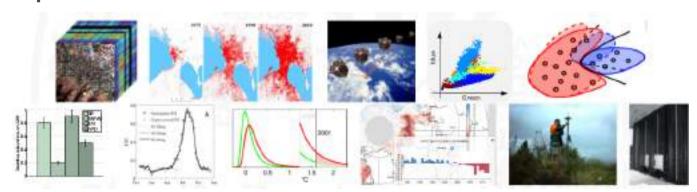
Big data challenges

- 1. Data size now exceeds 100 petabytes, and is growing quasi-exponentially
- 2. The speed of change exceeds 5 petabytes a year, and acquisition frequencies of 10 Hz or more;
- 3. Reprocessing and versioning are common challenges
- 4. Data sources can be multi-dimensional, spatially integrated, from the organ level (such as leaves) to the global level
- 5. Earth has diverse observational systems, from remote sensing to in situ observations
- 6. The uncertainty of data can stem from observational errors or conceptual inconsistencies



Statistical challenges

- 1. High dimensional data: multi-temporal, multi-angular and multi-source
- 2. Non-linear and non-Gaussian feature relations
- 3. Data misalignments and distortions
- 4. Irrelevant features and biased sampling strategies
- 5. Uneven sampling, skewed distributions and anomalies in the wild
- 6. Few supervised information is available



Philosophical challenges

Consistency issue: ML models do not respect Physics

Learning issue: ML are excellent approximators, yet no fundamental laws are learned

Interpretability issue: Big data is good to estimate correlations, what about causations?



The New Hork Times

Opinion

OP-ED CONTRIBUTORS

Eight (No, Nine!)
Problems With Big Data

By Gary Marcus and Ernest Davis

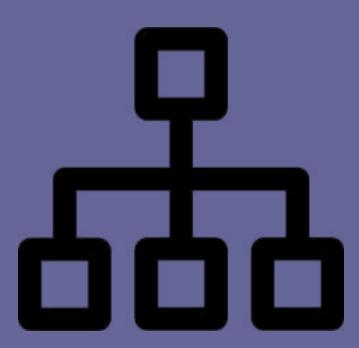


Outline

- 1. Advances in spatio-temporal data processing
 - Classification
 - Regression
 - Dimensionality reduction
- 2. Big data in the Google cloud
- 3. ML models should be consistent with Physics
- 4. Understanding is more important than predicting

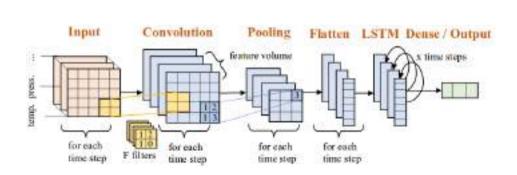


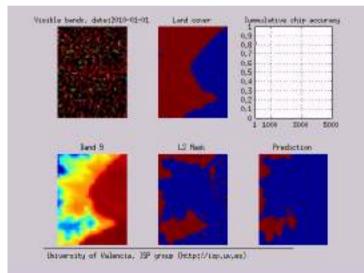
Spatio-temporal data classification



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



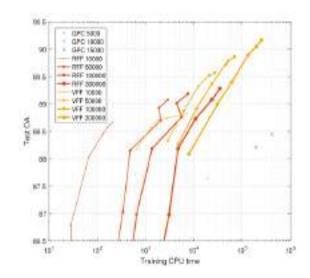


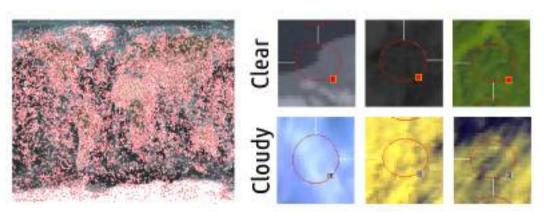
Tuia and Camps-Valls, IEEE IGARSS 2018, http://isp.uv.es/code/landmarks.html

[&]quot;A Deep Network Approach to Multitemporal Cloud Detection"

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

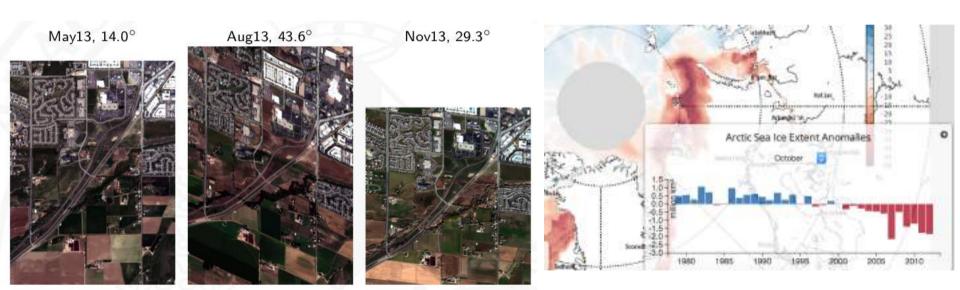
- Multiple inter-related outputs? Data from multiple sources?
- Learn to fuse heterogeneous information



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

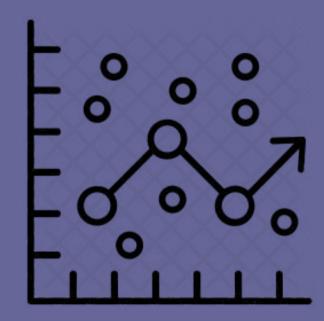
Anomalous change detection

Pervasive and anomaly changes in the wild



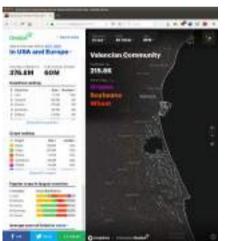
"A family of kernel anomaly change detectors" Longbotham and Camps-Valls, IEEE Whispers 2010.

