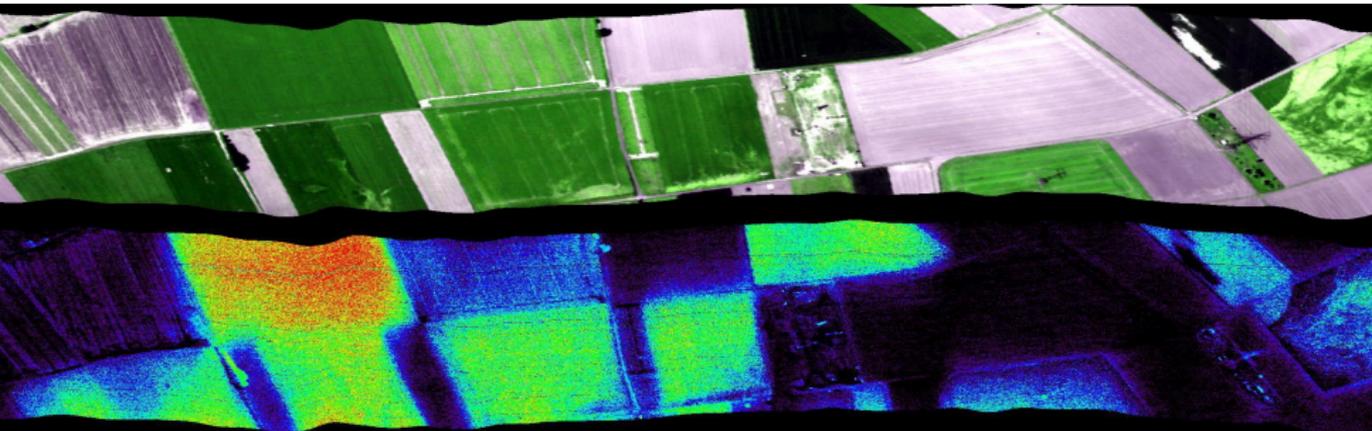


Monitoring Earth Climate Variables with Statistical Inference



Gustau Camps-Valls

Image Processing Laboratory (IPL)

Universitat de València, Spain

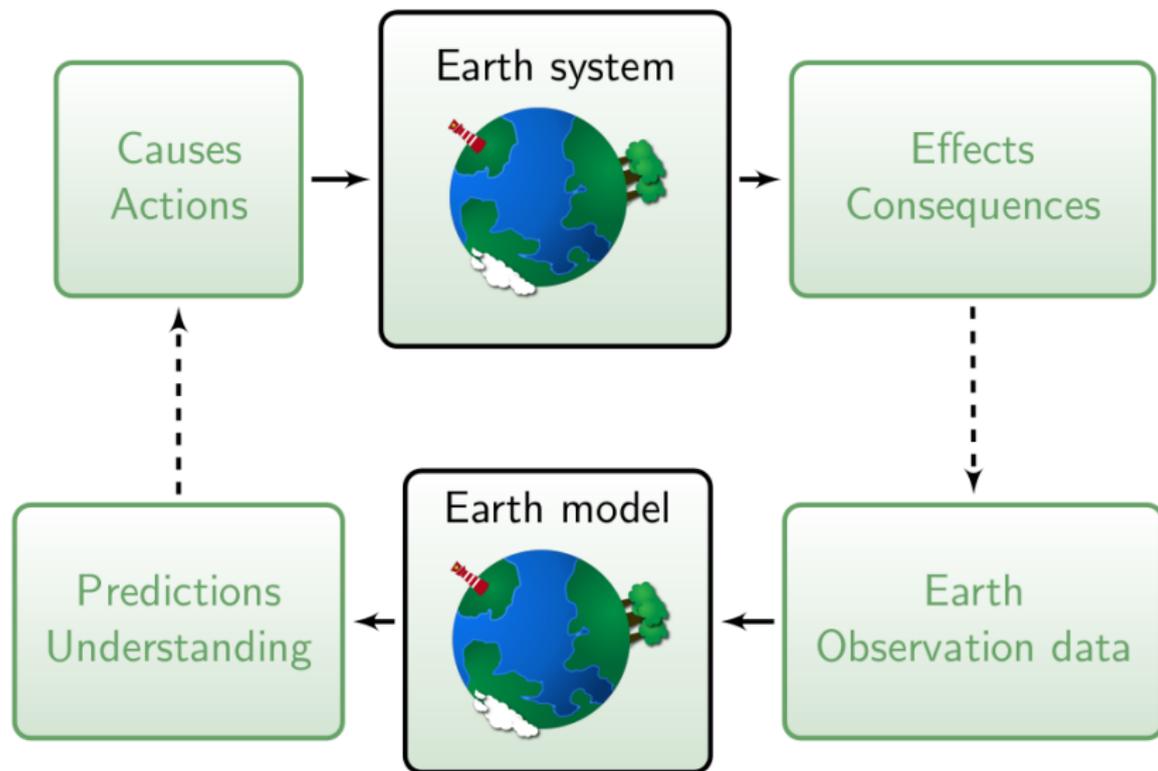
✉ gustau.camps@uv.es | <http://isp.uv.es>



Outline

- **Part 1: Earth observation from space**
- **Part 2: EO needs statistical learning**
- **Part 3: Advances in variable prediction and understanding**
 - 1 Temporal structures
 - 2 Learning the covariance
 - 3 Warping the function
 - 4 Heteroscedasticity
 - 5 Multi-output regression
 - 6 Computational efficiency
.....
 - 7 Sensitivity analysis
 - 8 From regression to causation
.....
 - 9 GPs in your smartphone
 - 10 GPs for weather forecasting
- **Part 4: Conclusions: references, code, ads**

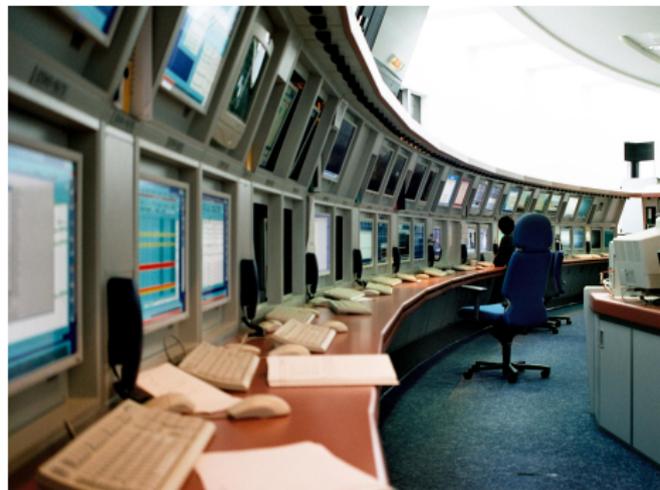
Part 1: Earth observation from space



We monitor the Earth constantly ...

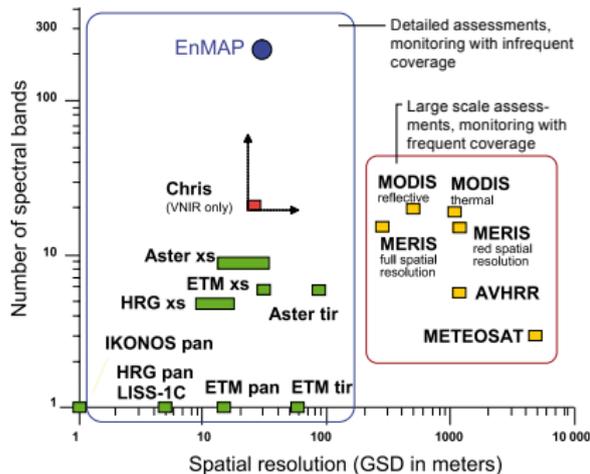


NASA Exploration Center, California

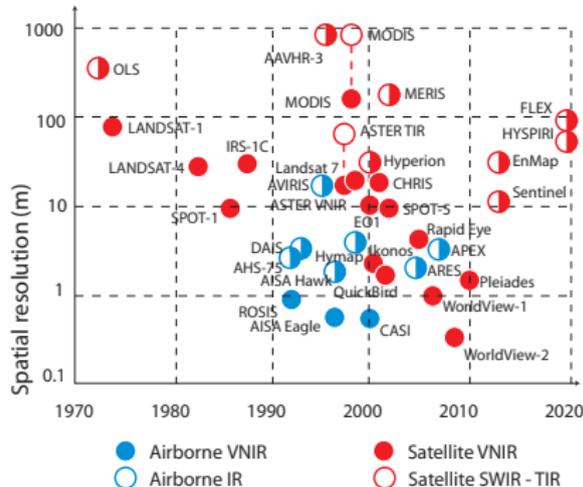


EUMETSAT Operations, Darmstadt

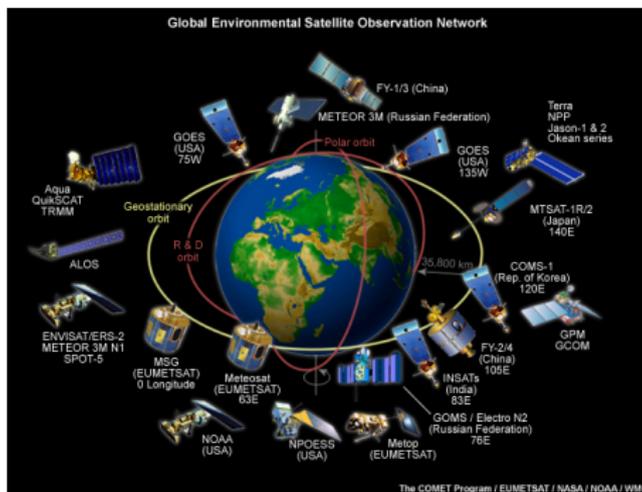
... and with many satellite sensors ...



