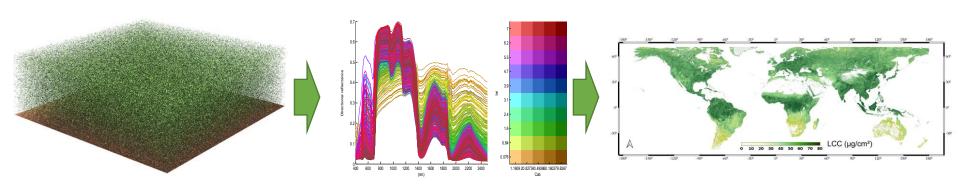




From model simulations towards vegetation properties mapping:

automating, optimizing & expanding



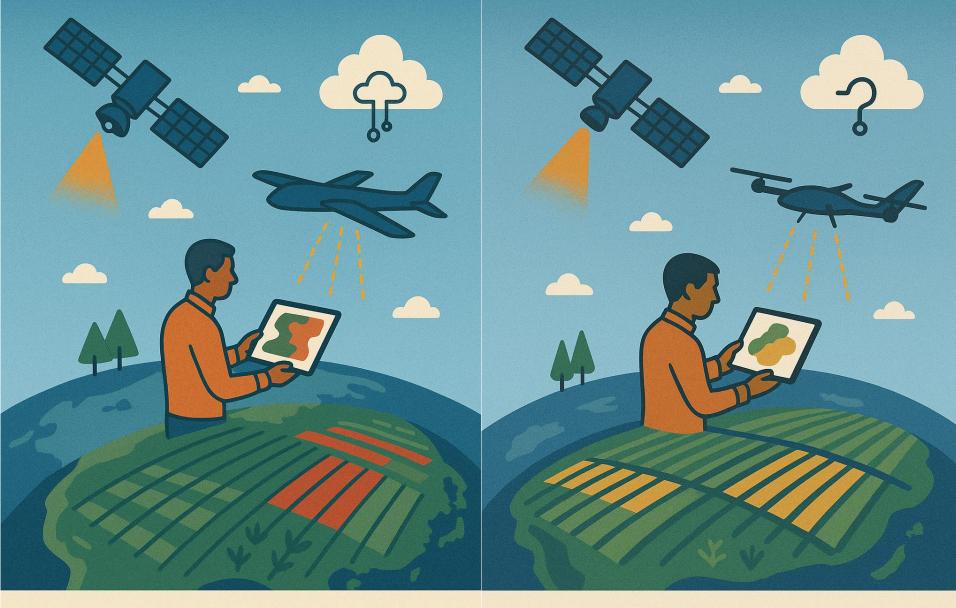
Jochem Verrelst

July 2025



QUANTITATIVE REMOTE SENSING OF VEGETATION

QUANTITATIVE REMOTE SENSING OF VEGETATION



VEGETATION CHANGE

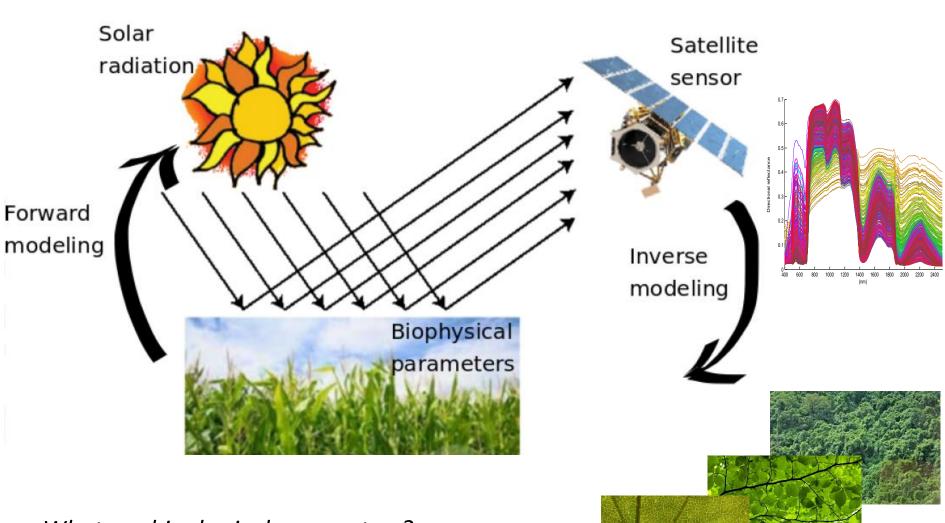
CROP YIELD PREDICTION

How to quantify vegetation properties?



Today we will learn:

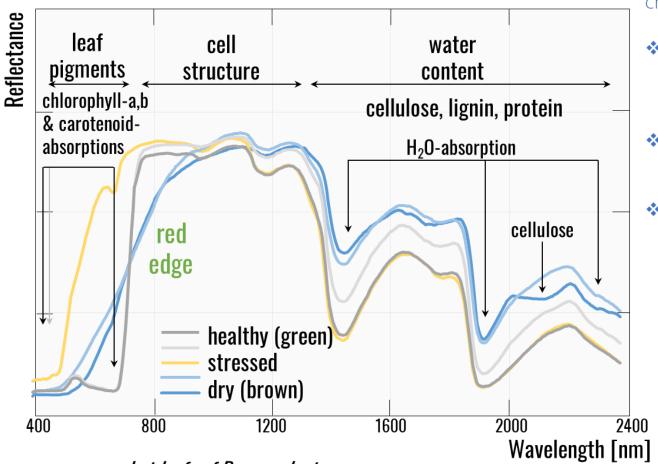
Semi-automated mapping of vegetation properties from optical RS data



5/61

- What are biophysical parameters?
- Why is it important to quantify them?

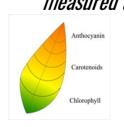
Factors controlling leaf reflectance

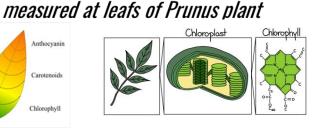


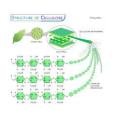
Shape of the leaf spectra is characterized by:

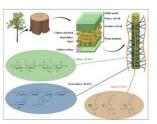
- Low reflectance across visible wavelengths (due to absorption by photosynthetic pigments).
- High reflectance in the NIR, with only ~ 10% of absorbed radiation.
- Intermediate reflectance in the SWIR, where energy is mainly absorbed by water or plant residues in case of dry/stressed leaves. Cell wall compounds (cellulose, lignin, proteins and sugars) lead to overlapping absorption features.

(Ustin & Jacquemoud 2020)



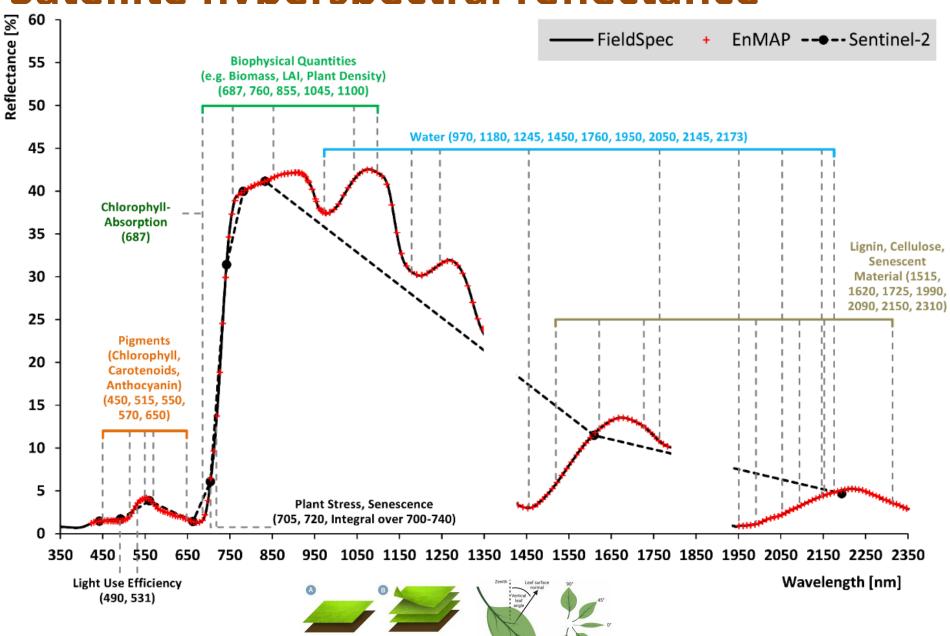








Satellite hyperspectral reflectance



The problem:

Biophysical parameter retrieval is an essential step in modeling the processes occurring on Earth and the interactions with the atmosphere.

The analysis can be done at **local** or **global** scales by looking at bio-geochemical cycles, atmospheric situations, ocean/river/ice states, and vegetation dynamics.

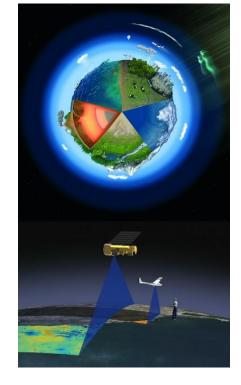
Main parameters: crop yield, biomass, leaf area coverage, chlorophyll content, fraction vegetation cover, GPP,....

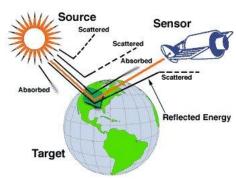
Land/vegetation parameters cannot be estimated directly from optical RS data. A model is required!

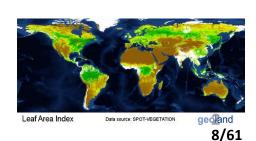
The objective: Transform measurements into biophysical parameter estimates.

The data:

- Input data: satellite/airborne spectra, in situ (field) radiometers, or simulated spectra by RTMs
- Output results: estimation of a biophysical parameter





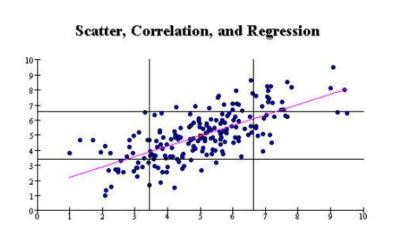


Introduction retrieval biophysical parameters

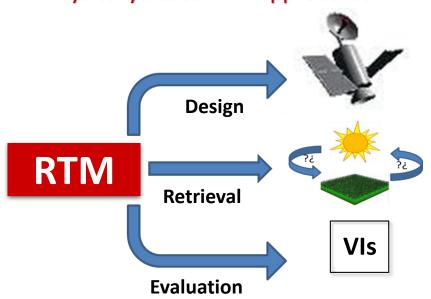


Retrieval of biophysical parameters from Remote Sensing (RS) data **always occurs through a model**, e.g. through statistical models or through inversion of physically-based radiative transfer models (RTM).