Regression, fitting, parameter retrieval



Some machine learning applications

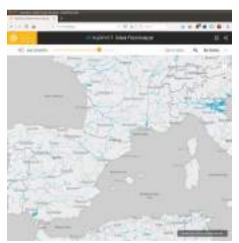
One soil map https://map.onesoil.ai



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



Flood analyzer http://floods.wri.org



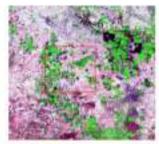
Disease mapping https://www.healthmap.org

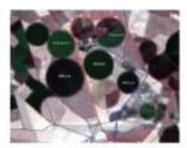


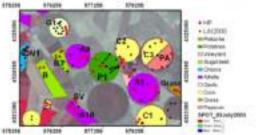
Spatializing vegetation parameters from space

Observations, x: CHRIS images: 62 bands, 400-1050 nm, 34m Variables, y: In situ leaf-level ChI (CCM-200) and LAI (PocketLAI phone app!)





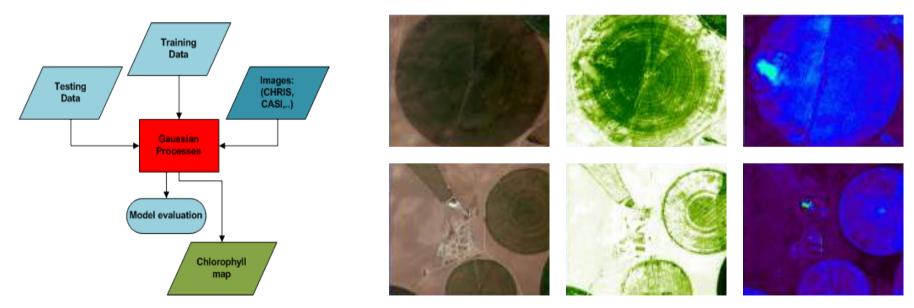






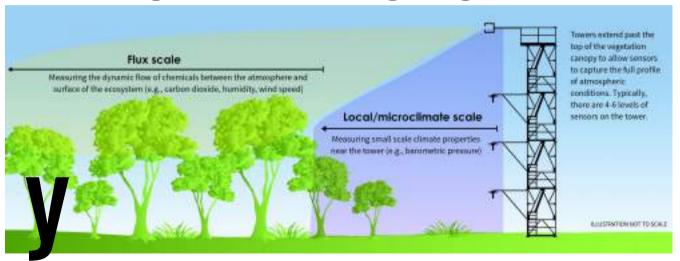
Spatializing vegetation parameters from space

Vegetation parameters from remote sensing data: chlorophyll content, LAI, vegetation cover



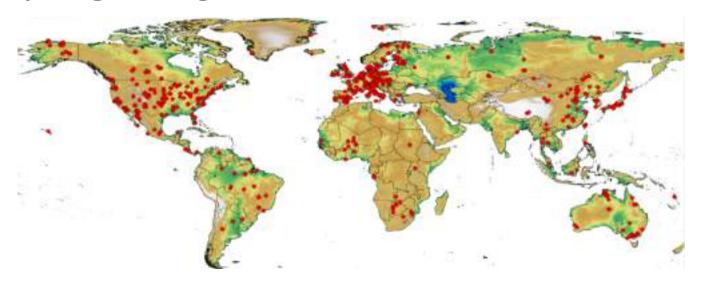
[&]quot;A Survey on Gaussian Processes for Earth Observation Data Analysis: A Comprehensive Investigation" Camps-Valls, G. and Verrelst, J. and Muñoz-Marí, et al. IEEE Geoscience and Remote Sensing Magazine 2016

 Sensors allow estimating turbulent exchange of carbon dioxide (CO2), latent and sensible heat, CO2 storage, net ecosystem exchange, energy balance, ...

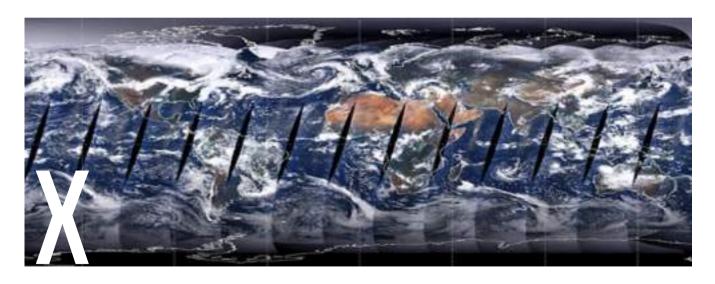


- Gross primary productivity
- Terrestrial ecosystem respiration
- Net ecosystem exchange

- FLUXNET: a sensor network of eddy covariances
- Upscaling CO2, energy and heat fluxes

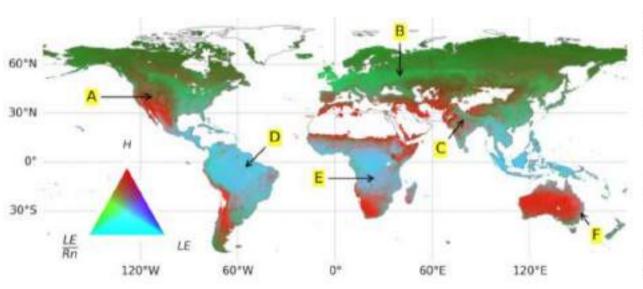


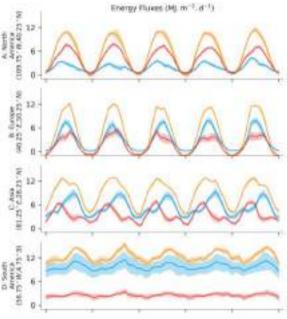
Upscaling CO2, energy and heat fluxes from eddy covariances