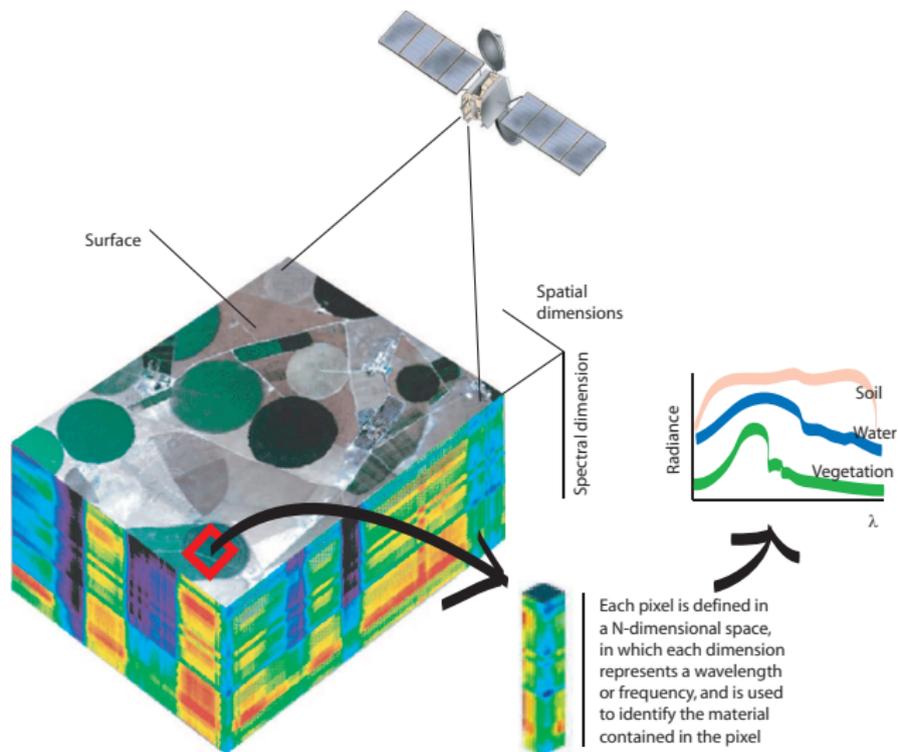
Credits: <http://www.enmap.de/>

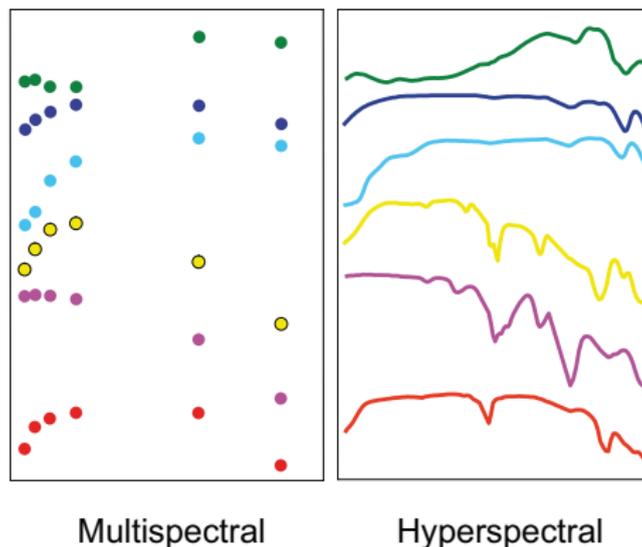


... and many more almost ready to come!



ESA Sentinels, NASA A-train, EnMAP, FLEX, MTG-IRS, HypIRI, MEOS, ZASat, HIS, HERO, etc.





- Hyperspectral signals allow finer material characterization
- Absorption, depth, re-emissions and modulated spectral features
- Identification of chemical components and bio-chemical processes
- Estimation of bio-geo-physical parameters

What can we do with these signals?

Geology

- Mineral detection
- Cover homogeneity

Forestry

- Infected trees
- Status monitoring
- Forest clearing

Sea/ice/coastal

- Oil spills monitoring
- Water quality

Precision agriculture

- Crop stress location
- Crop productivity

Atmosphere

- Air quality, pollutants
- Global/local change

Land management

- Crop monitoring/phenology
- Land use/cover change

Defense

- Target detection
- Mine detection

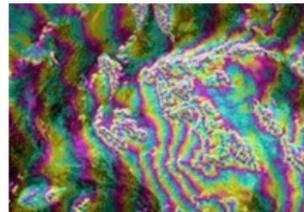
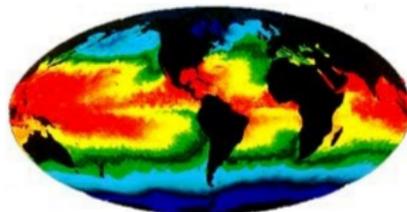
Public safety

- Logistics & operations
- Fire risk, floods

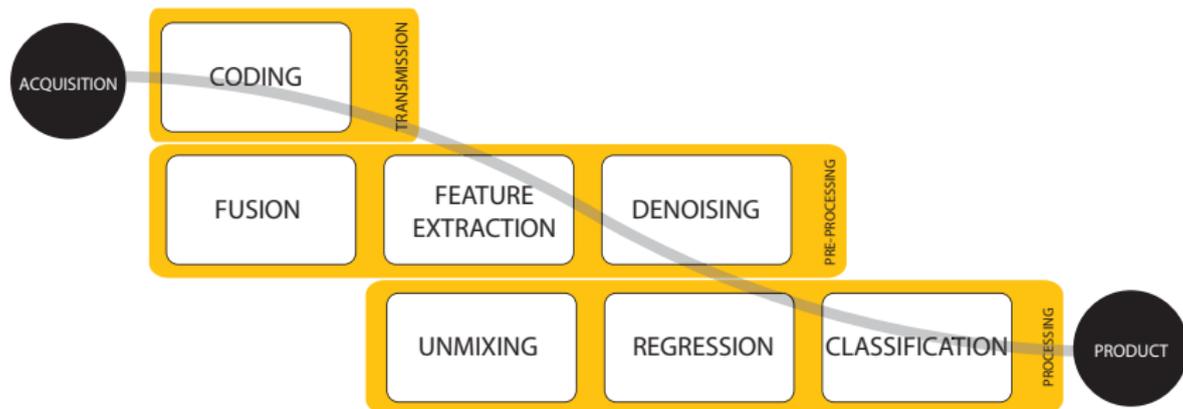
Regulation & Policy making

- Urban growth
- Settlements, population movements

- Visible / NIR / MIR – only day, no clouds
 - Vegetation dynamics and covers
 - Geological maps (structure, mineralogy, oil)
 - Agriculture, urban, forests use
 - Ocean temperature, fitoplancton
 - Meteorology of clouds
 - Layer dynamics
- Thermal Infrared – day and night
 - Clouds temperature and height
 - Forest fires
 - Temperature maps
 - Plumes
 - Heat islands
- Active microwaves – day and night
 - Surface characterization, structure of trees and leaves
 - Moisture, deformation by earthquakes, ...
 - Military applications



A standard image processing chain:



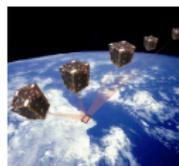
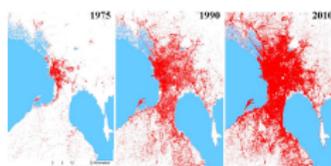
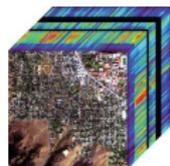
Characteristics of remote sensing data

- High spectral resolution → moderate spatial resolutions



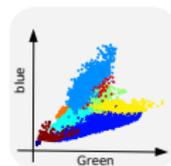
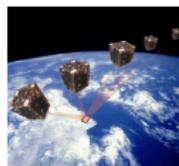
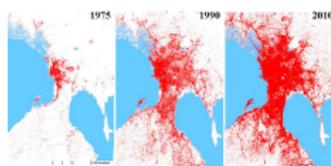
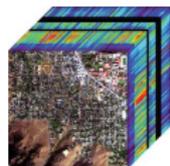
Characteristics of remote sensing data

- High spectral resolution → moderate spatial resolutions
- High dimensional: multi-temporal, angular and source



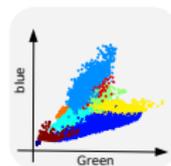
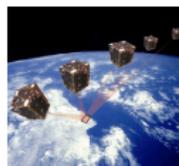
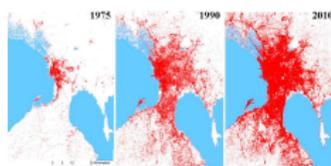
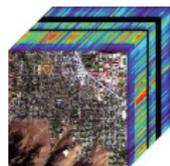
Characteristics of remote sensing data

- High spectral resolution → moderate spatial resolutions
- High dimensional: multi-temporal, angular and source
- Non-linear feature relations



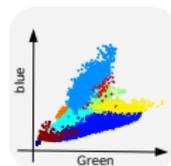
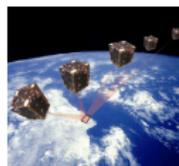
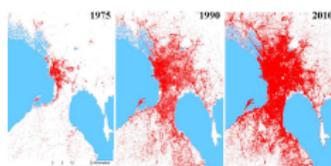
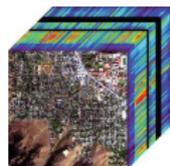
Characteristics of remote sensing data

- High spectral resolution \rightarrow moderate spatial resolutions
- High dimensional: multi-temporal, angular and source
- Non-linear feature relations
- Non-Gaussian data distributions



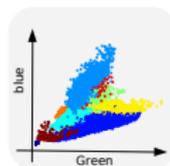
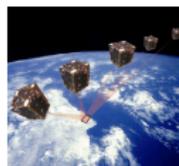
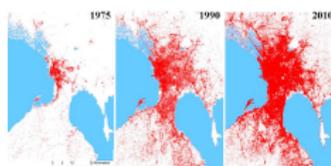
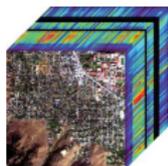
Characteristics of remote sensing data

- High spectral resolution → moderate spatial resolutions
- High dimensional: multi-temporal, angular and source
- Non-linear feature relations
- Non-Gaussian data distributions
- Dependent noise, uneven sampling