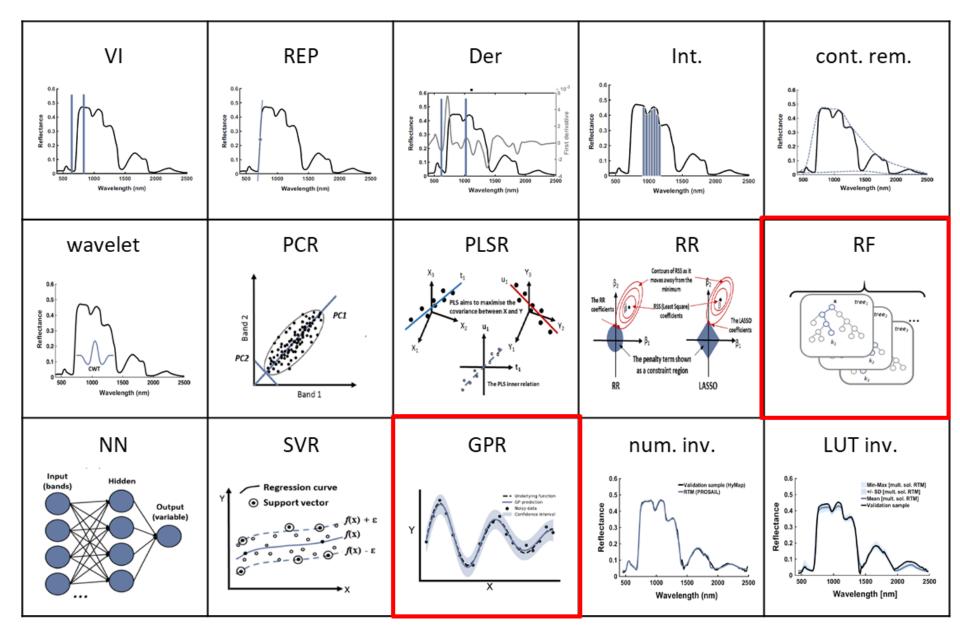
Statistical approaches



Physically based RTM approaches



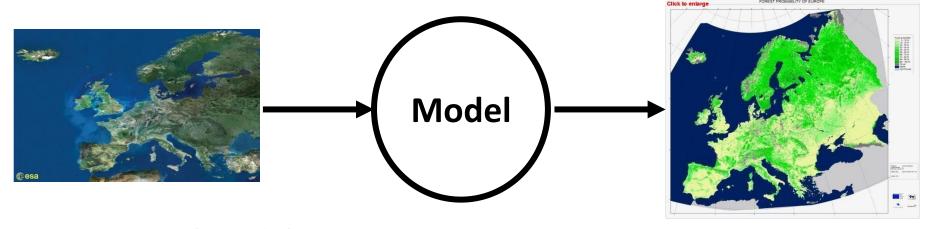
Some retrieval methods....



Retrieval of (continuous) vegetation properties

Remote sensing image

Map of a vegetation property



1. Statistical models

- 1. Parametric regression models
- 2. Nonparametric regression models
 - Linear
 - Nonlinear: ML

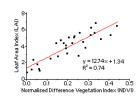
2. Inversion of physically based radiative transfer models

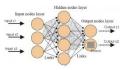
- 1. Numerical optimization
- 2. Lookup-table (LUT)-based inversion

Taxonomy of retrieval methods, three main families:

1. Statistical: parametric and non-parametric:

- Parametric models rely on *some* physical knowledge of the problem and build explicit parametrized expressions that relate a few spectral bands with the biophysical parameter(s) of interest.
- Non-parametric models are data-driven models. They are adjusted to predict a variable of interest using a training dataset of input-output data pairs.





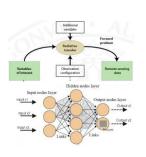
2. Physical: try to reverse RTMs.

• Physically based algorithms are applications of physical laws establishing photon interaction *cause–effect relationships*. Model variables are inferred based on specific knowledge, typically obtained with *radiative transfer functions*.



3. Hybrid:

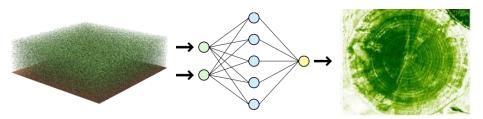
 A hybrid-method combines elements of nonparametric statistics and physically based methods. Hybrid models rely on the generic properties of physically based methods combined with the flexibility and computational efficiency of nonparametric nonlinear regression methods.



Retrieval families

RTM inversion Parametric regression Non-parametric regression Spectral relationships that are Advanced techniques that Models that simulate sensitive to specific search for relationships interactions between vegetation properties between spectral data and vegetation and radiation biophysical variables leaf $NDVI = \frac{(\rho_{NIR} - \rho_{RED})}{(\rho_{NIR} + \rho_{RED})}$ **Normalized Difference Vegetation Index** canopy

Methods of these different families can be combined: hybrid methods



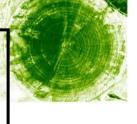
Statistical interpretation of RS



Statistical relationship

- Parametric regression
- Non-parametric regression

Variable of Interest



- Simple statistical relationships (VIs) constitute the **BULK of RS analysis**.
- These analyses allow to determine **IF** there is a relationship, **not WHY** there is a relationship.
- Linear methods such as VIs are **useful indicators** of biophysical (e.g. structure) or biochemical (e.g. chlorophyll) parameters, however in natural, complex environments indices are **confounded** by additional abiotic and biotic factors.
- VIs lack generality for estimating biophysical parameters.
- Apart from VIs a large number of powerful **alternative statistical retrieval** methods exists (e.g. non-parametric regression methods).

Parametric regression

Parametric regression assume an explicit model for retrieval **BODY MEDITY STREETS AND ST

• Discrete band methods(VIs):

- 2-band: SR, NDVI, PRI, OSAVI
- 3-band: TVI, MCARI, SIPI
- 4-band: TCARI/OSAVI

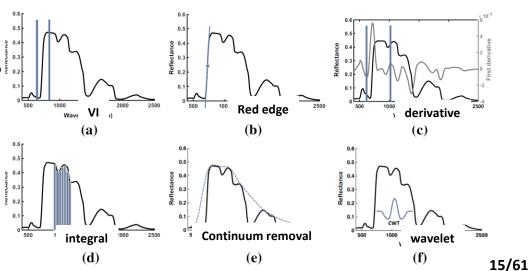
$$PRI = \frac{(\rho 570 - \rho 531)}{(\rho 570 + \rho 531)}$$

$$TCARI / OSAVI = 3 \cdot \left[\left(\rho_{\mu 700} - \rho_{\mu 670} \right) - 0.2 \cdot \left(\rho_{\mu 700} - \rho_{\mu 550} \right) \cdot \right]$$

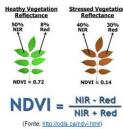
$$\left(\rho_{\mu 700} - \rho_{\mu 670} \right) \left(1 + 0.16 \right) \cdot \left(\rho_{\mu 800} - \rho_{\mu 670} \right) / \left(\rho_{\mu 800} - \rho_{\mu 670} + 0.16 \right) \tag{2}$$

Shape-based methods (hyperspectral data):

- Red-edge position (REP)
- Derivative/Integral indices
- Continuum removal
- wavelet



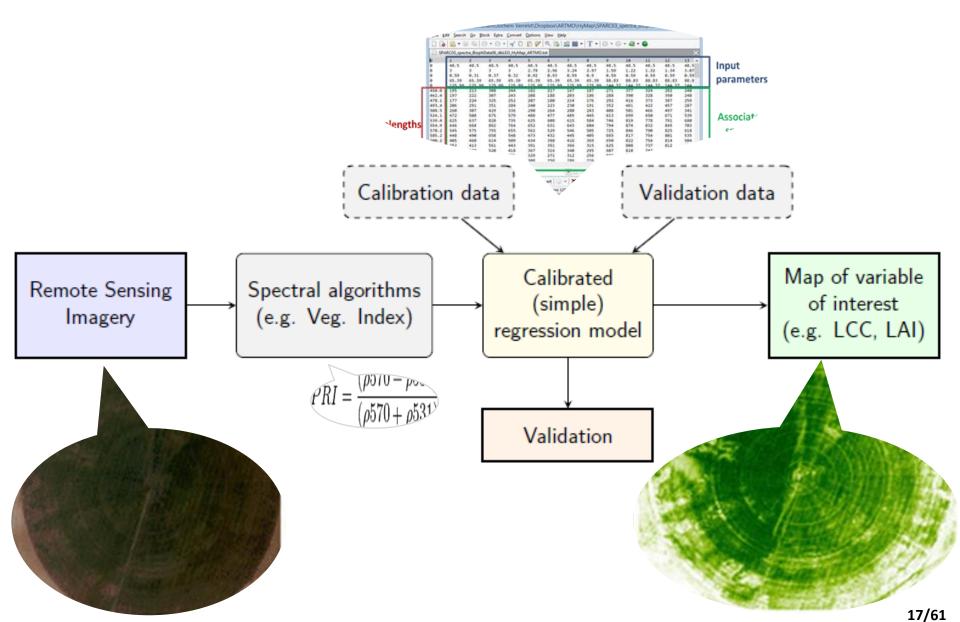
Parametric regression:



			(Fonte: http://odis.ca/ndvi.html)	
	Strengths ©		Weaknesses ⊗	
•	Simple and comprehensive regression models;	•	Makes only poorly use of the available information	
	little knowledge of user required.		within the spectral observation; at most a spectral	
			subset is used. Therefore, they tend to be more noise-	
•	Fast in processing		sensitive as compared to full-spectrum methods	
•	Computationally inexpensive	•	Parametric regression puts boundary conditions at the	
			level of chosen bands, formulations and regression	
			function.	
		•	Statistical function accounts for one variable at a time.	
		•	A limited portability to different measurement	
			conditions or sensor characteristics	
		•	No uncertainty estimates are provided. Hence the	
			quality of the output maps remains unknown.	