- LAI
- EVI
- NDVI
- LST-Night
- MSC-Day
- LST-Day
- NDWI

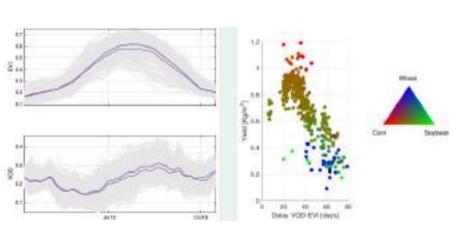
• Upscaling CO2, energy and heat fluxes from eddy covariances

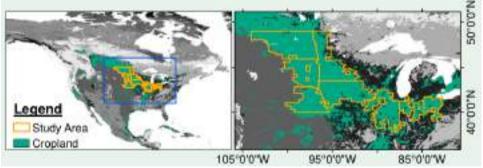


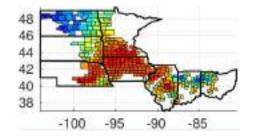


Crop yield prediction from space

• Crop yield (corn, soybean, wheat) & crop production





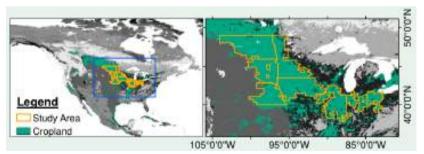


"Nonlinear Distribution Regression for Remote Sensing Applications"
Adsuara, Perez, Muñoz, Mateo, Piles, Camps-Valls, IEEE TGARS 2019

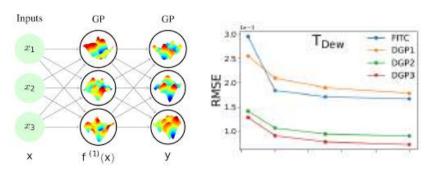
Spatio-temporal variable prediction

- 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

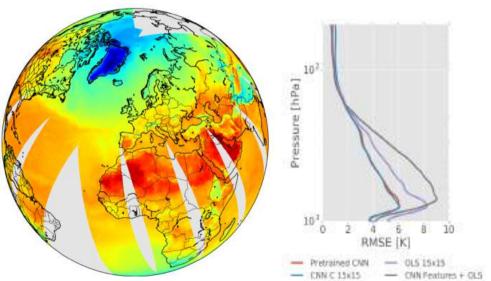


"A Survey on Gaussian Processes for Earth Observation Data Analysis"
Camps-Valls et al. IEEE Geoscience and Remote Sensing Magazine 2016

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

Multioutput and transfer learning

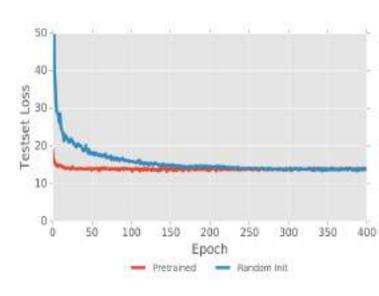
Multioutput regression: compactness & speed



"Statistical Retrieval of Atmospheric Profiles with Deep Convolutional Neural Networks",

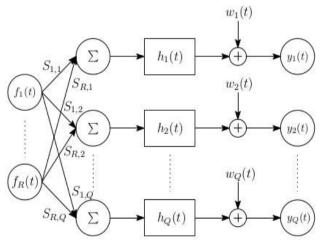
Malmgren-Hansen, Laparra and Camps-Valls et al, IEEE Trans Geosc. Rem. Sens.. 2019.

Transfer learning



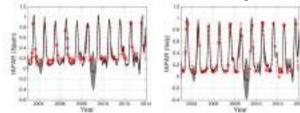
Multioutput regression and gap filling

Transfer learning across time, sensors and space

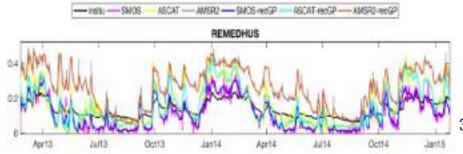


"Gap filling of biophysical parameters with multi-output GPs"
Mateo, Camps-Valls et al, IEEE IGARSS. 2018.
"Latent force GP models for EO time series prediction"
Luengo, Muñoz, Piles, Camps-Valls, IEEE TGARS, 2019