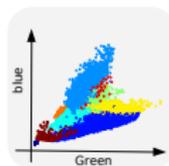
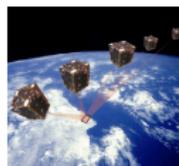
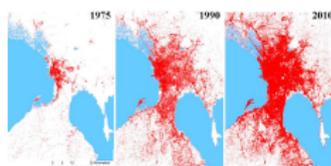
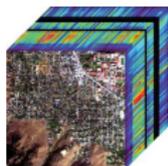
Characteristics of remote sensing data

- High spectral resolution → moderate spatial resolutions
- High dimensional: multi-temporal, angular and source
- Non-linear feature relations
- Non-Gaussian data distributions
- Dependent noise, uneven sampling
- Few supervised (labeled) information is available (high cost)

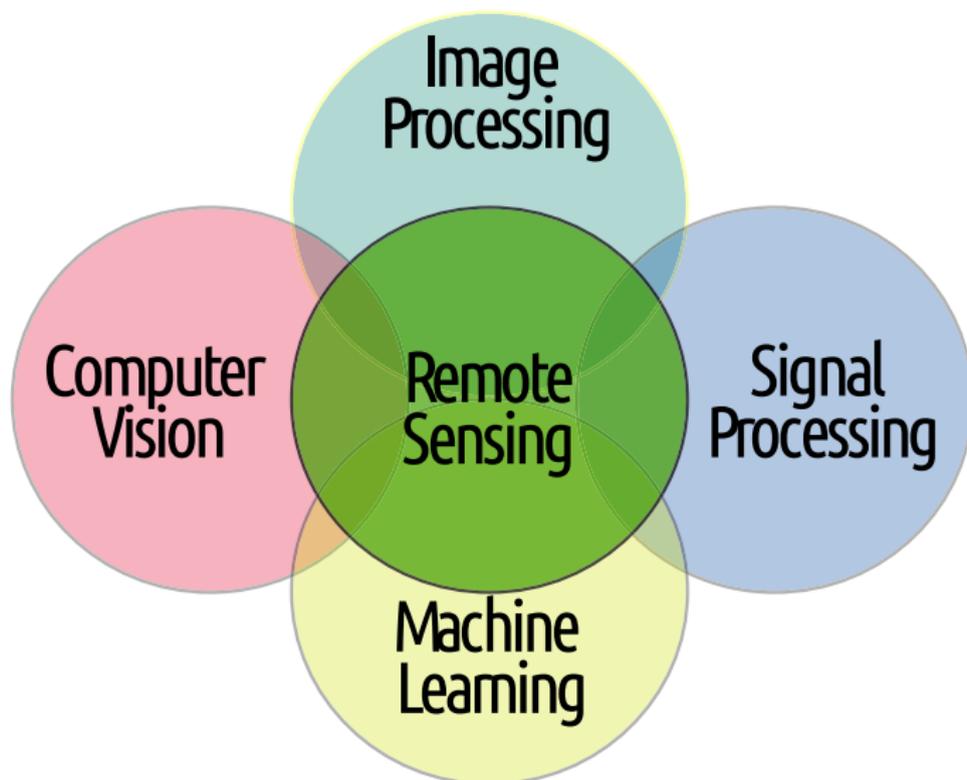


Characteristics of remote sensing data

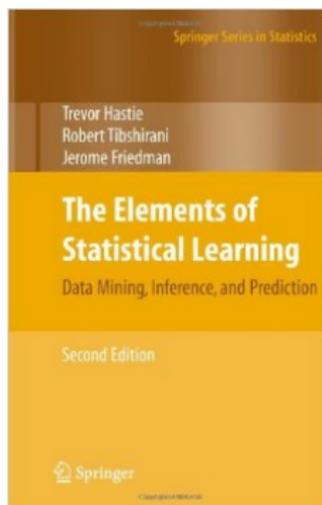
- High spectral resolution → moderate spatial resolutions
- High dimensional: multi-temporal, angular and source
- Non-linear feature relations
- Non-Gaussian data distributions
- Dependent noise, uneven sampling
- Few supervised (labeled) information is available (high cost)
- Tons of data to process in (near) real-time



We live at the intersection ...



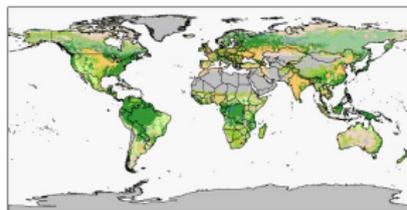
Part 2: Statistical learning



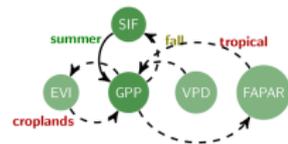
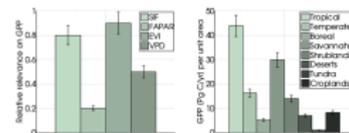
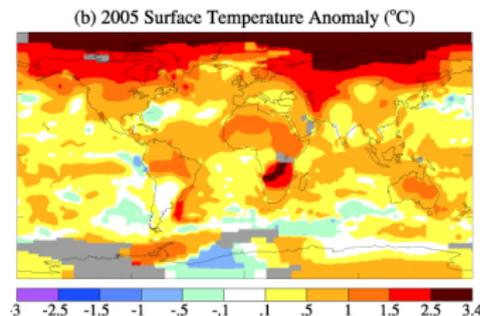
- Statistical learning theory is a framework for machine learning drawing from the fields of statistics and functional analysis
- Statistical learning theory deals with the problem of finding a predictive function based on data
- Given a set of input-output pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i) | i = 1, \dots, N\}$, learn a function $f(\cdot)$ that predicts outputs for new inputs well, $y^* = f(\mathbf{x}^*)$

Earth Observation needs Statistical Learning

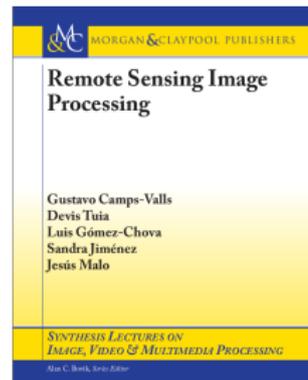
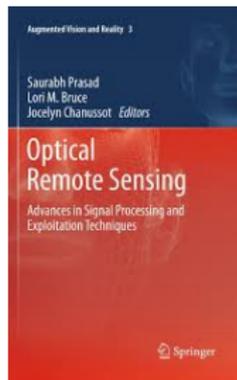
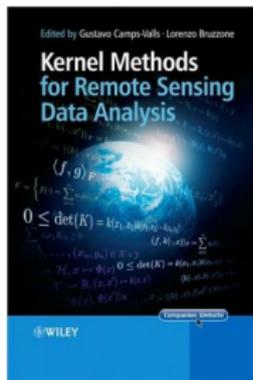
- ① Identify objects and detect changes
- ② Estimate the content of bio-geo-physical parameters
- ③ Assess relative relevance of variables
- ④ Infer (causal) relations between variables and observations



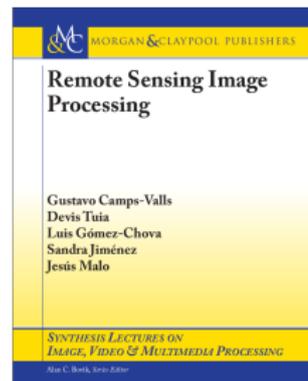
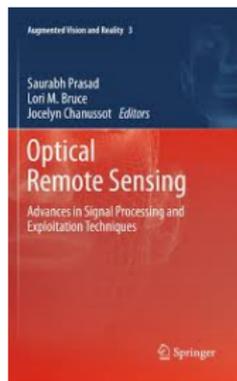
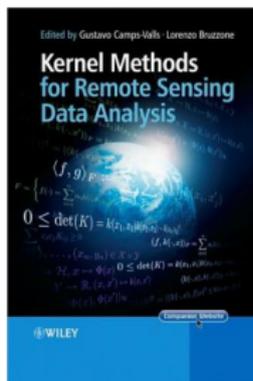
Dominant GlobCover Land Use / Cover after RED Classification



Last decade was dominated by kernel methods ...

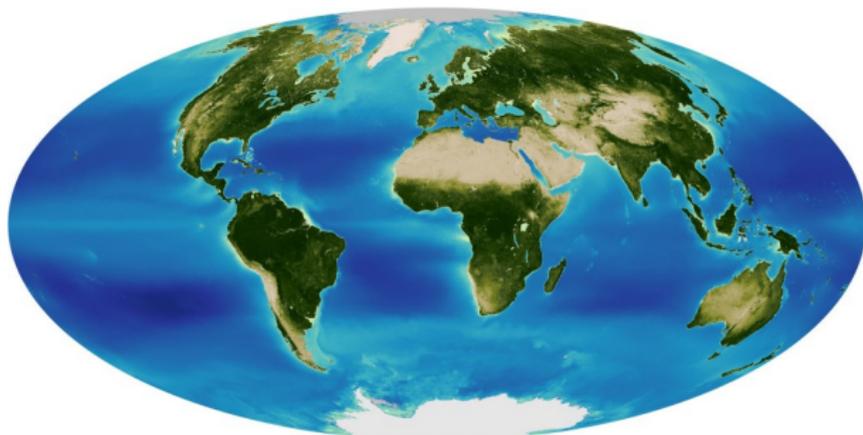


Last decade was dominated by kernel methods ...