Parametric regression

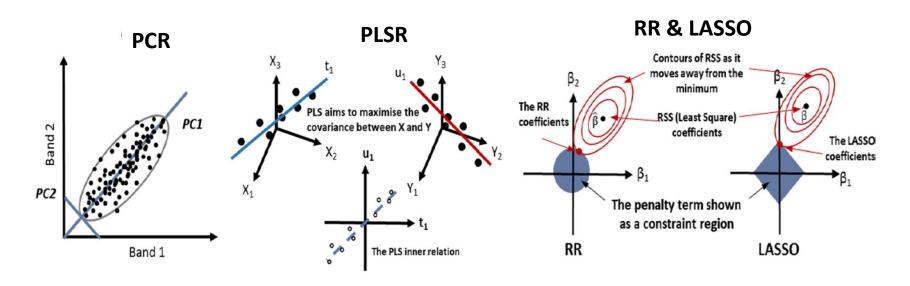


Non-parametric models (1/2):

Data-driven methods: Do not assume explicit feature relations

Linear nonparametric models:

- Stepwise multiple linear regression (SMLR)
- Principal component regression (PCR)
- Partial least squares regression (PLSR)
- Ridge regression (RR)
- Least Absolute Shrinkage and Selection Operator (LASSO)

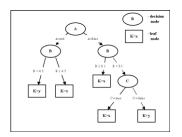


Non-parametric models (2/2):

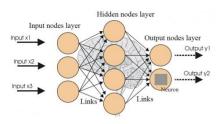
Data-driven methods: Do not assume explicit feature relations

Non-linear nonparametric models:

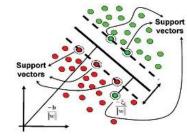
Decision Trees (DT)



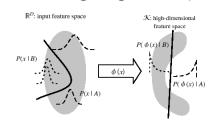
Neural networks (NN)



Support vector regression (SVR)

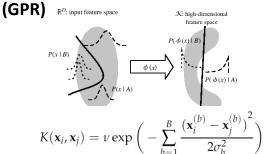


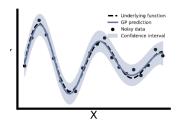
Kernel ridge regression (KRR)



$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/(2\sigma^2)).$$

Gaussian processes regression





Also:

- Elastic Net (ELASTICNET)
- Bagging trees (BAGTREE)
- Boosting trees (BOOST)
- Neural networks (NN)

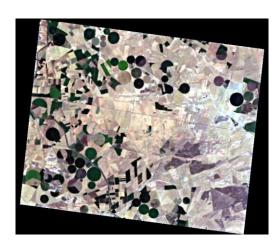
- Extreme Learning Machines (ELM)
- Relevance Vector Machine (RVM)
- Gaussian process Regression (GPR)
- Variational Heteroscedastic Gaussian Process Regression (VHGPR)

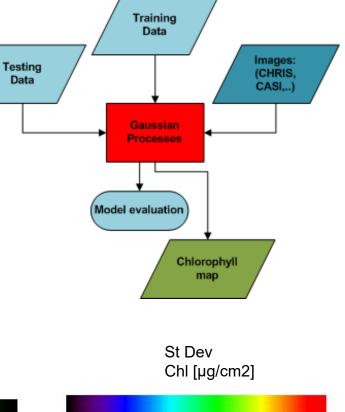
Gaussian Processes Regression (GPR)

- A **GPR** model is a **probabilistic** (**Bayesian**) model directly in function space, with no intermediate model or model parameters.
- GPR are equivalent to kernel ridge regression, least square suport vector machines (SVM), Kriging, large neural networks (NN) and very closely related to SVM regulazation networks.
- **GPR alleviates** some **shortcomings** of the previous methods, while maintaining very good numerical performance and stability:
 - GPR is far simpler than NN, and needs fewer sample points
 - Not only a mean prediction for each sample (pixel), but also a full distribution over the output values including an uncertainty of the prediction (confidence interval).
 - GPR provide a ranking of features (bands) and samples (spectra), thus partly overcoming the blackbox problem.
 - http://www.rainsoft.de/projects/gausspro.html

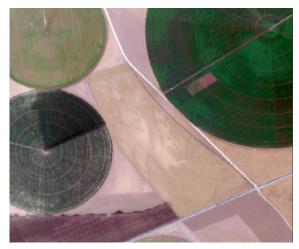
Example GPR

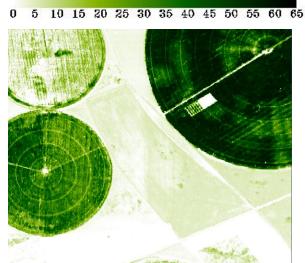




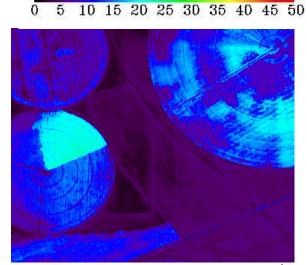


RGB CASI





Chl [µg/cm²]



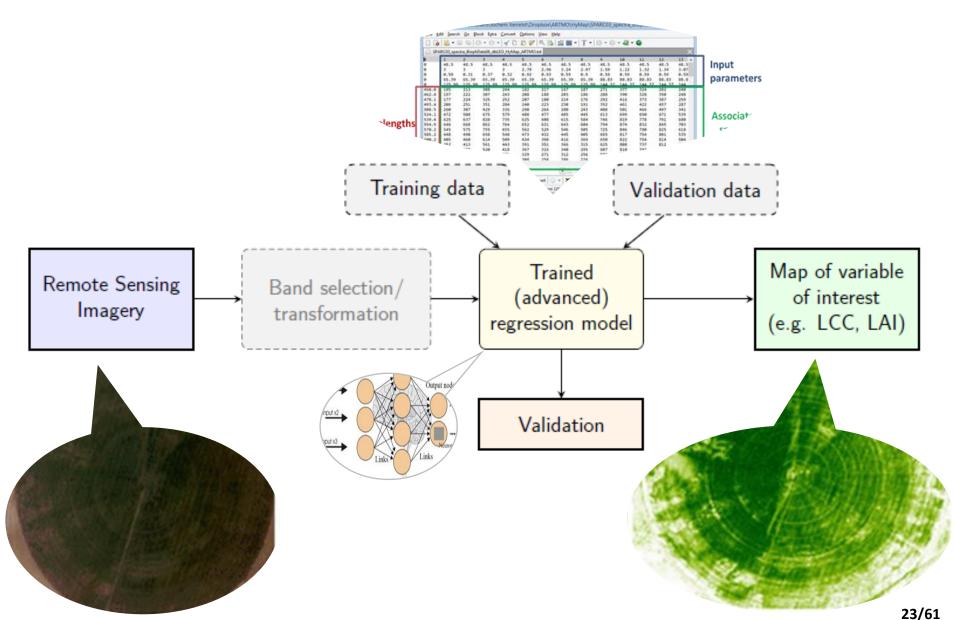
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Non-parametric regression:

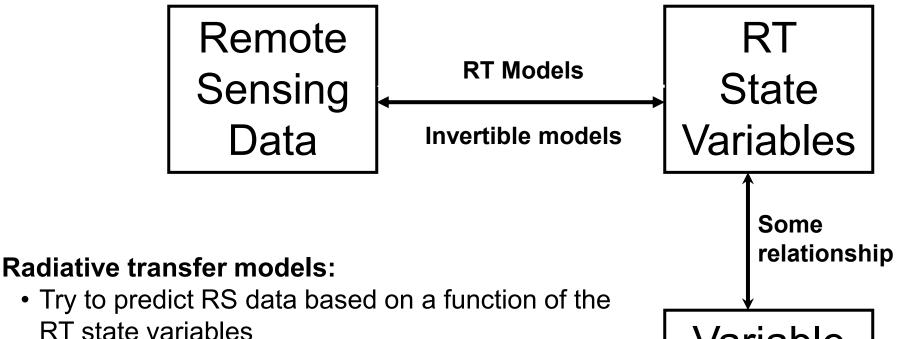
	Strengths ©		Weaknesses ⊗
•	Full-spectrum methods. They make use of the complete	•	Training can be computational expensive.
	spectral information.	•	Hypercomplex models can be generated. Their generic
•	Advanced, adaptive (non-linear) models are built.		potential is limited and hence they do not generalize well,
•	Methodologically, accurate and robust performance is		based on the training data (problem of over-fitting).
	enabled.	•	Some regression algorithms are difficult (or even impossible)
•	Some MLRAs cope well with datasets showing redundancy		to train with a high number of samples.
	and high noise levels.	•	Expert knowledge is required, e.g. for tuning. However,
•	Once trained, imagery can be processed time efficient.		toolboxes exist automating some of the steps in this sub- process.
•	Some of the non-parametric methods (e.g. ANNs, decision trees) can be trained with a high number of samples	•	Some of the methods can be considered as black boxes.
	(typically >1,000,000).	•	Some regression algorithms elicit instability when applied
•	Some MLRAs provide insight in model development (e.g. GPR: relevant bands; decision trees: model structure).		with datasets statistically deviating from the datasets used for training.
•	Some MLRAs can provide multiple-outputs (e.g. PLRS, ANN,		
	SVR, GPR and KRR)		
•	Some MLRAs provide uncertainty intervals (e.g. GPR).		22/6



Non-parametric regression



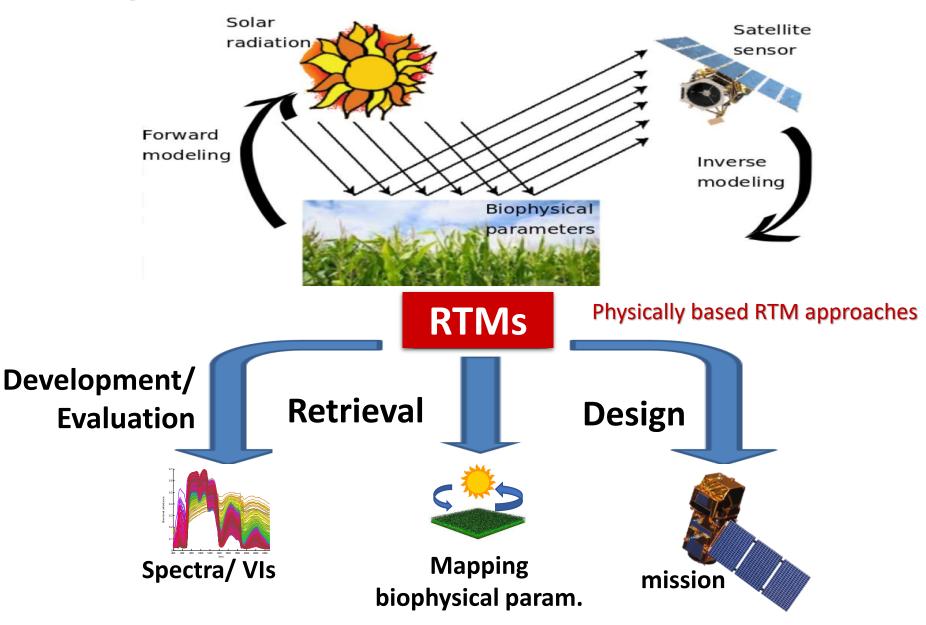
Physical interpretation of RS



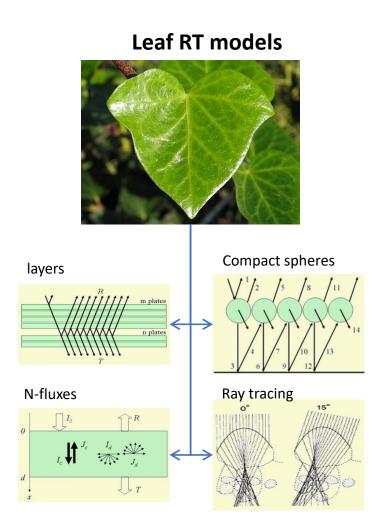
- Two categories of RT models:
 - <u>Economically invertible models</u>: typically designed for simple scenes, have a few number of state variables (e.g. SAIL, RPV)
 - Non-economically invertible models: typically designed for complex scenes, have a large number of state variables (e.g. DART, Drat)