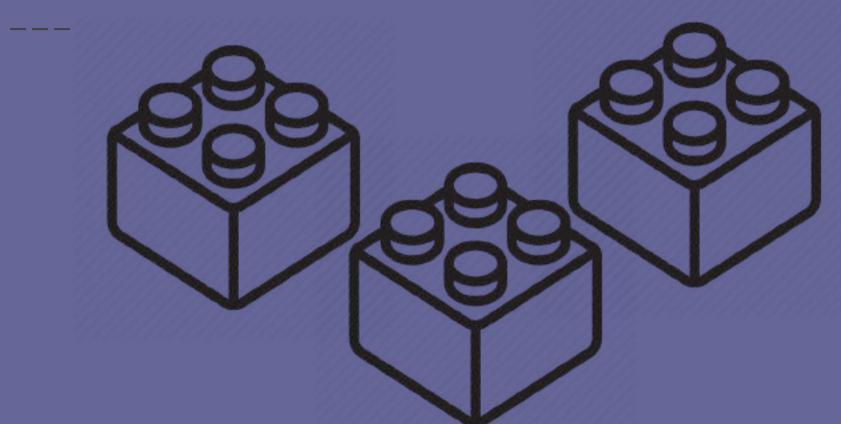
LAI and FAPAR across time and space



Soil moisture and sensor fusion

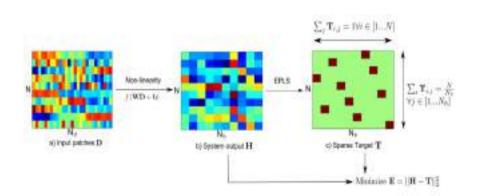


Dimensionality reduction and modes of variability



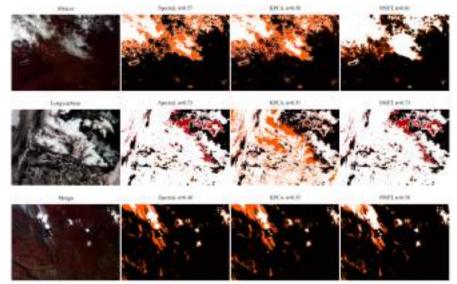
Sparse coding in unsupervised deep nets

CNN trained to extract sparse features → features+linear classifier suffice!



PS: for each sample only one output must be active

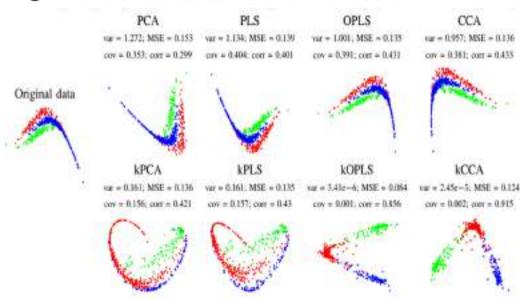
LS: even distribution of outputs, no dead outputs



[&]quot;Unsupervised Deep Feature Extraction for Remote Sensing Image Classification"
Romero, A. and Gatta, C. and Camps-Valls, IEEE Trans. Geosc. Rem. Sens, 2016

Kernel multivariate data analysis

Transform data to max var/corr/covar



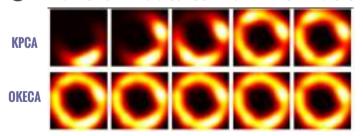
"Kernel multivariate analysis framework for supervised subspace learning: A tutorial on linear and kernel multivariate methods", Arenas and Camps-Valls et al, IEEE Signal Proc. Mag. 2013.

Transform data to max SNR



"Signal-to-Noise Ratio in reproducing kernel Hilbert spaces"
Gomez, Santos and Camps-Valls et al, Patt. Recog. Lett.. 2018.

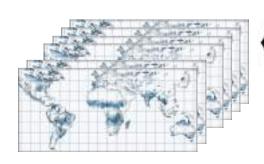
Transform data to max information



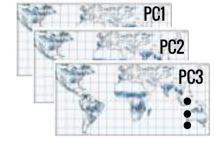
"Optimized Kernel Entropy Components"
Izquierdo, Jenssen and Camps-Valls et al, IEEE Trans. Neur. Nets. 20140

Spatio-temporal analysis of the Earth cubes

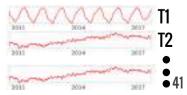
- PCA/EOF is popular, yet cannot cope with nonlinear spatio-temporal relations
- ROCK PCA
 - copes with nonlinearities
 - extracts spatial and temporal components
 - very fast



Spatial components



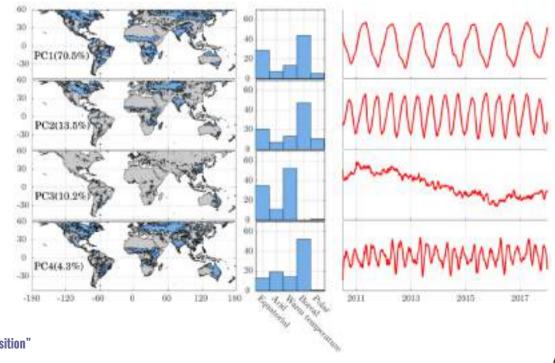
Temporal modes



"Rotated Complex Kernel PCA for spatio-temporal data decomposition"
Bueso, Piles, Camps-Valls, IEEE TGARS, 2018

Spatio-temporal analysis of the Earth cubes

- SM decomposition
 - Meaningful compression
 - Climate-specific modes of variability
 - Boreal and Equatorial modes of SM variability dominate
 - Seasonal and ENSO related temporal modes

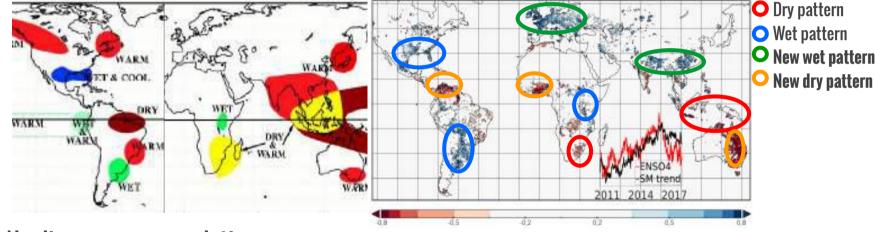


"Rotated Complex Kernel PCA for spatio-temporal data decomposition"