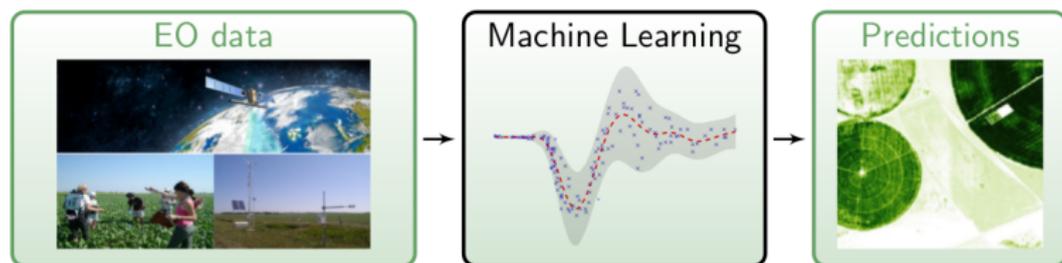


- RS problems are typically nonlinear
- KMs are efficient in high-dimensional low-sampled problems
- KMs allow combination of multi- source/temporal/angular data
- KMs are simple and clean to design, understand and apply
- We have 130 years of solid mathematics, theorems, and bounds

- Estimate biophysical parameters is key to monitor our Planet
- Monitoring land is the most challenging (and interesting) problem:
 - Phenological stage of crops and forests
 - Health status (e.g., development, productivity, stress)
- Implications on agriculture, biofuels and food
- Models typically resort to *in situ* data + remote sensing data



Goal: Transform measurements into biophysical parameter estimates



Data:

• **Input data:**

- satellite/airborne spectra
- *in situ* (field) radiometers
- simulated spectra from RTMs

• **Output results:** estimation of a bio/geo-physical parameter

Taxonomy of retrieval methods

- ① The *statistical* inversion models: parametric and non-parametric.
 - Parametric models rely on physical knowledge of the problem and build explicit parametrized expressions that relate a few spectral channels with the bio-geo-physical parameter(s) of interest.
 - Non-parametric models are adjusted to predict a variable of interest using a training dataset of input-output data pairs.
- ② *Physical* inversion models: try to reverse RTMs.
 - After generating input-output (parameter-radiance) datasets, the problem reduces to, given new spectra, searching for similar spectra in the dataset and assigning the most plausible ('closest') parameter.
- ③ *Hybrid* inversion models try to combine the previous approaches.

- **Parametric models based on band ratios are typically used:**
 - Simple
 - Understandable
 - Fast
- **Problems:**
 - Too general and simplistic, not suited to all scenarios
 - Require prior information (and solid physical knowledge)
- **Nonlinear, nonparametric regression typically performs better:**
 - More flexible, adaptive
 - No assumptions about data relations
 - Many methods: neural networks, random forests, SVR ...

What is a Gaussian process?

- It is a probability density over functions
- It is defined by
 - A mean function $m(\mathbf{x})$
 - A covariance function $k(\mathbf{x}, \mathbf{x}')$
- It is expressed as

$$f(\mathbf{x}) \sim GP(m(\mathbf{x}), k_{\theta}(\mathbf{x}, \mathbf{x}'))$$

- The joint pdf of any subset of points of $f(\mathbf{x})$ is a Gaussian:

$$\begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} m(\mathbf{x}_1) \\ \vdots \\ m(\mathbf{x}_N) \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \cdots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix} \right)$$

Gaussian processes regression in a nutshell

- Input-output data: $\{\mathbf{x}_n \in \mathbb{R}^D, y_n\}_{n=1}^N$
- Observation model:

$$y_n = f(\mathbf{x}_n) + \varepsilon_n, \quad \varepsilon_n \sim \mathcal{N}(0, \sigma^2)$$

- Test point \mathbf{x}_* with corresponding output y_*
- Posterior over the unknown output:

$$p(y_* | \mathbf{x}_*, \mathcal{D}) = \mathcal{N}(y_* | \mu_{\text{GP}*}, \sigma_{\text{GP}*}^2)$$

$$\mu_{\text{GP}*} = \mathbf{k}_{\mathbf{f}*}^\top (\mathbf{K} + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{y} = \mathbf{k}_{\mathbf{f}*}^\top \boldsymbol{\alpha}$$

$$\sigma_{\text{GP}*}^2 = \sigma^2 + k_{**} - \mathbf{k}_{\mathbf{f}*}^\top (\mathbf{K} + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{k}_{\mathbf{f}*}.$$

- Marginal likelihood (aka evidence)

$$\log p(\mathbf{y}) = -\frac{1}{2} \mathbf{y}^\top (\mathbf{K} + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K} + \sigma^2 \mathbf{I}_n| - \frac{N}{2} \log(2\pi)$$

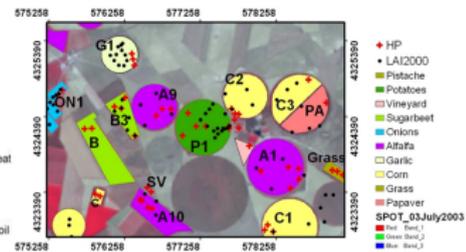
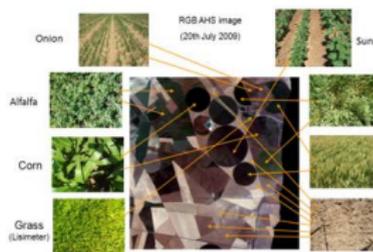
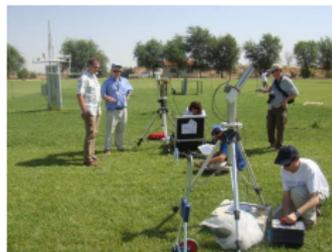
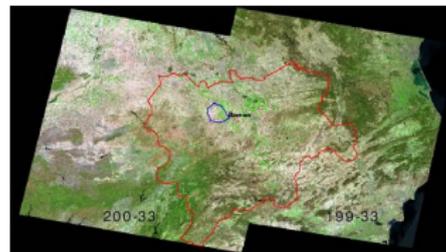
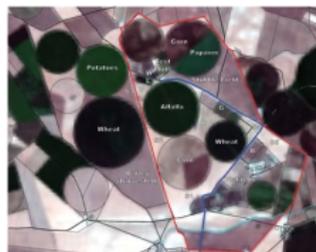
- Slow: $\mathcal{O}(N^2)$ storage and $\mathcal{O}(N^3)$ computing cost



- Nonlinear regression tool
- No assumption about the data relations
- Serious competitor to other nonparametric methods
- Provides confidence intervals
- Learns the relevance of the input bands
- Allows for flexible kernels that encode priors
- Automatic tuning of parameters

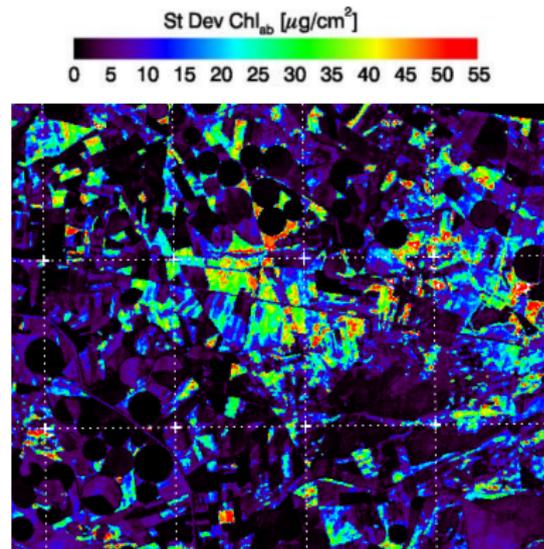
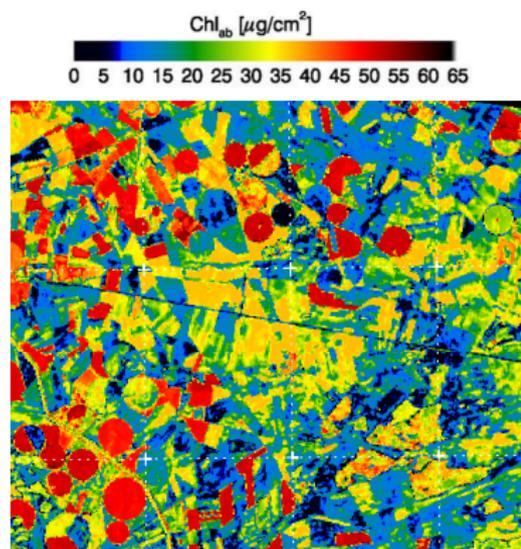
An illustrative real example: Retrieve vegetation chlorophyll content

- *In situ* leaf-level *Chl* measured with a calibrated CCM-200 Chlorophyll Content Meter in the field
- CHRIS images (62 bands, 400-1050 nm, 34m nadir res.) –corrected geometrically and atmospherically



Method	Formulation	ME	RMSE	MAE	R
GI	R_{672}/R_{550}	12.97	28.77	26.58	0.74
mNDVI	$(R_{800}-R_{680})/(R_{800}+R_{680}-2R_{445})$	1.20	9.27	7.06	0.79
mNDVI ₇₀₅	$(R_{750}-R_{705})/(R_{750}+R_{705}-2R_{445})$	1.22	9.13	6.30	0.80
mSR ₇₀₅	$(R_{750}-R_{445})/(R_{705}+R_{445})$	2.52	10.94	7.99	0.76
NDVI	$(R_{800}-R_{670})/(R_{800}+R_{670})$	1.72	9.85	7.34	0.78
NDVI2	$(R_{750}-R_{705})/(R_{750}+R_{705})$	1.81	9.56	6.79	0.80
OSAVI	$1.16(R_{800}-R_{670})/(R_{800}+R_{670}+0.16)$	1.72	9.85	7.34	0.78
PRI	$(R_{531}-R_{570})/(R_{531}+R_{570})$	25.58	35.96	32.14	0.77
PRI2	$(R_{570}-R_{539})/(R_{570}+R_{539})$	37.84	39.19	37.84	0.76
PSRI	$(R_{680}-R_{500})/R_{750}$	28.07	37.10	34.18	0.80
RDVI	$(R_{800} - R_{670})/\sqrt{(R_{800} + R_{670})}$	2.12	10.67	8.21	0.76
SIPI	$(R_{800}-R_{445})/(R_{800}-R_{680})$	17.18	31.54	28.62	0.76
SR1	R_{750}/R_{700}	3.16	11.76	8.49	0.75
SR3	R_{750}/R_{550}	0.87	9.78	7.51	0.75
SR4	R_{672}/R_{550}	12.97	28.77	26.58	0.74
VOG	R_{740}/R_{720}	0.61	9.68	7.44	0.76
LR	ℓ_2 least squares	4.56	11.52	8.94	0.77
LASSO	ℓ_1 least squares	3.46	12.39	9.56	0.73
TREE	Pruning, min. split = 30	0.14	6.98	4.59	0.86
NN	Sigmoid links, one hidden layer	0.93	9.19	6.49	0.77
KRR	RBF kernel	0.73	6.22	5.24	0.89
GPR	Anisotropic RBF kernel	1.69	6.57	5.19	0.95

simpleR: <http://www.uv.es/gcampes/code/simpleR.html>



- High confidences (west) were the most sampled fields
- Low confidences (center) in underrepresented areas
e.g. dry barley, harvested barley, and bright bare soils