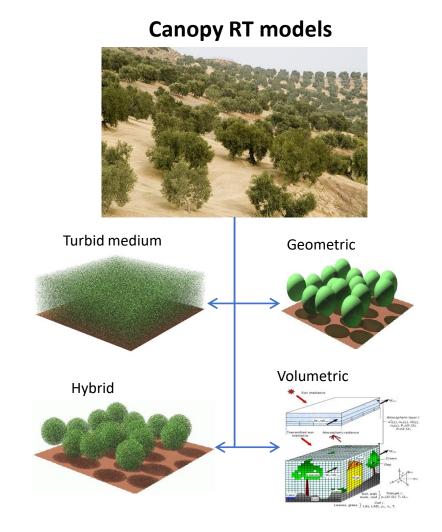


Background



Radiative transfer models



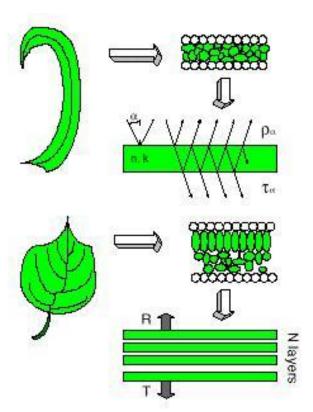


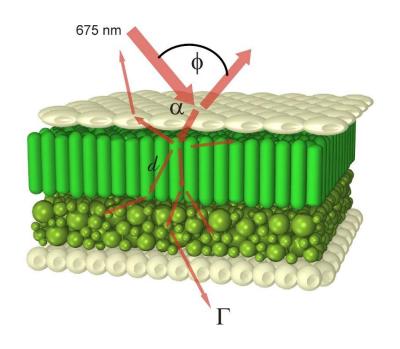


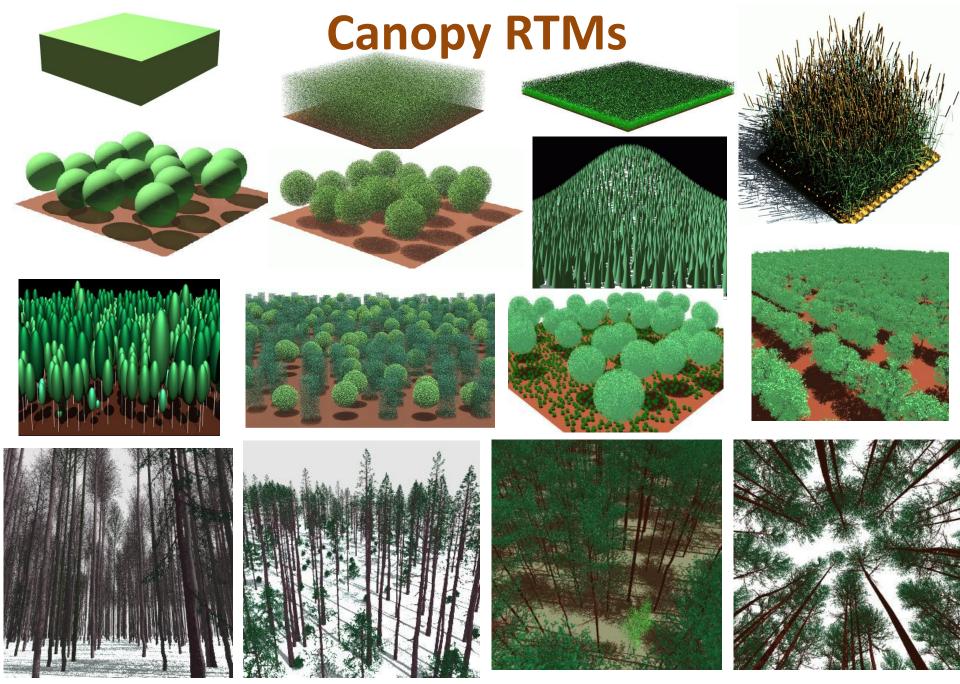
Multiple models exist with diverse complexity.

Leaf optical models

- A leaf is not opaque but transparent.
- Leaf as composed out of layers and empty spaces



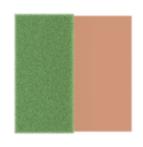


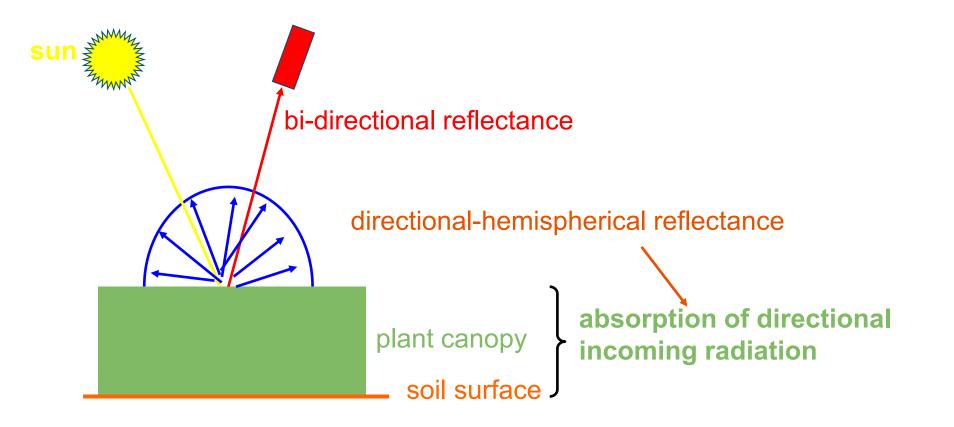


http://rami-benchmark.jrc.ec.europa.eu

Examples of canopy RTMs(1/4)



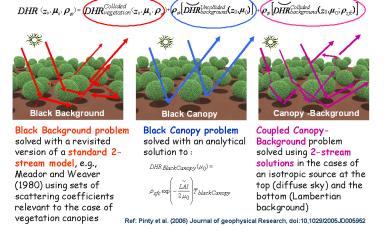


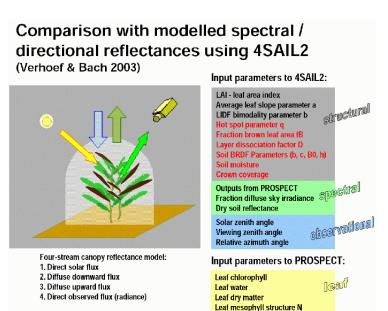


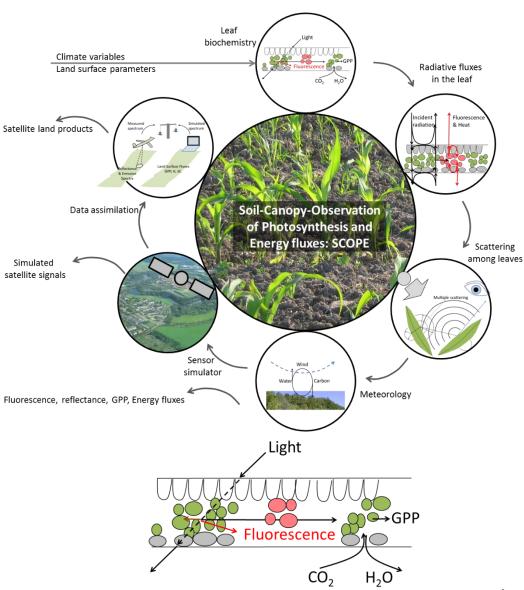
Examples of canopy RTMs (2/4)

Canopy models can be coupled with leaf, soil and atmospheric models

Solutions to the simpler problems







Examples of canopy RTMs (3/4)

Ray tracing models

Drat -the aDvanced Radiometric Ray Tracer.

P. Lewis, 1999; Saich et al., 2001. University College, Dept. Geography, London

Vegetation is built using The Botanical Plant Modelling System (BPMS) BPMS is a form of L-systems - the branches of a tree as geometric primitives

ARARAT - the advanced radiometric ray tracer, reverce ray tracing, a variety of camera models implemented



(Dürer, 1525)



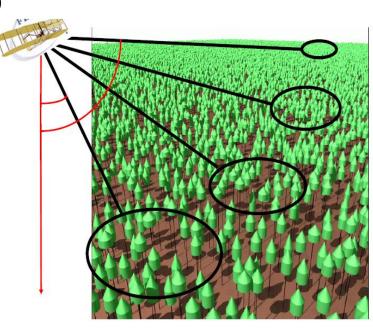
(http://www.geog.ucl.ac.uk/~plewis/)

Examples of canopy RTMs (4/4)

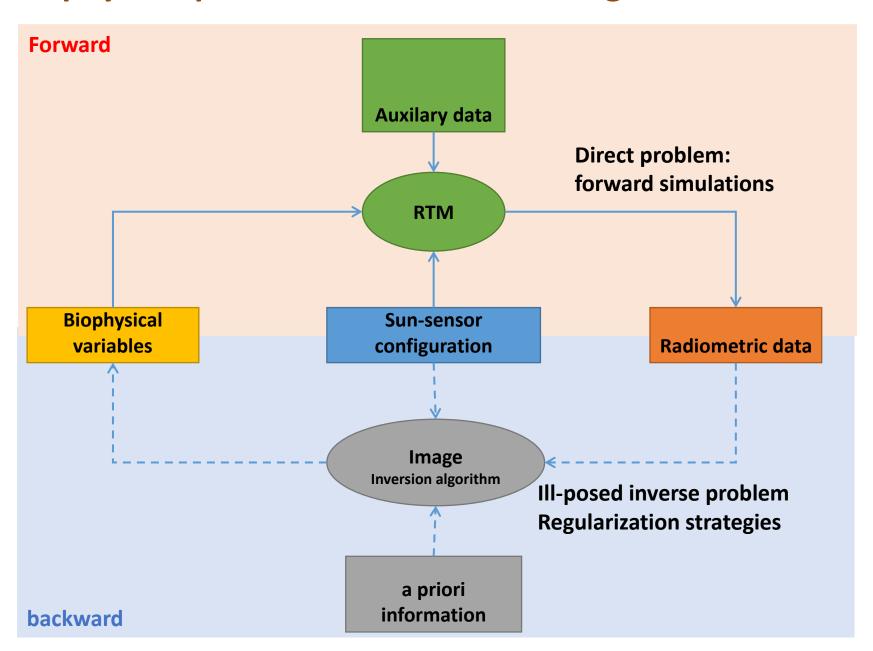
FLIGHT (North, 1996): A 3-D model

FLIGHT MC ray tracing approach

- Large scale structure by geometric primitives (e.g. cone)
- Foliage within crowns described by volume-averaged parameters
- 3D photon trajectories are simulated, accounting for the probabilities of free path, absorption and scattering
- Individual photon trajectories are traced from a solar source, through successive interactions, to a predetermined sensor view angle.