Bueso, Piles, Camps-Valls, IEEE TGARS, 2018

Spatio-temporal analysis of the Earth cubes

PC3 highly correlates with ENSO + new spatial patterns uncovered



 Nonlinear cross-correlation uncovers unreported SM-ENSO lags

ENSO 1.2
 ENSO 3
 ENSO 3.4
 ENSO 4

 Lag [days]
 60
 30
 25
 5

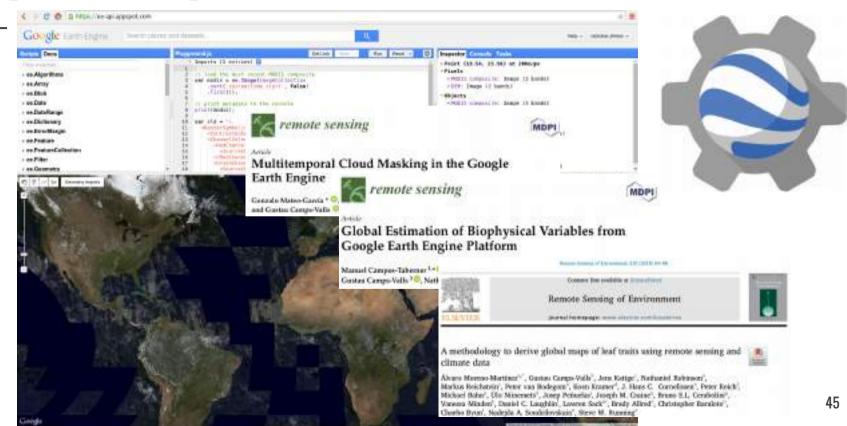
 Max Corr
 0.56
 0.68
 0.66
 0.8

[&]quot;Rotated Complex Kernel PCA for spatio-temporal data decomposition"
Bueso, Piles, Camps-Valls, IEEE TGARS, 2018

Efficiency

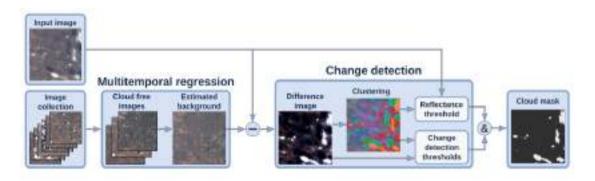


Google Earth Engine (something that Europeans love)



Google Earth Engine: cloud detection in the cloud

Exploit temporal information and change detection

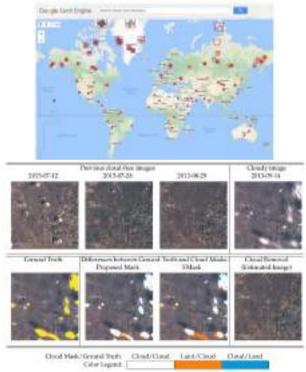


"Multitemporal Cloud Masking in the Google Earth Engine"

Mateo, Gómez, Amorós, Muñoz. and Camps-Valls. Remote Sensing 7 (10):1079, 2018

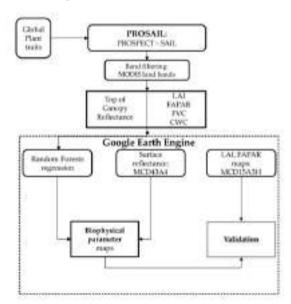
"Cloud masking and removal in remote sensing image time series"

Gómez, Amorós, Mateo, Muñoz-Marí and Camps-Valls. Journal of Applied Remote Sensing 11 (1):015005, 2017



Google Earth Engine: biophysical parameter retrieval

Global maps of LAI, FAPAR, FVC, canopy water content by inverting PROSAIL with ML ...



Parameter

CWC [kg/m²]

CWC [kg/m²]

CWC [kg/m²]

CWC [kg/m²]

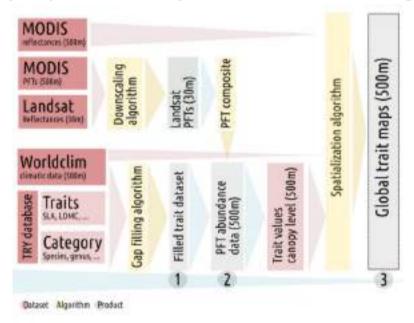
CWC [kg/m²]

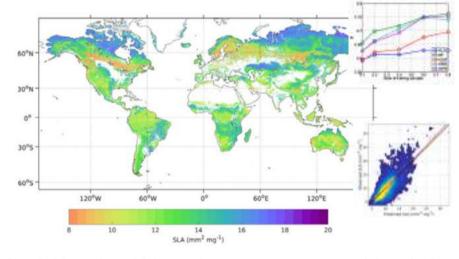
CWC [kg/m²]

[&]quot;Global estimation of biophysical variables from Google Earth Engine platform" Campos, Moreno, Garcia, Camps-Valls, G. et al, Remote Sensing (10):1167, 2018

Google Earth Engine: spatialization of plant traits

Global maps at 500 m resolution of specific leaf area, leaf dry matter content, leaf nitrogen and phosphorus content per dry mass, and leaf nitrogen/phosphorus ratio.



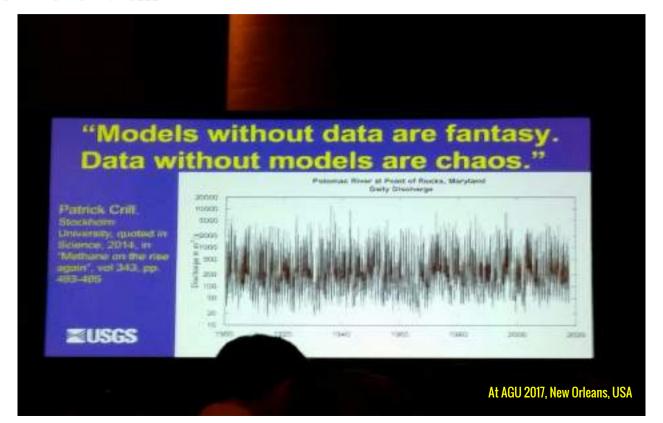


"A methodology to derive global maps of leaf traits using remote sensing and climate data" Moreno, Camps-Valls, Kattge, Robinson, Reichstein, ... and Running. Remote Sensing of Environment 218 (12):69-88, 2018

Physics-aware machine learning

$$F(X_{\bullet}H(t)|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle) = Y$$

The truth is that...