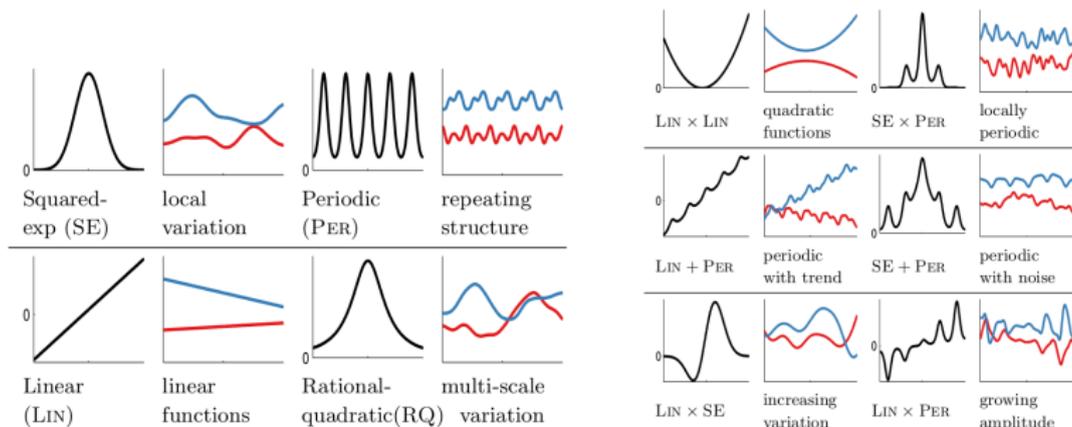
Part 3: Advances in variable prediction and understanding

Structured, non-stationary and multiscale

- Typical kernel (covariance) function:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \nu \exp \left(- \sum_{f=1}^F \frac{(\mathbf{x}_i^f - \mathbf{x}_j^f)^2}{2\sigma_f^2} \right) + \sigma_n^2 \delta_{ij}$$

- Combine kernels:



Time-based covariance for GP regression

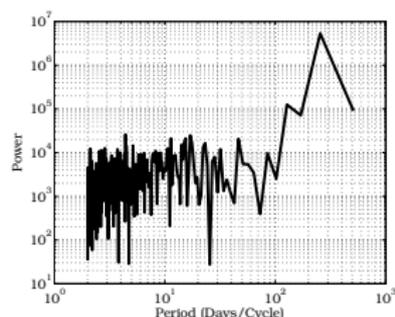
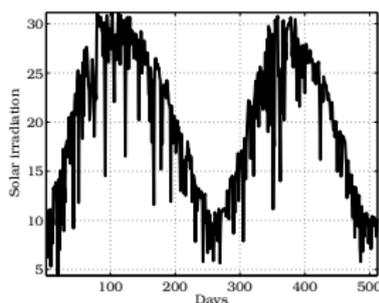
- Standard local relations:

$$k_1(\mathbf{x}_i, \mathbf{x}_j) = \nu \exp \left(- \sum_{f=1}^F \frac{(\mathbf{x}_i^f - \mathbf{x}_j^f)^2}{2\sigma_f^2} \right) + \sigma_n^2 \delta_{ij}$$

- Stationary covariance to capture (inexact) periodicity:

$$k_2(t_i, t_j) = \gamma \exp \left(- \frac{2 \sin^2[\pi(t_i - t_j)]}{\sigma_t^2} \right) \times \exp \left(- \frac{(t_i - t_j)^2}{2\sigma_d^2} \right)$$

- Combine kernels: $k([\mathbf{x}_i, t_i], [\mathbf{x}_j, t_j]) = k_1(\mathbf{x}_i, \mathbf{x}_j) + k_2(t_i, t_j)$

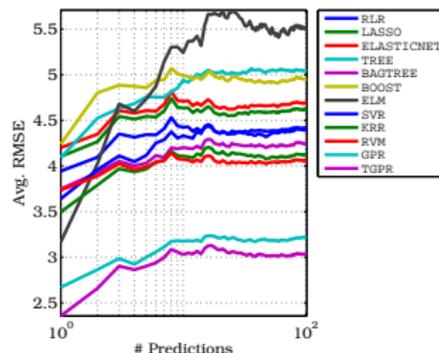


Time-based covariance for GP regression

Prediction of Daily global solar irradiation

Source	Data	Units	min-max
Cimel sunphotometer	Aerosol Optical Depth	-	0.01-1.38
Brewer spectrophotometer	Total Ozone	Dobson	242.50-443.50
Atmospheric sounding	Total Precip. Water	mm	1.33-41.53
GFS	Cloud amount	%	2-79.2
Pyranometer	Measured global solar irradiation	kJ/m^2	4.38-31.15

Method	ME	RMSE	MAE	ρ
RLR	0.27	4.42	3.51	0.76
RLR_t	0.25	4.33	3.42	0.78
SVR	0.54	4.40	3.35	0.77
SVR_t	0.42	4.23	3.12	0.79
GPR	0.14	3.22	2.47	0.88
GPR_t	0.13	3.15	2.27	0.88
TGPR	0.11	3.14	2.19	0.90



Parameter-free covariance

PCK: Probabilistic cluster kernel:

- 1: Run EM-GMM clustering T times with K clusters
- 2: Obtain the posterior probability vector $\pi_i(t, k)$ for \mathbf{x}_i :
- 3: Compute:

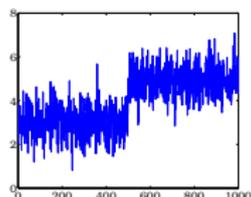
$$K(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{Z} \sum_{t=1}^T \sum_{k=2}^K \pi_i(t, k)^\top \pi_j(t, k) \quad i, j = 1, \dots, n$$

- 4: Done!

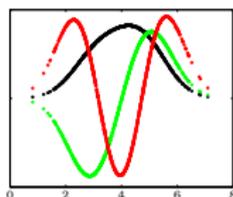
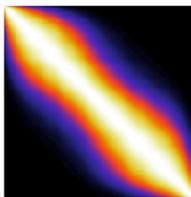
[Izquierdo and Camps-Valls, NEUCOM, 2013]

Parameter-free covariance

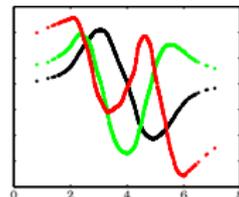
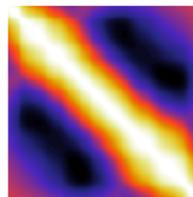
Original Data



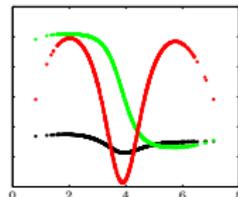
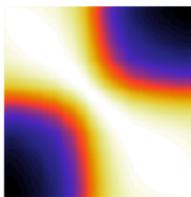
RBF



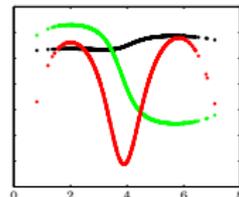
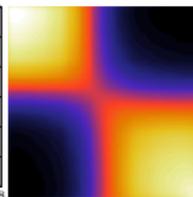
Fisher



Jensen-Shannon



PCK



[Izquierdo and Camps-Valls, NEUCOM, 2013]

Parameter-free covariance

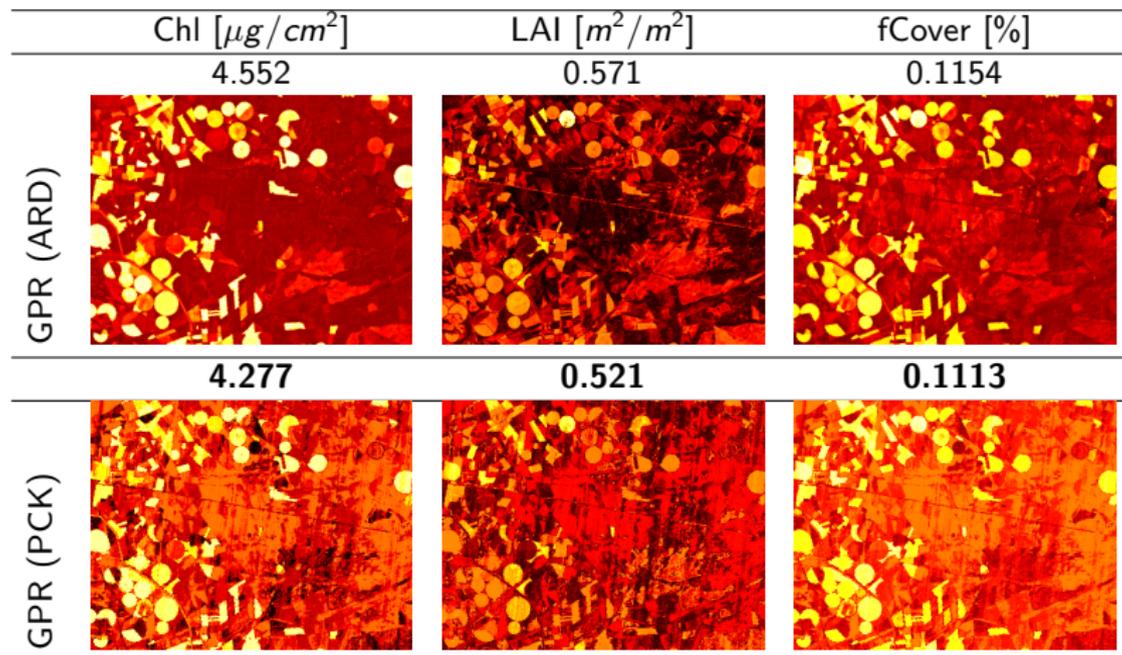


Figure : Estimation maps for Chl, LAI and FCV using CHRIS/PROBA data.