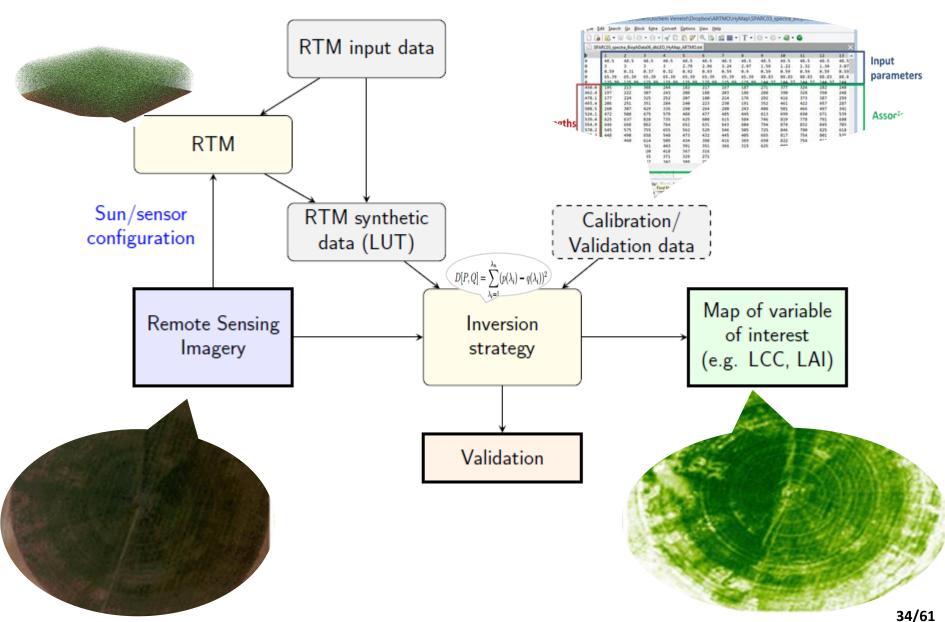


Biophysical parameters retrieval through RTM inversion:



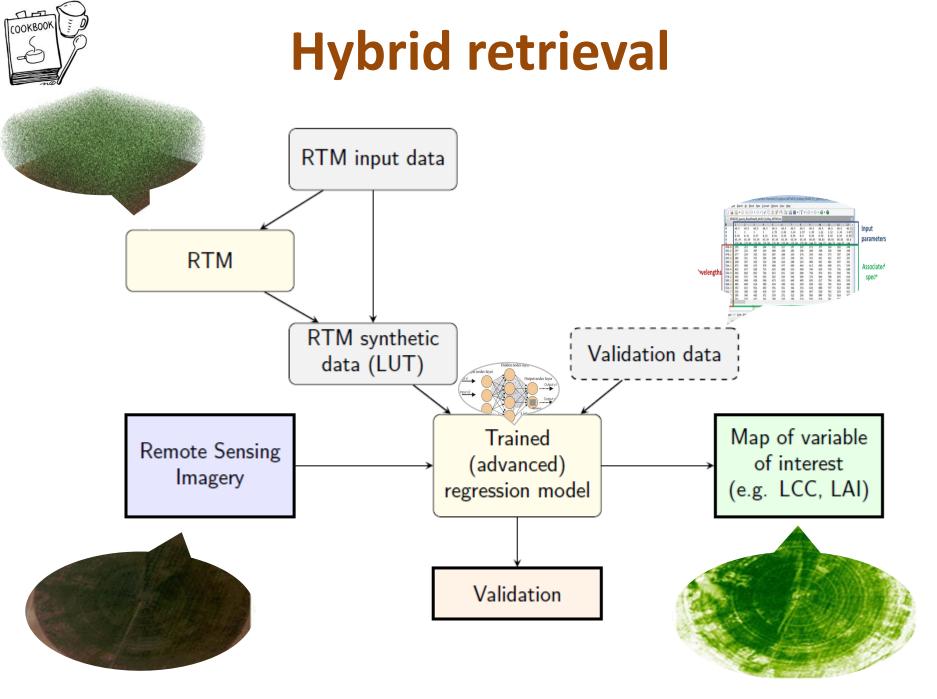


LUT-based RTM inversion



LUT-based inversion:

	Strengths ©	Weaknesses ⊗
•	Full-spectrum methods Reputation of physically-based (however, note the impact of regularization factors) Generally and globally applicable (e.g. MODIS products). Capability to provide multiple outputs	 Computationally demanding due to the per-pixel based approach (however, solutions based on a priori information have been developed). Retrieval quality depends on the quality of the RT models, prior knowledge and regularization. Quite complex approach: requires parameterization
•	uncertainty of the retrievals (e.g. residuals).	 The imposed upper/lower boundaries in the LUT have a logical consequence in that estimated variables cannot go beyond the boundaries imposed. This contradicts somewhat the physical approach as the prior information has an overwhelming influence. LUT-based inversion methods are often strongly affected by noise and measurement uncertainty.



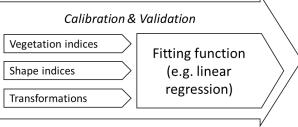
Non-parametric regression: hybrid

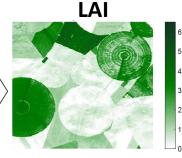
	Strengths ©		Weaknesses ⊗
•	Full-spectrum methods. They make use of the complete	•	Training can be computational expensive.
	spectral information.	•	Hypercomplex models can be generated. Their generic
•	Advanced, adaptive (non-linear) models are built.		potential is limited and hence they do not generalize well,
•	Methodologically, accurate and robust performance is		based on the training data (problem of over-fitting).
	enabled.	•	Some regression algorithms are difficult (or even impossible)
•	Some MLRAs cope well with datasets showing redundancy		to train with a high number of samples.
	and high noise levels.	•	Expert knowledge is required, e.g. for tuning. However,
•	Once trained, imagery can be processed time efficient.		toolboxes exist automating some of the steps in this sub- process.
•	Some of the non-parametric methods (e.g. ANNs, decision trees) can be trained with a high number of samples	•	Some of the methods can be considered as black boxes.
	(typically >1,000,000).	•	Some regression algorithms elicit instability when applied
•	Some MLRAs provide insight in model development (e.g. GPR: relevant bands; decision trees: model structure).		with datasets statistically deviating from the datasets used for training.
•	Some MLRAs can provide multiple-outputs (e.g. PLRS, ANN, SVR, GPR and KRR)		
•	Some MLRAs provide uncertainty intervals (e.g. GPR).		27/