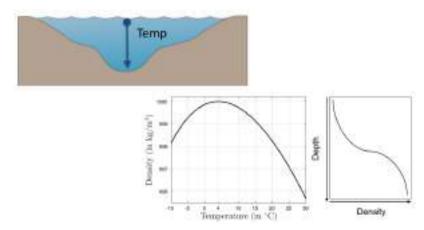


Physics-driven ML: constrained optimization

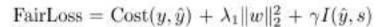
ML that minimizes model violations and predictions are dependent of physical laws

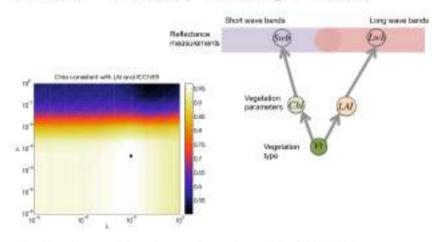
PhysLoss = Cost
$$(y, \hat{y}) + \lambda_1 ||w||_2^2 + \gamma \Omega(\hat{y}, \Phi)$$

 $\Omega(\hat{y}, \Phi) = \text{sum of physical violations of } \hat{y}$



"Theory-guided Data Science", Karpatne, A. et al. IEEE Trans. Know. Data Eng., 2017.





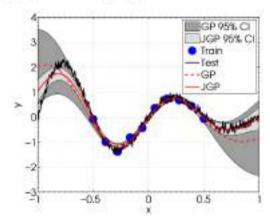
"Fair Kernel Learning" Perez, Laparra, Gomez, Camps-Valls, G. ECML, 2017. **"Consistent Regression of Biophysical Parameters with Kernel Methods"** Díaz, Peréz-Suay, Laparra, Camps-Valls, IGARSS 2018

Physics-driven ML: joint model-data ML

Let ML talk to physical models

JointLoss = Cost
$$(y, \hat{y}) + \lambda_1 ||w||_2^2 + \gamma \Omega(\hat{y}, \Phi)$$

 $\Omega(\hat{y}, \Phi) = \text{Cost}_s(y_s, \hat{y}_s)$

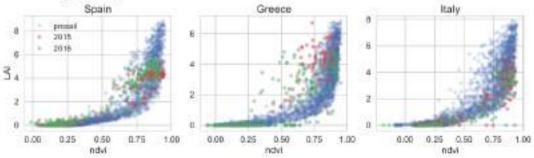


"Joint Gaussian Processes for Biophysical Parameter Retrieval" Svendsen, Martino, Camps-Valls, IEEE TGARS 2018

Setup

- ERMES project: 3 rice sites, 85% European production
- Landsat 8 + in situ measurements + PROSAIL simulations
- In situ LAI measurements: r = 70-300 (3 countries, 2 years)
- Simulations: s = 2000 (Landsat 8 spectra and LAI)

Filling the space ...



[&]quot;Physics-aware Gaussian processes in remote sensing" Camps-Valls, G. et al. Applied Soft Computing, 2018.

Physics-driven ML: hybrid modeling framework

PERSPECTIVE

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

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

Markus Reichstein^{1,2a}, Gustau Camps-Valls³, Bjorn Stevens⁴, Martin Jung¹, Joachim Denzler^{2,5}, Nuno Carvalhais^{1,6} & Prabhat⁷

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.

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

Physics-driven ML: hybrid modeling framework

ML that learns laws of physics (e.g. consistency model-data, convection, advection, mass and energy conservation)

A: "Physisizing" a deep learning architecture by adding one or several physical layers after the multilayer neural network Physical output Physical model Physical model 'parameters' More abstract Ligarroad mapping 2...n+1Simple features Leamed mepping T Input

B: A motion field is learned with a convolutional-deconvolutional net, and the motion field is further processed with a physical model

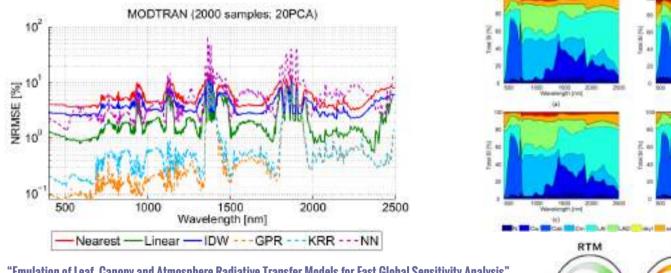
Predicted future temperature field Physical warping model Motion field Convolutionaldeconvolutional neural network Input: past temperature fields

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

"Deep Learning for Physical Processes: Incorporating Prior Scientific Knowledge". de Bezenac. Paiot, & Gallinari, arXiv:1711.07970 (2017)

Physics-driven ML: emulation of complex codes

GP Emulation = Mathematical tractability + Global sensitivity analysis + Speed



[&]quot;Emulation of Leaf, Canopy and Atmosphere Radiative Transfer Models for Fast Global Sensitivity Analysis", Verrelst, Camps-Valls et al Remote Sensing of Environment, 2016

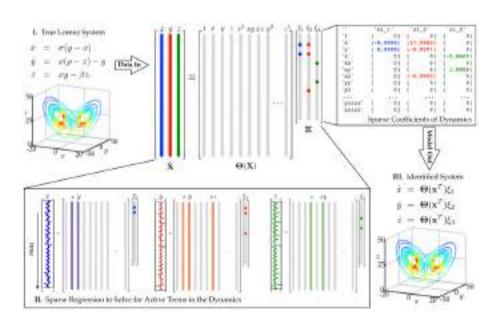
2.3-24.5 s/pix

RMSE = 0.1 - 5%

[&]quot;Emulation as an accurate alternative to interpolation in sampling radiative transfer codes", Vicent and Camps-Valls, IEEE Journal Sel. Topics Rem. Sens, Apps. 2018

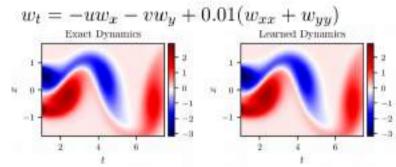
Physics-driven ML: encoding and learning ODE/PDEs

Who needs Lorenz?