Warped GPR: Learning the output transformation

- No more *ad-hoc* transformations of the observed variable
- Data can be “warped” to look more like a GP:

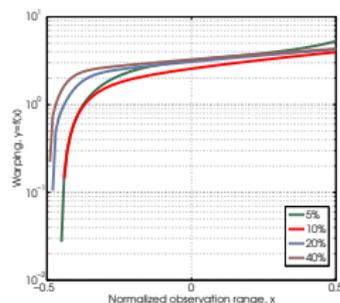
$$y_i = g(f(\mathbf{x}_i) + \varepsilon_i)$$

- Warped GP places another prior for $g(\mathbf{x}) \sim \mathcal{GP}(f, c(f, f'))$

$$g^{-1}(y_i) = y_i + \sum_{\ell=1}^L a_{\ell} \tanh(b_{\ell}(y_i + c_{\ell})), \quad a_{\ell}, b_{\ell} \geq 0,$$

- Evidence is analytical, posterior mean is easy to find
- Improved results and some knowledge about the target

METHOD	ME	RMSE	MAE	R
GPR	0.285	2.312	0.451	0.618
WGPR	0.298	2.344	0.445	0.638



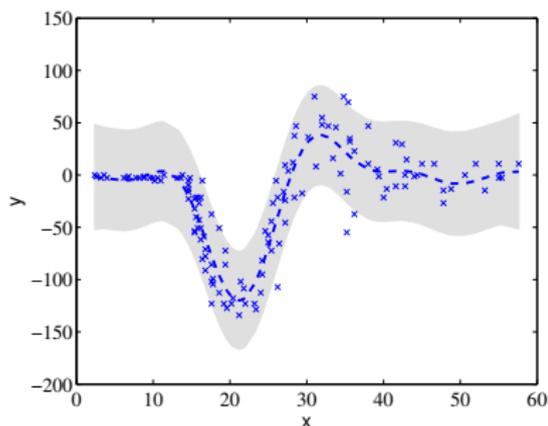
Heteroscedastic GPR

- Heteroscedasticity: Signal and noise relations exist
- Standard GP prior does not capture these relations, $\varepsilon_n \sim i.i.d$
- The GP prior is

$$f(\mathbf{x}) \sim \mathcal{GP}(\mu_0 \mathbf{1}, k_{\theta_f}(\mathbf{x}, \mathbf{x}'))$$

- Good results, but unreasonable uncertainties!

METHOD	ME	RMSE	MAE	R
GPR	0.285	2.312	0.451	0.618
WGPR	0.298	2.344	0.445	0.638



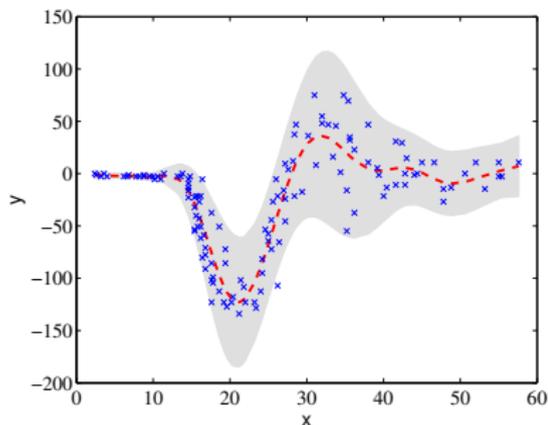
Heteroscedastic GPR

- Heteroscedasticity: Signal and noise relations exist
- Change the GP prior over ε_n to $\varepsilon_n \sim \mathcal{N}(0, e^{\mathbf{g}(\mathbf{x}_n)})$
- We place an additional GP prior

$$f(\mathbf{x}) \sim \mathcal{GP}(\mu_0 \mathbf{1}, k_{\theta_f}(\mathbf{x}, \mathbf{x}')) \quad \mathbf{g}(\mathbf{x}) \sim \mathcal{GP}(\mu_0 \mathbf{1}, k_{\theta_g}(\mathbf{x}, \mathbf{x}'))$$

- Improved results and some knowledge about the noise

METHOD	ME	RMSE	MAE	R
GPR	0.285	2.312	0.451	0.618
WGPR	0.298	2.344	0.445	0.638
VHGPR	0.271	2.309	0.442	0.684



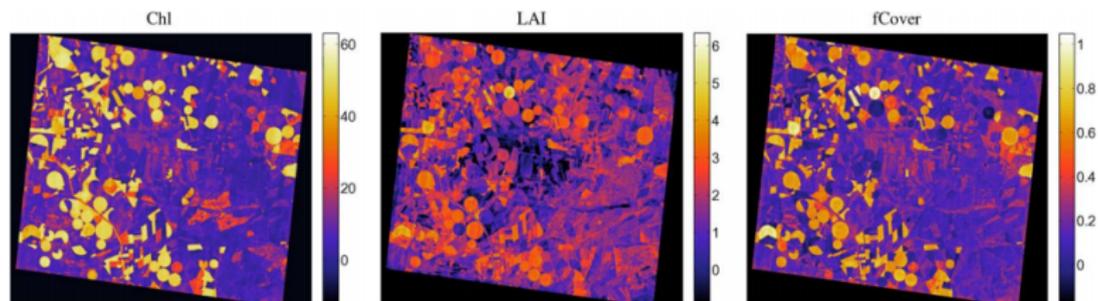
Multioutput GPR

- A model to predict several variables simultaneously
- Constrain the outputs to be physically-meaningful
- Posterior over the unknown output:

$$p(y_* | \mathbf{x}_*, \mathcal{D}) = \mathcal{N}(y_* | \mu_{\text{GP}*}, \sigma_{\text{GP}*}^2)$$

$$\mu_{\text{GP}*} = \mathbf{k}_{\mathbf{f}*}^\top (\mathbf{K} + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{Y} = \mathbf{k}_{\mathbf{f}*}^\top \mathbf{A}$$

- Just efficiency, no actual cross-relations



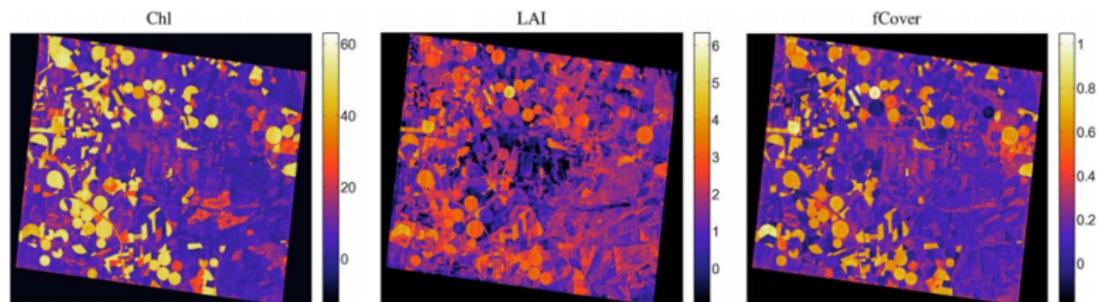
Multioutput GPR

- Constrain the outputs to be physically-meaningful
- Response vector as a linear combination of a set of M latent GPs
- Gives a block covariance matrix $[\tilde{\mathbf{K}}_{ij}^m] = k_m(\mathbf{x}_i, \mathbf{x}_j)$, $m = 1, \dots, M$

$$p(y_* | \mathbf{x}_*, \mathcal{D}) = \mathcal{N}(y_* | \mu_{\text{GP}*}, \sigma_{\text{GP}*}^2)$$

$$\mu_{\text{GP}*}^m = \tilde{\mathbf{k}}_{\mathbf{f}*}^\top (\tilde{\mathbf{K}} + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{Y} = \tilde{\mathbf{k}}_{\mathbf{f}*}^\top \mathbf{A}$$

- Promising results in biophysical parameter retrieval



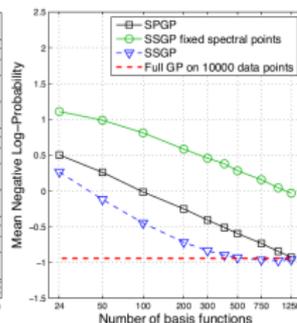
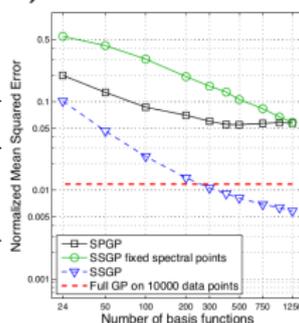
Sparse spectrum Gaussian Processes Regression (SSGPR)

- Speeding up GP is mandatory
- Sparse spectrum GP = standard GP with covariance:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \sum_{m=1}^M \cos(\mathbf{w}_m^\top (\mathbf{x}_i - \mathbf{x}_j)), \quad M \text{ basis functions}$$

- Computation time goes from $\mathcal{O}(N^3)$ to $\mathcal{O}(M \cdot N^2)$
- Storage goes from $\mathcal{O}(N^2)$ to $\mathcal{O}(M \cdot N)$

METHOD	ME	RMSE	R	CPU [s]
GPR	0.285	2.312	0.618	1.150
SSGPR	0.296	2.194	0.684	0.530



Sparse spectrum Gaussian Processes Regression (SSGPR)

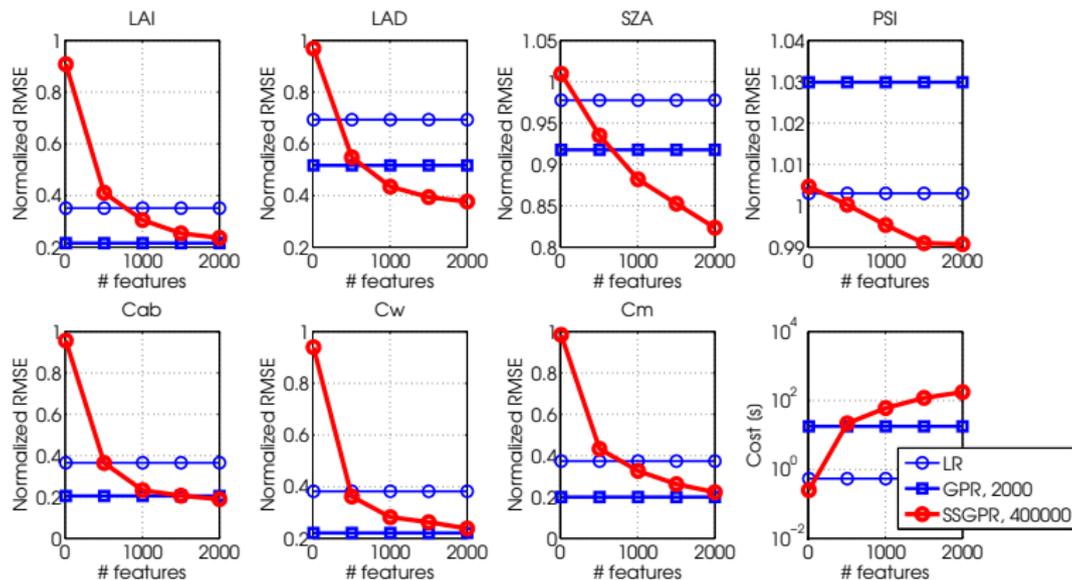
- Inversion of PROSAIL radiative transfer model
- PROSAIL models leaf properties and canopy bidirectional reflectance
- 10^6 points; train with 400,000 samples and cosine basis
- Prediction of 7 vegetation variables

Table : Configuration parameters of the simulated data.