Summary mapping methods

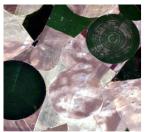
Parametric regression

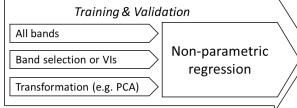


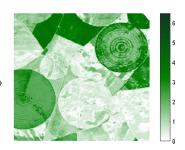




Non-parametric regression

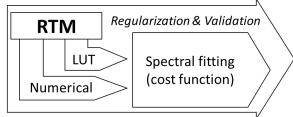






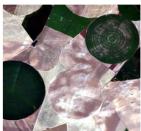
RTM inversion

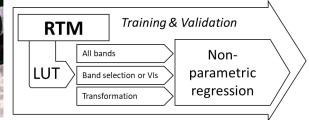


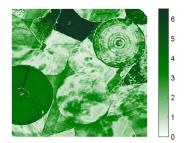




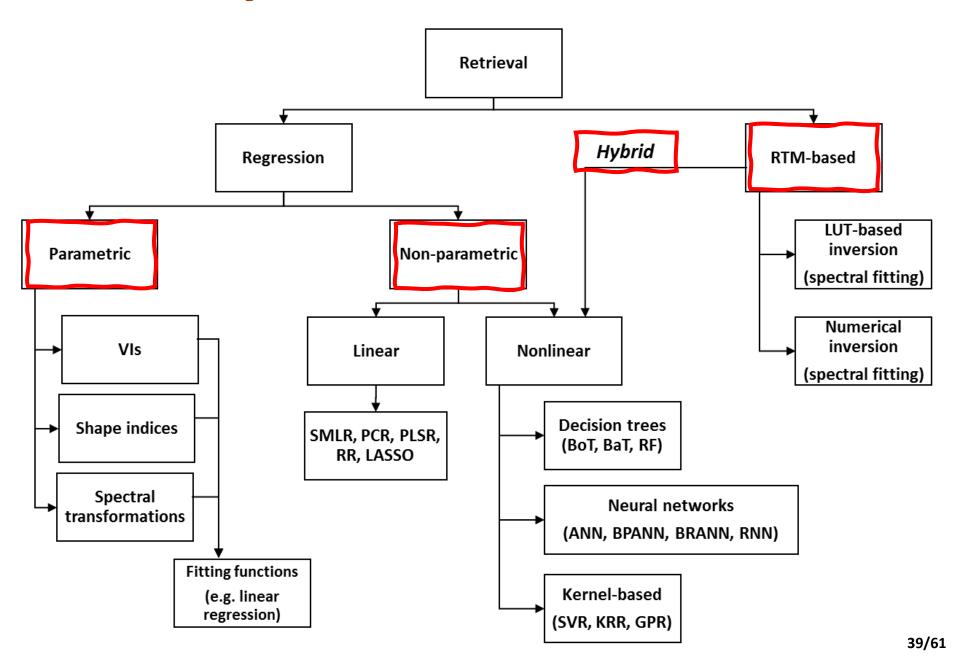
Hybrid regression







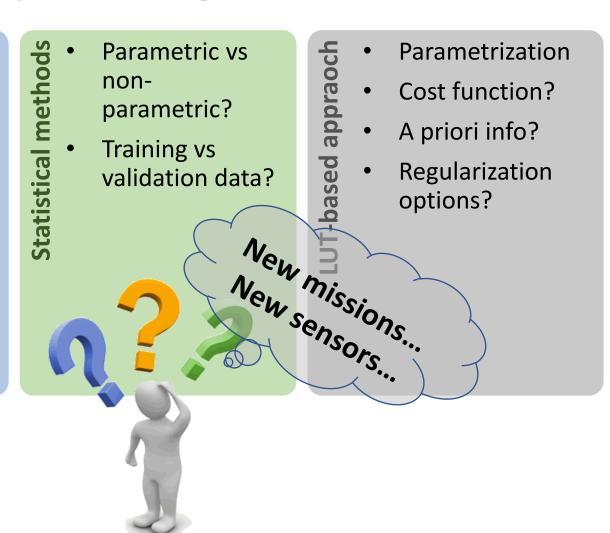
Taxonomy retrieval methods



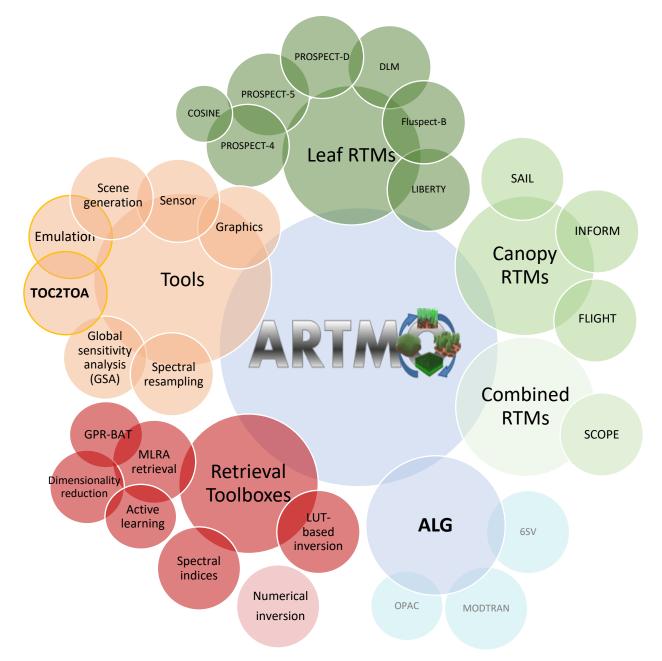
Optimizing retrieval

Spoectral indices

- Band combination?
- Formulation?
- Fitting function?

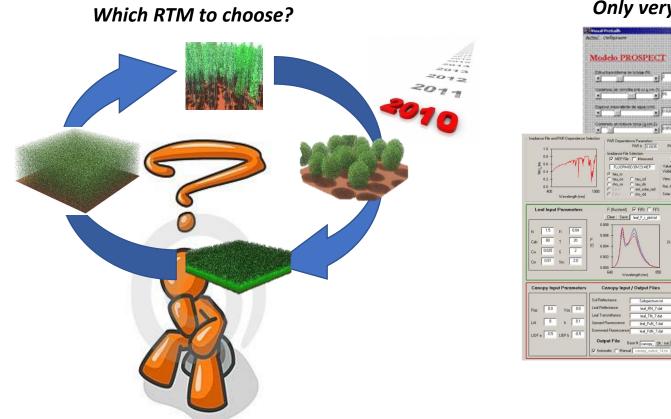


The many decisions to be taken require a systematic evaluation ARTM© automates retrieval optimization

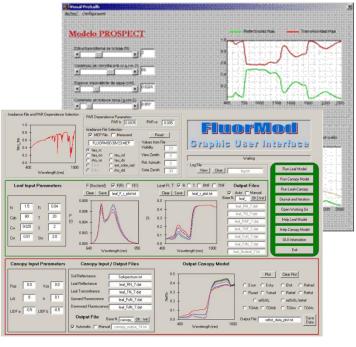




RTMs are important tools in EO research but for the broader community these models are perceived as complicated. Only very few of them offer user-friendly interfaces (GUIs).



Only very few offer a GUI.



- No interface exists that brings multiple RTMs together in one GUI.
- None of existing (publicly available) GUIs provide post-processing tools.

To fill up this gap:



- > To develop a GUI toolbox that:
 - operates various RTMs in an intuitive interface
 - provides a comprehensive visualization of model outputs
 - works both for multispectral and hyperspectral data
 - enables to retrieve biophysical parameters through various retrieval methods
 - takes different land cover classes into account.

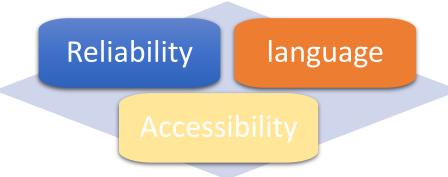
Toolbox for EO applications:

ARTM

Automated
Radiative
Transfer
Models
Operator



Selection RTMs & programming language



Model	Reference	Source code	
PROSPECT-4	Feret et al., 2008	Matlab	
PROSPECT-5	Feret et al., 2008	Matlab	
PROSPECT-D	Feret et al., 2017	Matlab	
DLM	Stuckens et al., 2009	Matlab	
LIBERTY	Dawson et al., 1998	Matlab	
FLUSPECT	Vilfan et al., 2016	Matlab	
4SAIL	Verhoef et al., 2007	Matlab	
FLIGHT	North, 1996	Executable file	
INFORM	Atzberger, 2000	Matlab	
SCOPE	Van der Tol et al., 2009	Matlab	

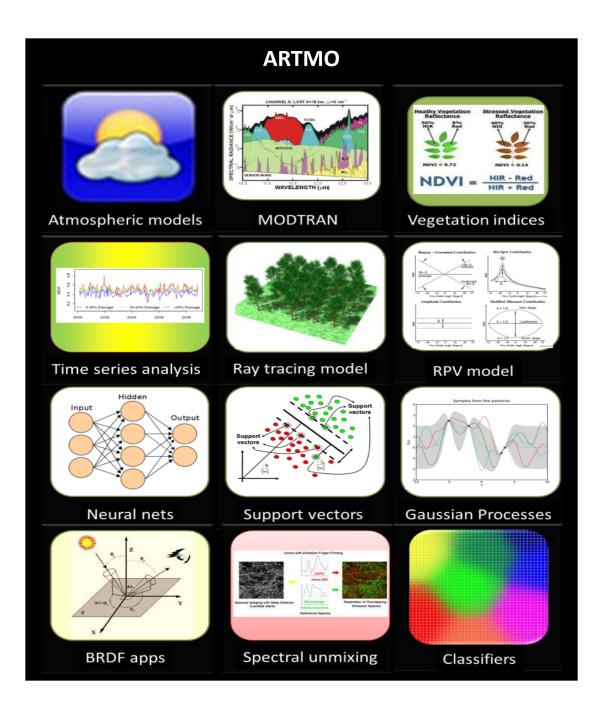
Software packages:

Programming language: Matlab®

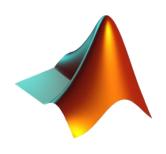
Database: MySQL®

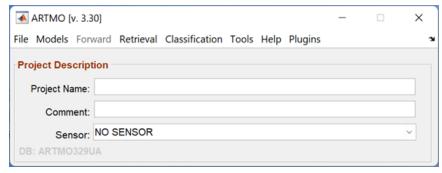
Image processing software: ENVI®



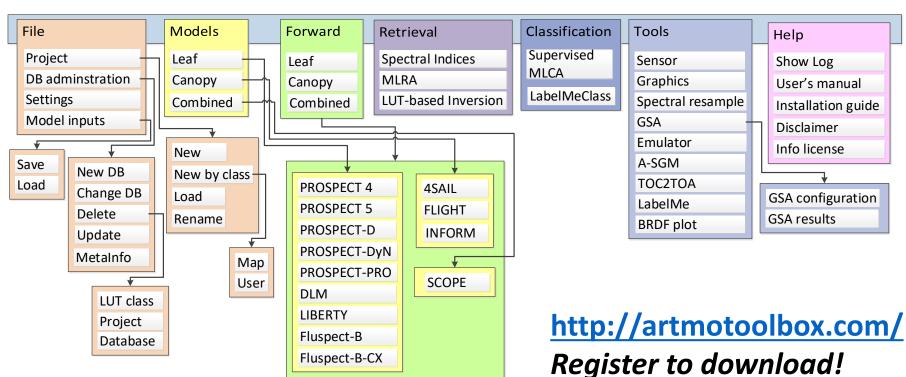


ARTMO v. 3.33







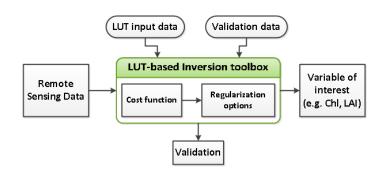


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ARTMO's retrieval toolboxes:

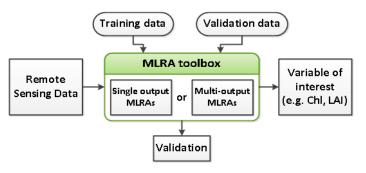
LUT-based inversion toolbox



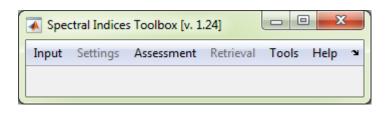


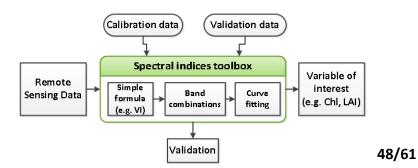
Machine learning regression algorithm toolbox (MLRA)





Spectral indices toolbox







ISPRS Journal of Photogrammetry and Remote Sensing



journal homepage: www.elsevier.com/locate/isprsjprs

Experimental Sentinel-2 LAI estimation using parametric, non-parametric and physical retrieval methods – A comparison

Jochem Verrelst ^{a,*}, Juan Pablo Rivera ^a, Frank Veroustraete ^b, Jordi Muñoz-Marí ^a, Jan G.P.W. Clevers ^c, Gustau Camps-Valls ^a, José Moreno ^a

Table 9Best performing parametric, non-parametric and LUT-based inversion method and associated mapping speed.