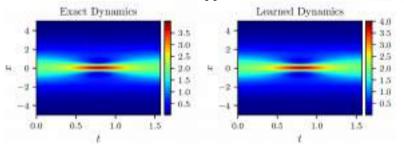


"Discovering governing equations from data by sparse identification of nonlinear dynamical systems" Brunton, Proctor, Kutz, PNAS 2016

Who needs Navier Stokes?



• Who needs Schrödinger? $\psi_t = 0.5i\psi_{xx} + i|\psi|^2\psi$

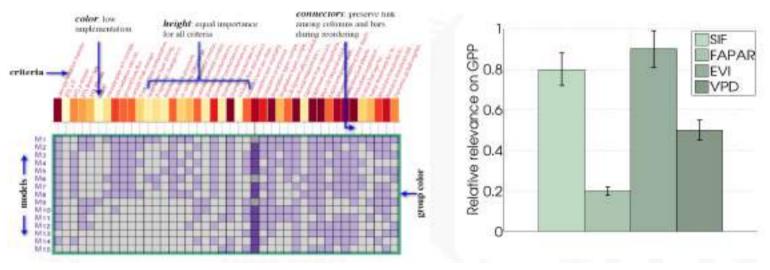


"Deep Hidden Physics Models: Deep Learning of Nonlinear Partial Differential Equa**tio**ns" Raissi, JMLR 2018

Understanding is more important than fitting

Feature selection & ranking

Filters & wrappers



[&]quot;Remote Sensing Feature Selection by Kernel Dependence Estimation", Camps-Valls, G. Mooij, JM. Schölkopf, IEEE-GRSL, 2010.

[&]quot;A guided hybrid genetic algorithm for feature selection with expensive cost functions", M. Jung, J. Zscheischler, Procedia, 2013.

Neuron and bases visualization

- What did the network learn?
- How do bases change in time, with real/simulations/together, under extremes?



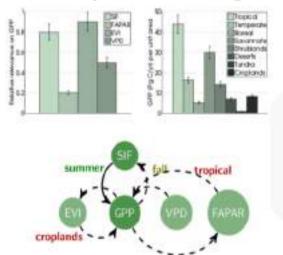
[&]quot;Visualizing and Understanding Convolutional Networks", Zeriler, et al 2013

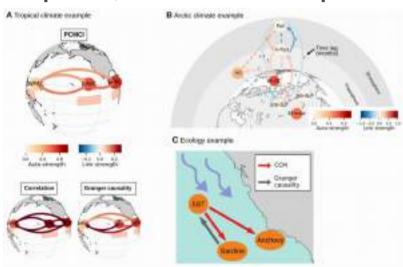
[&]quot;Processing of Extremely high resolution LiDAR and optical data", Campos-Taberner, Camps-Valls et al, 2016

[&]quot;What did your network learn under anomalies and adaptation?," Camps-Valls et al, in preparation (2018)

Graphical models and causal discovery

- Causality discovery learns cause and effects relations from data
- What for? Hypothesis testing, model-data comparison, causes of extreme impacts



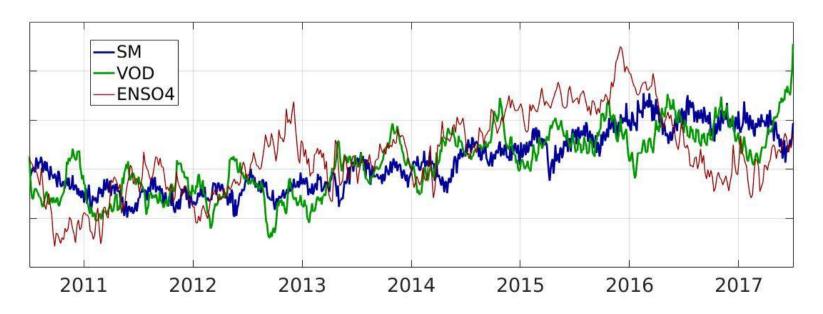


[&]quot;Inferring causation from time series with perspectives in Earth system sciences", Runge, Bathiany, Bollt, Camps-Valls, et al. Nat Comm (submitted), 2018.

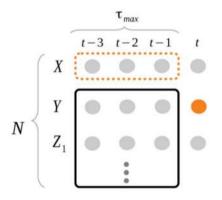
[&]quot;Causal Inference in Geoscience and Remote Sensing from Observational Data," Pérez-Suay and Camps-Valls, IEEE Trans. Geosc. Rem. Sens, 2018

[&]quot;CauseMe: An online system for benchmarking causal inference methods," Muñoz-Marí, Mateo, Runge, Camps-Valls. In preparation (2019). CauseMe: http://causeme.uv.es

- ENSO4 index and the inter-annual component extracted from VOD and SM
- High correlations, yet ... correlation does not imply causation