Parameter	Sampling	Min	Max
RTM model: Prospect 4			
Leaf Structural Parameter	Fixed	1.50	1.50
C_{ab} , chlorophyll a+b [$\mu\text{g}/\text{cm}^2$]	$\mathcal{U}(14, 49)$	0.067	79.97
C_w , equivalent water thickness [mg/cm^2]	$\mathcal{U}(10, 31)$	2	50
C_m , dry matter [mg/cm^2]	$\mathcal{U}(5.9, 19)$	1.0	3.0
RTM model: 4SAIL			
Diffuse/direct light	Fixed	10	10
Soil Coefficient	Fixed	0	0
Hot spot	Fixed	0.01	0.01
Observer zenith angle	Fixed	0	0
LAI, Leaf Area Index	$\mathcal{U}(1.2, 4.3)$	0.01	6.99
LAD, Leaf Angle Distribution	$\mathcal{U}(28, 51)$	20.04	69.93
SZA, Solar Zenit Angle	$\mathcal{U}(8.5, 31)$	0.082	49.96
PSI, Azimut Angle	$\mathcal{U}(30, 100)$	0.099	179.83

Sparse spectrum Gaussian Processes Regression (SSGPR)

- Inversion of PROSAIL radiative transfer model
- PROSAIL models leaf optical properties model and canopy bidirectional reflectance
- 1 million points; train with 400,000 samples and cosine basis



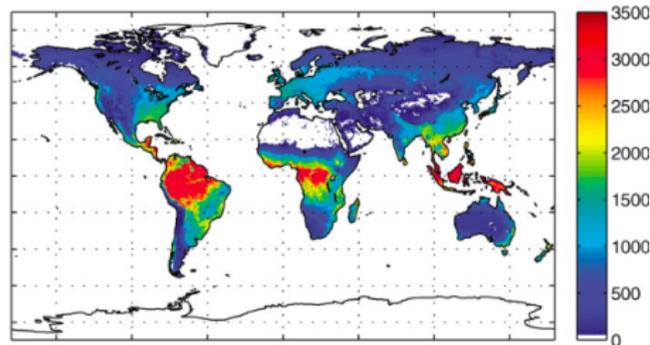
Sensitivity analysis

- Derivatives of the predictive mean $\phi(\mathbf{x})$ wrt features
- Sensitivity of feature j is defined as

$$s_j = \int \left(\frac{\partial \phi(\mathbf{x})}{\partial \mathbf{x}_j} \right)^2 p(\mathbf{x}) d\mathbf{x} = \dots = \frac{1}{N} \sum_{q=1}^N \left(\sum_{p=1}^N \frac{\alpha_p (\mathbf{x}_{p,j} - \mathbf{x}_{q,j})}{\sigma_j^2} k(\mathbf{x}_p, \mathbf{x}_q) \right)^2$$

- Gross Primary Production (GPP) is the largest global CO₂ flux driving several ecosystem functions

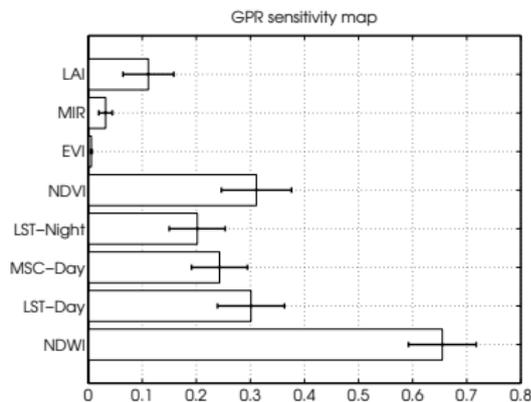
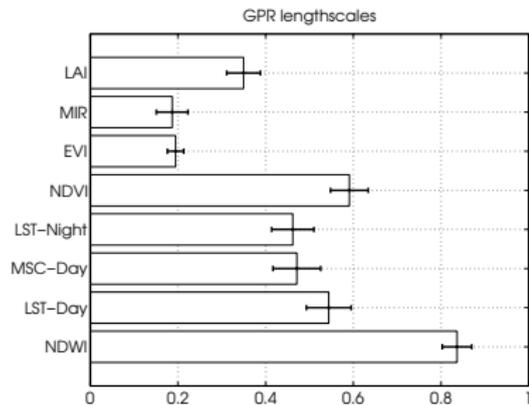
GPP	ME	RMSE	MAE	ρ
LR	-0.01	1.83	1.30	0.78
MLP	+0.04	1.92	1.39	0.73
SVR	+0.01	1.80	1.23	0.78
GPR	+0.03	1.76	1.16	0.80



Sensitivity analysis

- Derivatives of the predictive mean $\phi(\mathbf{x})$ wrt features
- Sensitivity of feature j is defined as

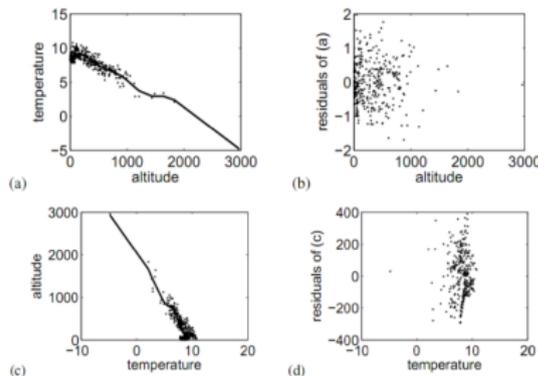
$$s_j = \int \left(\frac{\partial \phi(\mathbf{x})}{\partial \mathbf{x}_j} \right)^2 p(\mathbf{x}) d\mathbf{x} = \dots = \frac{1}{N} \sum_{q=1}^N \left(\sum_{p=1}^N \frac{\alpha_p (\mathbf{x}_{p,j} - \mathbf{x}_{q,j})}{\sigma_j^2} k(\mathbf{x}_p, \mathbf{x}_q) \right)^2$$



From regression to causation

Hoyer (2008) regression-based framework:

- Perform nonlinear regression from $x \rightarrow y$ (and vice-versa, $y \rightarrow x$)
- Independent forward residuals? $(y - f(x)) \perp\!\!\!\perp x$
- Independent backward residuals? $(x - g(y)) \perp\!\!\!\perp y$
- p -value of independence tells the right direction of causation

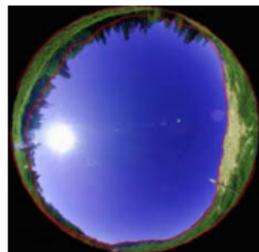
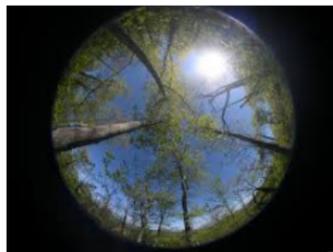


Method	p_f	p_b	Conclusion
GP	2.88×10^{-2}	3.54×10^{-12}	alt \rightarrow temp
WGPR	7.47×10^{-4}	9.28×10^{-11}	alt \rightarrow temp
VHGPR	2.94×10^{-16}	8.83×10^{-23}	alt \rightarrow temp
GP	3.86×10^{-61}	1.57×10^{-119}	PPFD(tot) \rightarrow NEP
WGPR	2.09×10^{-52}	4.18×10^{-112}	PPFD(tot) \rightarrow NEP
VHGPR	5.09×10^{-61}	2.51×10^{-108}	PPFD(tot) \rightarrow NEP
GP	1.59×10^{-11}	1.24×10^{-79}	PPFD(diff) \rightarrow NEP
WGPR	1.16×10^{-12}	9.00×10^{-79}	PPFD(diff) \rightarrow NEP
VHGPR	2.94×10^{-13}	9.90×10^{-78}	PPFD(diff) \rightarrow NEP
GP	2.05×10^{-8}	1.56×10^{-112}	PPFD(dir) \rightarrow NEP
WGPR	1.30×10^{-15}	3.33×10^{-111}	PPFD(dir) \rightarrow NEP
VHGPR	4.53×10^{-16}	1.12×10^{-115}	PPFD(dir) \rightarrow NEP

[Camps-Valls, 2012]

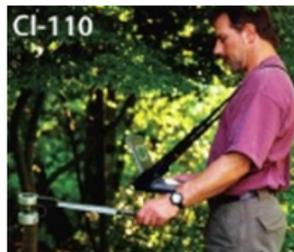
Explicit mapping LAI with GPR and your smartphone

- Leaf area index (LAI) characterizes plant canopies
- LAI: one-sided green leaf area per unit ground surface area
- LAI: Key variable to analyze plants-atmosphere interaction
 - amount of radiation intercepted
 - plant water requirements
 - CO₂ sequestration
 - assimilation of exogenous information in simulation models
 - forecasting purposes
- Hemispherical photography estimates LAI from upward-looking fisheye photographs taken beneath the plant canopy