Retrieval algorithm	RMSE	R^2	Mapping speed (s)
Tian 3-band formulation	0.615	0.823	3.847
VH-GPR	0.436	0.902	73.884
Pearson chi-square inversion	0.802	0.745	3706.965

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Inversion GPR VI 1 1.5 2 2.5 3 1 2 3 4 5 RGB HyMap LAI $[m^2/m^2]$ LAI (μ) [m²/m²] $SD [m^2/m^2]$ LAI (μ) [m²/m²] % CV Residues

^a Image Processing Laboratory (IPL), Universitat de València, València, Spain

^b Department of Bioscience Engineering, Faculty of Sciences, University of Antwerp, Antwerp, Belgium

^cLaboratory of Geo-information Science and Remote Sensing, Wageningen University, Wageningen, The Netherlands



Operational processing?



Characteristic	Parametric	Non- parametric	RTM-based	Hybrid
Generalization capacity		-	++	++
Mapping Speed	++	+		+
Uncertainties		++*	+	++*
Accuracy	+	++	+	++
Variables	++	++	+	+

^{*} Some machine learning methods (e.g. probabilistic or ensemble methods)

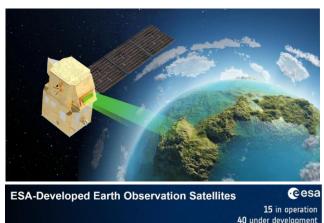
CHIME: Copernicus Hyperspectral Imaging Mission

CHIME will carry a visible to shortwave infrared spectrometer to provide global routine hyperspectral observations. The mission will support new and enhanced services for sustainable agricultural and biodiversity management, as well as soil property characterisation.

Technical concept:

Routine spectroscopic observation in contiguous spectral bands:

- Instrument: Pushbroom Imaging
 Spectrometer 400 2500 nm, Δλ
 = 10nm
- Revisit 10 15 days
- GSD (spatial resolution): 30 m
- Sun synchronous orbit (LTDN 10:30 11:30)
- Nadir view covering land and coastal areas
- High radiometric accuracy, low spectral/spatial misregistration





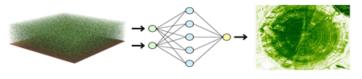
CORE Data Products:

The mission shall provide access to Level-1B, Level-1C and Level-2A products accessible via DIAS and with API support:

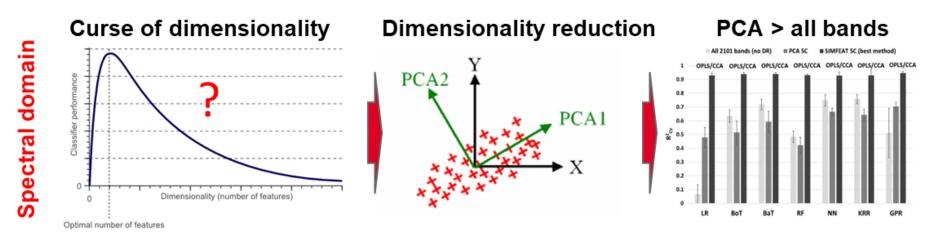
- Bottom-of-Atmosphere (BOA) reflectance (atmospherically corrected)
- Ortho rectified geometry
- Basic pixel classification (opaque clouds, thin clouds, cloud shadows, vegetation, water, snow etc.)
- Additionally –>
 Vegetation products
 (Level-2B)

Hybrid methods: data-driven methods

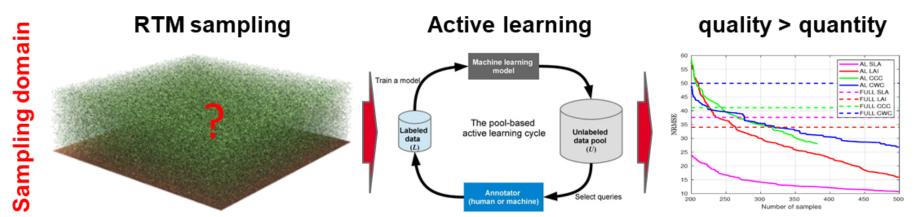




Many factors play a role. Spectral variability: quantity & quality & applied ML algorithm



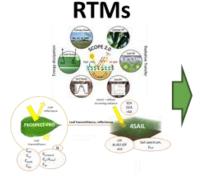
Rivera-Caicedo, J. P., Verrelst, J., Muñoz-Marí, J., Camps-Valls, G., & Moreno, J. (2017). Hyperspectral dimensionality reduction for biophysical variable statistical retrieval. ISPRS journal of photogrammetry and remote sensing, 132, 88-101.



Verrelst, J., Berger, K., & Rivera-Caicedo, J. P. (2020). Intelligent sampling for vegetation nitrogen mapping based on hybrid machine learning algorithms. *IEEE Geoscience an* 2/61 *Remote Sensing Letters*. 18(12), 2038-2042.

Workflow CHIME vegetation traits models:

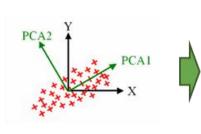




Active learning

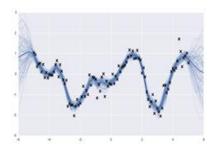


PCA



Okay?

Train GPR algorithms



Use RTMs (e.g. PROSPECT-PRO – SAIL) to generate a LUT composed by pairs (e.g. 1000) of vegetation parameters and spectra.

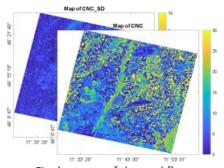
Select the **most representative** samples from the training dataset via a **diversity** or entropy criteria. Later, add non-vegetated spectra.

Dimensionality reduction with **PCA** (20 components).

With the **LUT optimized** for vegetation and non-vegetated surfaces, train probabilistic ML algorithms.

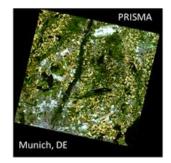
ilgoritiilis.

Maps + uncertainties



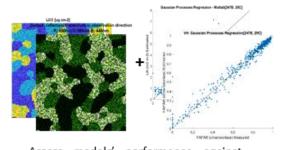
Final outputs of the workflow.

Apply to new observations



PRISMA images resampled to CHIME band settings

Validate the models



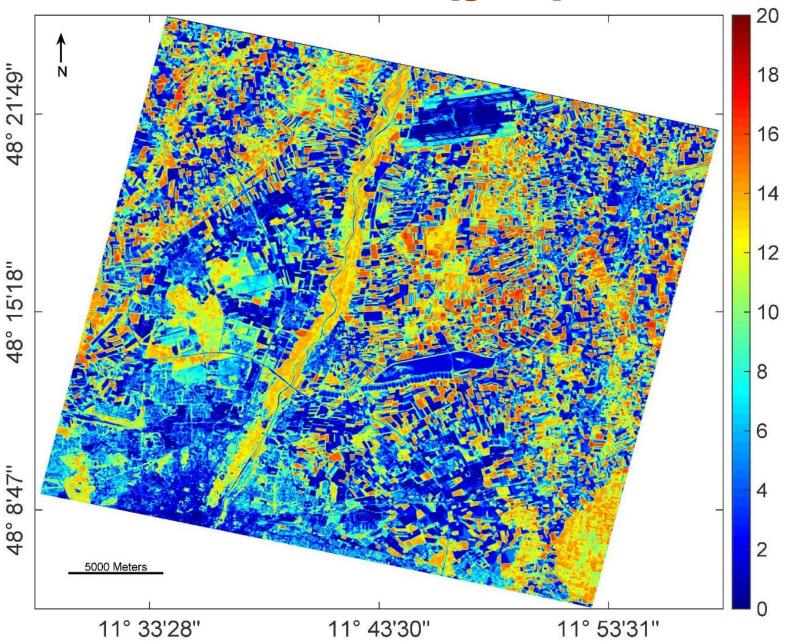
Assess models' performance against field data and vegetation reference scenes.



Verification and Validation vegetation models through E2E using CHIME-like data

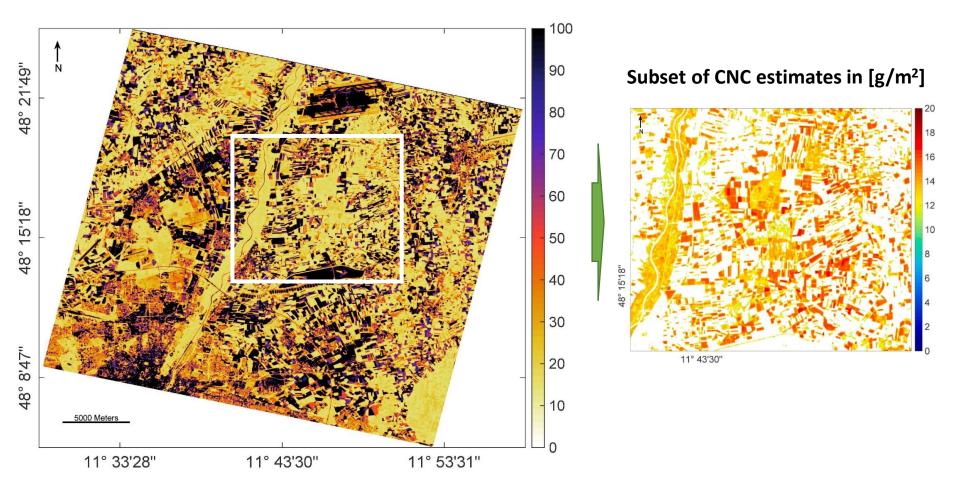
Page. 35

CNC estimates in [g/m²]



Verrelst, J., Rivera-Caicedo, J. P., Reyes-Muñoz, P., Morata, M., Amin, E., Tagliabue, G., ... & Berger, K. (2021). Mapping landscape canopy nitrogen content from space using PRISMA data. *ISPRS Journal of Photogrammetry and Remote Sensing*, 178, 382-395.