- Causal inference goes beyond correlation analysis
- Granger causality tests whether the past of X is useful to predict the future of Y



$$Y_{t+1} = a^{\top} X_t + \varepsilon_t^Y$$

$$Y_{t+1} = b_1^{\top} Y_t + b_2^{\top} X_t + \varepsilon_t^{Y|X}$$

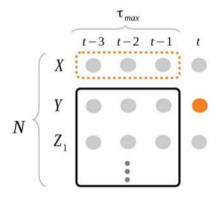
$$X \to Y \leftrightarrow \mathbb{V}[\varepsilon_t^Y] \ll \mathbb{V}[\varepsilon_t^{Y|X}]$$

Perez-Suay and Camps-Valls, IEEE TGARS 2019

[&]quot;Causal inference from Observational Data in Remote Sensing and Geosciences"

[&]quot;Inferring causation from time series with perspectives in Earth system sciences"

- Causal inference goes beyond correlation analysis
- Granger causality tests whether the past of X is useful to predict the future of Y
- We introduce a kernel Granger method to account for nonlinear Granger-causal relations



$$a_{H} = (K(X_{t}, X'_{t}) + \varepsilon_{t}^{Y})^{-1}Y_{t+1}$$

$$b_{H} = (L([Y_{t}, X_{t}], [Y'_{t}, X'_{t}]) + \varepsilon_{t}^{Y|X})^{-1}Y_{t+1}$$

$$X \to Y \leftrightarrow \mathbb{V}_{H}[\varepsilon_{t}^{Y}] \ll \mathbb{V}_{H}[\varepsilon_{t}^{Y|X}]$$

Perez-Suay and Camps-Valls, IEEE TGARS 2019

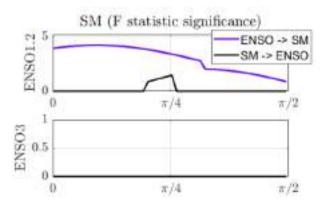
[&]quot;Causal inference from Observational Data in Remote Sensing and Geosciences"

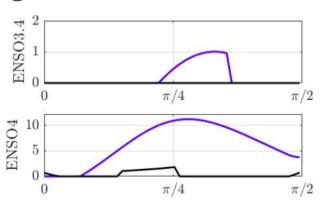
[&]quot;Inferring causation from time series with perspectives in Earth system sciences"

An ANOVA F-statistic summarizes kernel Granger causality

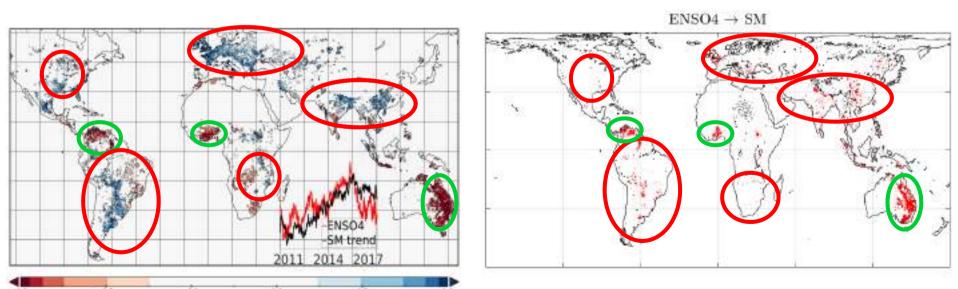
$$F = \frac{\text{explained variance}}{\text{unexplained variance}} \propto \frac{\mathbb{V}_H[\varepsilon_t^Y]}{\mathbb{V}_H[\varepsilon_t^{Y|X}]} - 1 \ge \theta$$

● ENSO1.2 and ENSO4 are the most "kernel Granger causal" indices





- Causality is sharper than mere correlation! Some impacts confirmed, others not!
- ENSO4 "causes" SM in very dry (Sahel) and very wet (tropical rain forests)



A platform for causal discovery

- CauseMe: http://causeme.uv.es
 - Download time series with ground truth
 - Run your causal discovery algorithm offline
 - Upload your causal graph
 - Get your results!

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[&]quot;Inferring causation from time series with perspectives in Earth system sciences"
Runge, Bathiany, Bollt, Camps-Valls, et al. Nat Comm (submitted), 2018.

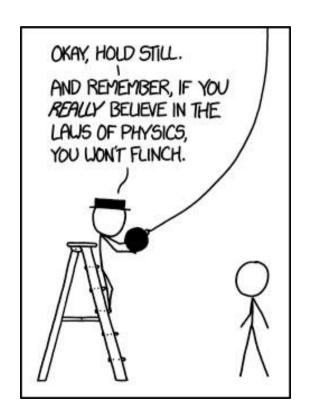
"Causal Inference in Geoscience and Remote Sensing from Observational Data,"
Pérez-Suav and Camps-Valls, IEEE Trans, Geosc. Rem. Sens. 2018

Conclusions



Conclusions

- Machine learning in EO and climate
 - Many techniques ready to use
 - Huge community, exciting tools
- Solid mathematical framework to deal with
 - Multivariate data
 - Multisource data
 - Structured spatio-temporal relations
 - Nonlinear feature relations
 - Fitting and classification
- Risks & remedies
 - Understanding is more complex
 - Physics consistency a must
 - Physics-driven ML & Explainable Al



Thanks!





http://isp.uv.es



@isp_uv_es



gustau.camps@uv.es



















Propaganda



ERC Consolidator Grant 2015-2020 Statistical Learning for Earth Observation Data Analysis

Gustau Camps-Valls, Universitat de València, Spain

⊠ gustau.camps@uv.es | ♠ http://isp.uv.es





1 PhD + 1 PostDoc positions!

- Remote sensing and geosciences
- Machine learning
 - Regression, time series analysis
 - Graphical models
 - Causal inference

E-mail me: gustau.camps@uv.es