Explicit mapping LAI with GPR and your smartphone

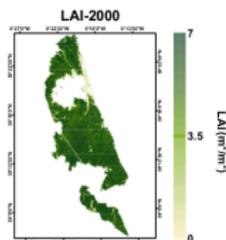
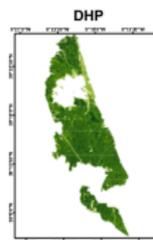
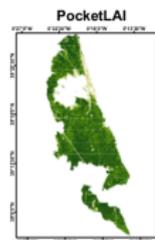
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 - plant water requirements
 - CO₂ sequestration
 - assimilation of exogenous information in simulation models
 - forecasting purposes
- Ceptometers invert light transmittance models, but expensive, heavy, maintenance



[Campos and Camps-Valls, 2015]

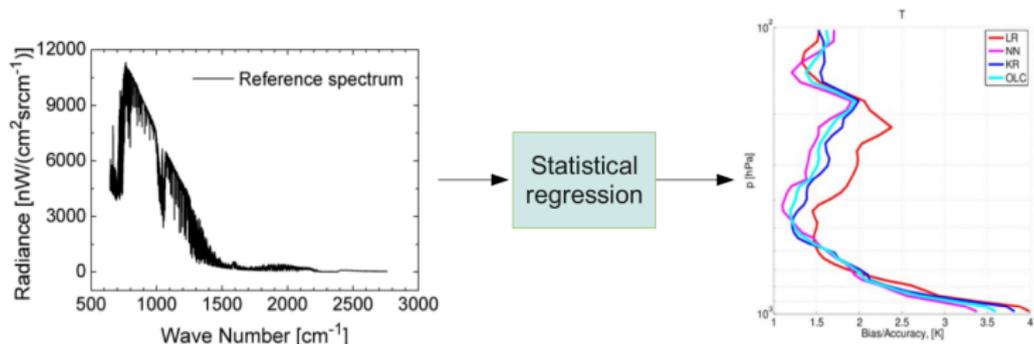
Explicit mapping LAI with GPR and your smartphone

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 - amount of radiation intercepted
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 - forecasting purposes
- PocketLAI app: Segmentation (color-based, sky conditions), accelerometer, Poisson model for random leaves spatial distribution



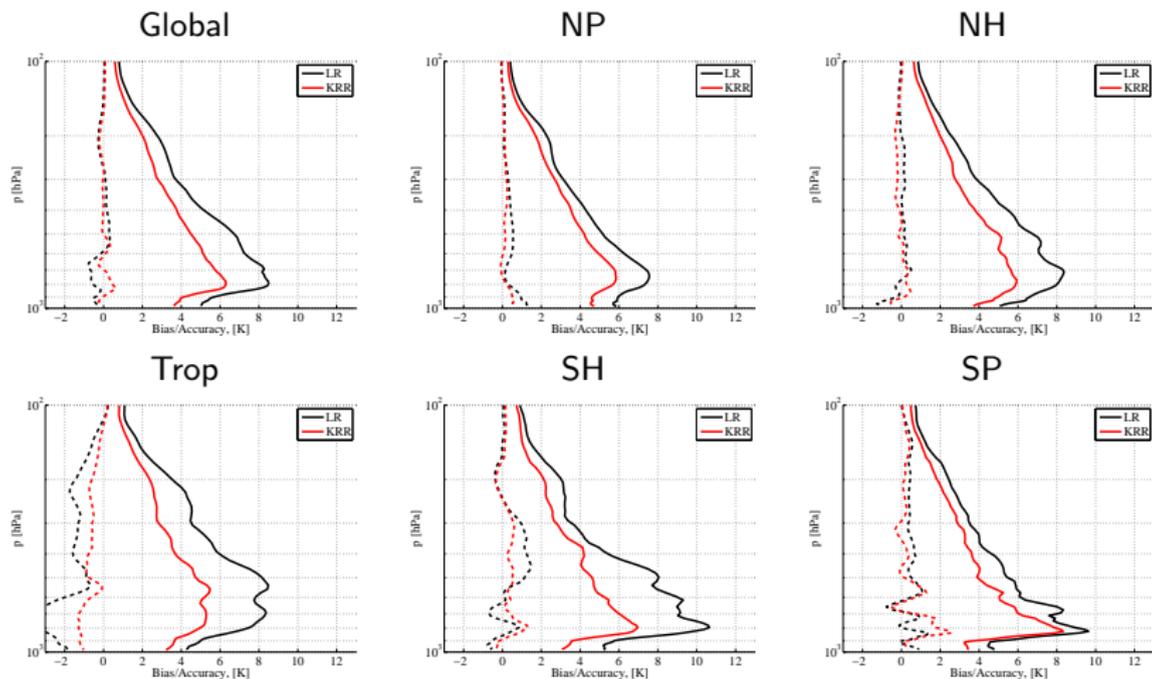
GPR for weather forecasting

- Meteorological satellites carry infrared sounders, e.g. AIRS or IASI
- Big data: terabytes/day, IASI pixels are 8000-dim, 100 atmos. levels
- We run multioutput GPR for predicting temperature, moisture and ozone concentration (among other parameters)
- Gain in RMSE (1.5K), CPU time (seconds vs hours), and cloud detection



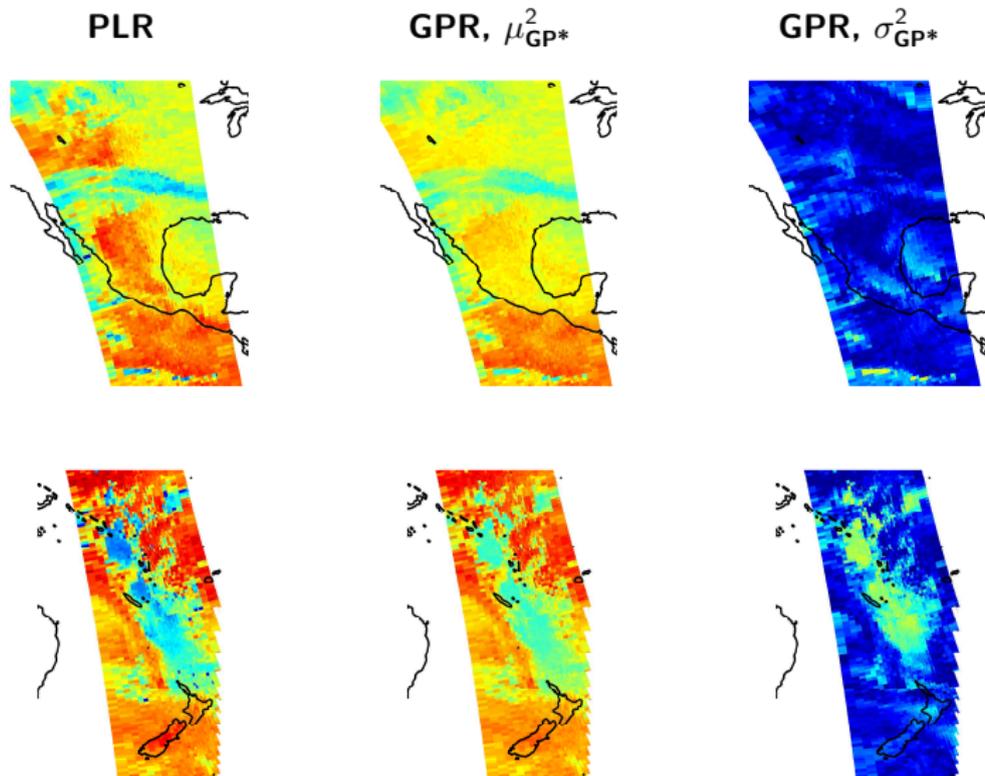
[Laparra, Calbet and Camps-Valls, 2015]

GPR for weather forecasting



- GPR largely improves PLR results over land (+1.5K)
- Big numerical and statistical differences in all regions

GPR for weather forecasting



Part 4: Conclusions

Conclusions

- **Advances in climate variable estimation from space**
- **Look at the signal structure and act!**
- **Bayesian nonparametrics is a proper framework**
 - Solid Bayesian foundation
 - Excellent prediction capabilities
 - Encoding of prior knowledge and structures
 - Deal efficiently with uncertainties
- **GPR allows feature ranking and causal inference**
- **Code, papers, demos: <http://isp.uv.es/>**

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Thanks! Tuia, Jensen, Jung, Reichstein, Laparra, Mooij, Schölkopf, Peters, Verrelst, Lázaro-Gredilla, Titsias, Pérez-Cruz, Calbet, Muñoz-Marí, Moreno, Salcedo, Izquierdo, Campos



-  *Global monitoring of crop photosynthesis with chlorophyll fluorescence*, PNAS 2014.
-  *Prediction of Daily Global Solar Irradiation*, IEEE-GRSL 2015.
-  *Kernel Framework for Supervised Subspace Learning*, IEEE SPM 2013
-  *Advances in Hyperspectral Image Classification*, IEEE SPM 2014
-  *Gaussian processes Uncertainty Estimates in Experimental Sentinel-2 LAI*, ISPRS, 2013
-  *Gaussian process retrieval of chlorophyll content*, IEEE JSTARS, 2013
-  *Retrieval of Canopy Parameters using Gaussian Processes Techniques*, IEEE TGRS, 2012
-  *Learning with the Kernel Signal To Noise Ratio*, IEEE PAMI, 2015
-  *Sensitivity Analysis of Chlorophyll content prediction*, IEEE TGRS, 2015
-  *Retrieval of Biophysical Parameters with Heteroscedastic GP*, IEEE GRSL, 2014
-  *Ranking drivers of global carbon and energy fluxes over land*, IEEE IGARSS, 2015
-  *Biophysical parameter retrieval with warped Gaussian processes*, IEEE IGARSS, 2015
-  *Large-scale random features kernel regression* , IEEE IGARSS, 2015
-  *Kernel methods for Remote Sensing Data Analysis*, Wiley and Sons, 2009
-  *Kernel methods for Digital Signal Processing*, Wiley and Sons, 2015