Relative uncertainties in [%]: used as mask (e.g. only ≤20%)

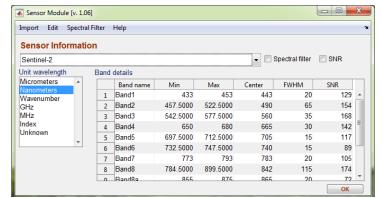


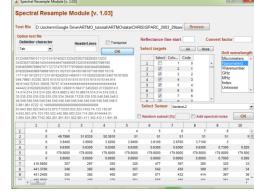
Conclusions CNC study:

- A workflow for operational mapping of CNC designed for spaceborne imaging spectroscopy missions
- Hybrid method based on PROSAIL-PRO and GPR
- GPR provides associated uncertainty estimates
- Model applied to PRISMA and successfully validated

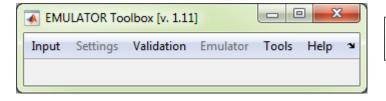
ARTMO's tools:

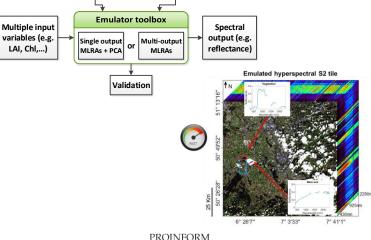
Sensor & spectral resample:





Emulation:

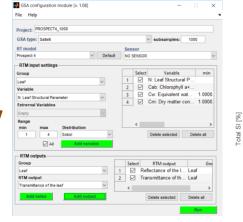


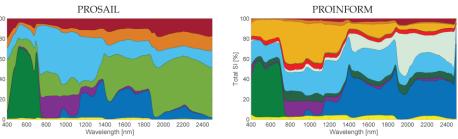


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Validation data

Global sensitivity analysis:





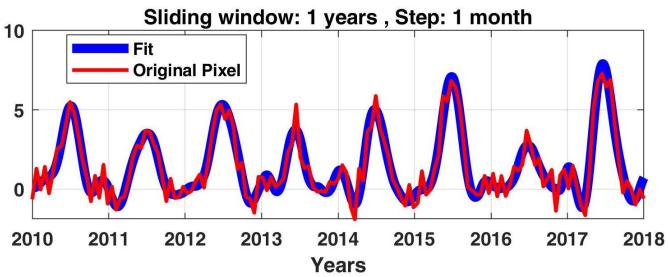
 \square N \square Cab \square Cw \square Cm \square LAI \square LAIs \square LAD \square LAIu \square SD \square H \square CD \square SZA \square Ps

Training data

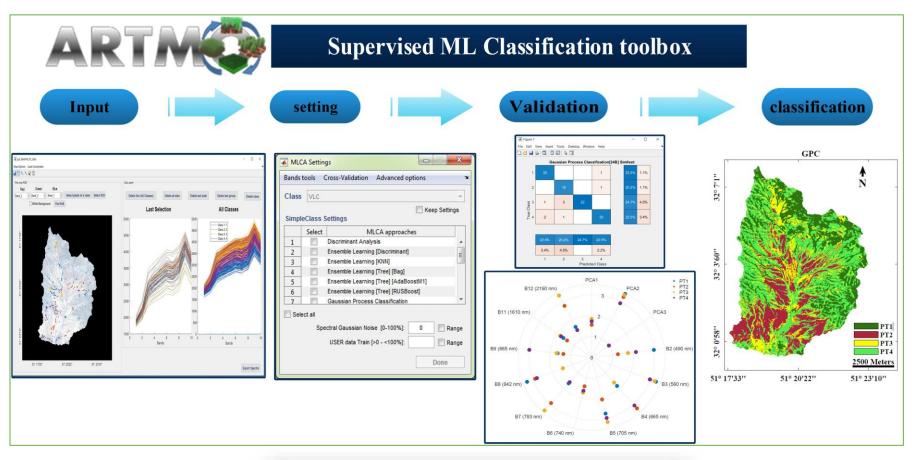


Dr. Santiago Belda Palazón Dr. Jochem Verrelst Dr. Juan Pablo Rivera Dr. Luca Pipia Pablo Morcillo

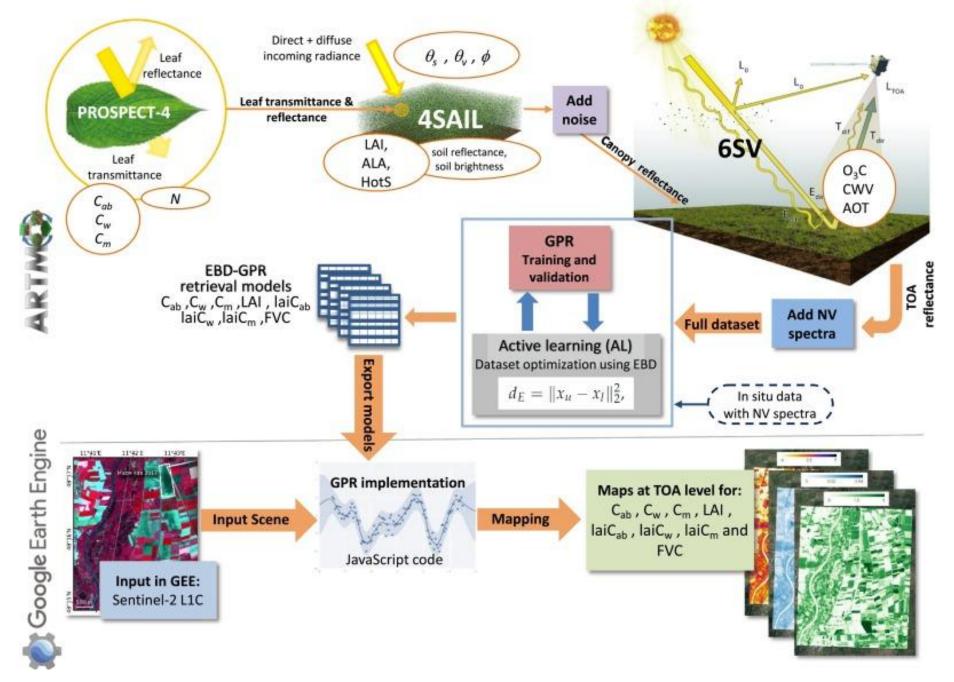




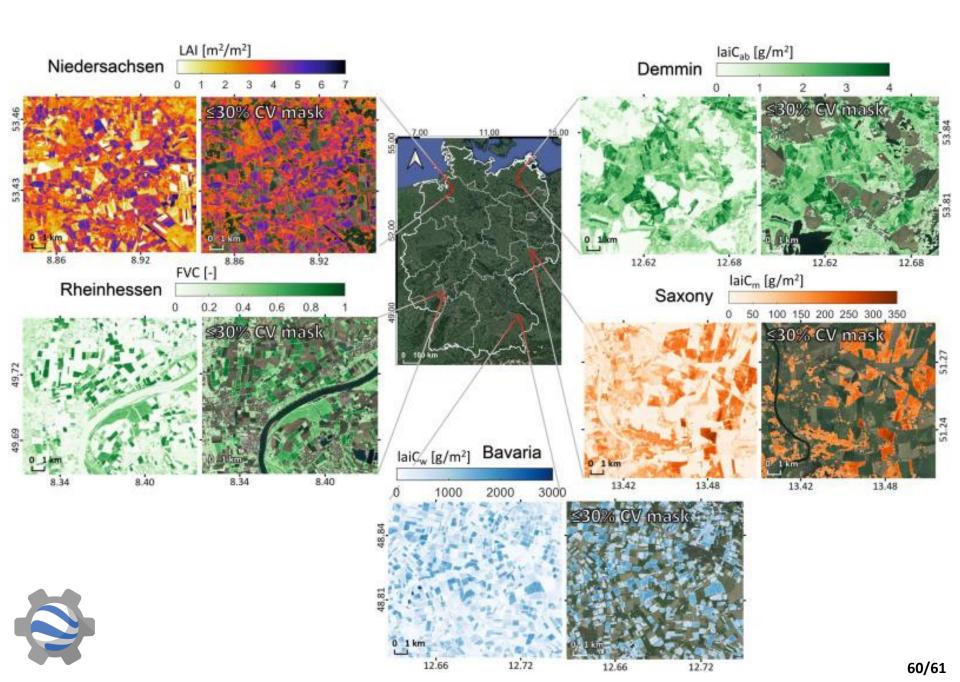
MLCA Classification toolbox - v.1.1



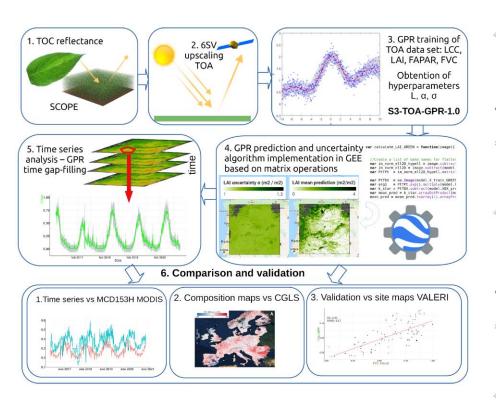


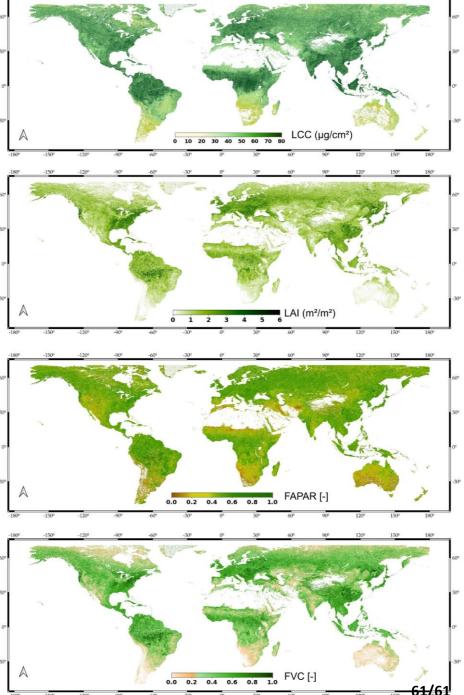


Estévez, J., Salinero-Delgado, M., Berger, K., Pipia, L., Rivera-Caicedo, J. P., Wocher, M., ... & Verrelst, J. (2022). Gaussian processes retrieval of crop traits in Google Earth Engine based on Sentinel-2 top-of-atmosphere data. *Remote Sensing of Environment*, 273, 112958.



GEE



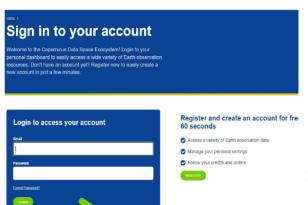


https://github.com/msalinero/ARTMOtoGEE

PyEOGPR

- 1. Free to use, registration to Copernicus Data Space Ecosystem required
- Open any Python IDE!
- pip install pyeogpr
- And you are ready to go!







https://pypi.org/project/pyeogpr/

Code snippet

