Recent advances in biophysical parameter retrieval methods – opportunities for Sentinel-2

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1. Introduction

New retrieval algorithms for Sentinel-2

The Copernicus Sentinel-2 (S2) satellite missions are designed to provide globally-available information on an operational basis for services and applications related to land. S2 is configured with improved spectral capabilities. Also **improved and robust algorithms for biophysical parameter retrieval are demanded**. This work present an overview of state-of-the-art retrieval methods dedicated to the quantification of terrestrial biophysical parameters. The rationale of all these methods is that spectral observations are in a way related to the parameters of interest. In all generality, retrieval methods can be categorized into three families: (*i*) ***parametric regression***, (*ii*) ***non-parametric regression***, and (*iii*) ***Inversion methods***.

We have recently developed retrieval modules within the **ARTMO toolbox** that provide a suite of methods of these three families. As such, consolidated findings can be achieved about which type of retrieval method is most accurate, robust and fast.

Objective:

To evaluate systematically 3 families of biophysical parameter retrieval methods for improved LAI estimation by using a local dataset (SPARC) and simulated S2 observations.

2. Data & Experimental setup

Ground truth data:

- SPARC dataset (Barrax, Spain): **103 LAI points** over various crop types and phenological stages.

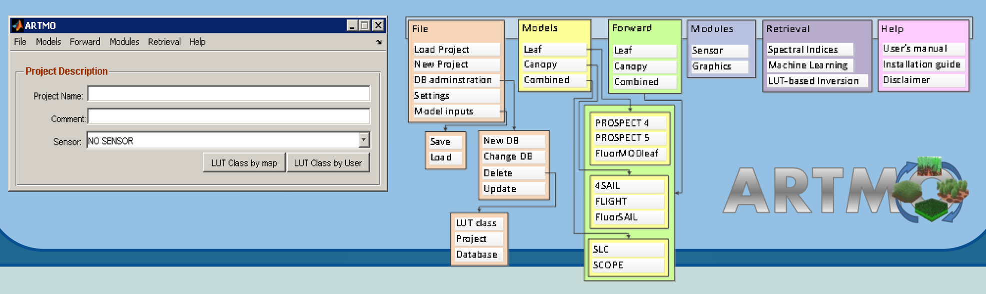
Simulated Sentinel-2 observations:

- **HyMap** flight line acquired during SPARC.
- **Resampled to Sentinel-2 settings**.

Band #	B1	**B2**	**B3**	**B4**	**B5**	**B6**	**B7**	**B8**	**B8a**	B9	B10	**B11**	**B12**
Band center (nm)	443	**490**	**560**	**665**	**705**	**740**	**783**	**842**	**865**	945	1375	**1610**	**2190**
Band width (nm)	20	**65**	**35**	**30**	**15**	**15**	**20**	**115**	**20**	20	30	**90**	**180**
Spatial resolution (m)	60	**10**	**10**	**10**	**20**	**20**	**20**	**10**	**20**	60	60	**20**	**20**

Experimental setup:

- Only S2 bands of 10 m (coarse-grained to 20 m) and 20 m were used (**10 bands**).
- 50% of data (ground truth & associated S2 spectra) for training (Spectral Indices, MLRA) and **50% for validation (same for all retrieval approaches).**
- Comparison through goodness-of-fit measures: R^2, RMSE, NRMSE



6. Conclusions

With view of biophysical parameters retrieval (e.g. LAI) from Sentinel-2 (20 m), three families of biophysical parameter retrieval methods have been systematically analyzed against the same validation dataset (SPARC, Barrax, Spain). Users typically require an accuracy with relative errors below 10%. It led to the following conclusions:

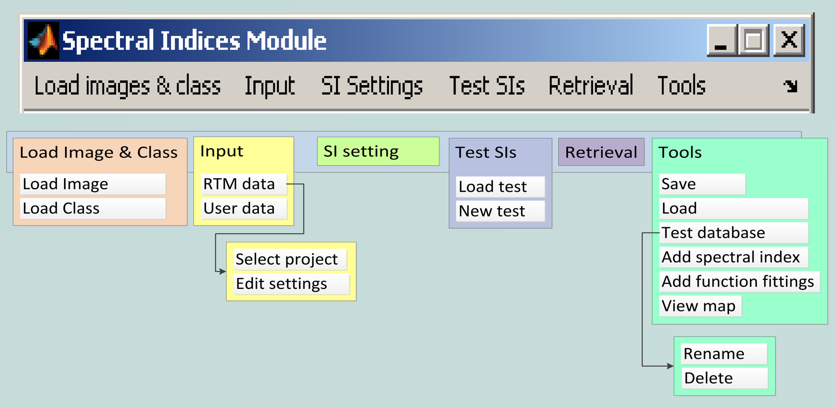
<u>Parametric - Spectral Indices</u>: All 2-, 3- and 4-band combinations according to normalized difference (ND) have been analyzed. A 4-band index with bands in SWIR was best performing, but the 10% error was not reached (NRMSE: 16.0%; R2: 0.79). Most critically, the absence of uncertainty estimates makes this method cannot be considered as reliable. Fast mapping (1s.).

<u>Nonparametric – MLRAs</u>: These are powerful and also fast regressors. Several yielded high accuracies with errors below 10% (KRR, GPR, VHGPR, ELR)! Particularly GPR (NRMSE: 8.2; R^2: 0.91) is of interest as it delivers insight in relevant bands and associated uncertainties. Hence, unreliable retrievals (e.g. <20%) can be masked out. Fast mapping (7s.).

<u>LUT-based Inversion</u>: A PROSAIL LUT of 100000 simulations has been prepared and various cost functions and regularization options were applied. Best cost functions performed on the same order as best 2-band SIs (16.6%; R2: 0.76). Because inverted against a LUT table pixel-by-pixel, biophysical parameter mapping went unacceptably slow (> 25h.).

3. (*i*) Parametric regression: Spectral Indices - LAI

ARTMO's *Spectral Indices* (SI) module:



In the ***Spectral Indices*** module the predictive power of all posible 2-, 3- or 4-band combinations according to an Index formulation (e.g. simple ratio (SR), normalized difference (ND)) to a biophysical parameter can be evaluated.

Applied SI formulations:

- 2-band SIs:
  - **SR (B2/B1)** (10^2 combinations)
  - **ND (B2-B1)/(B2+B1)** (10^2 combinations)
- ND 3-band **(B2-B1)/(B2+B3)** (10^3 combinations)
- ND 4-band **(B2-B1)/(B3+B4)** (10^4 combinations)

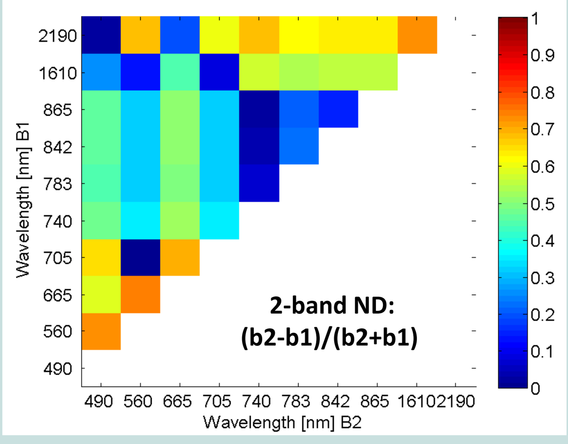
A Linear regression was applied.

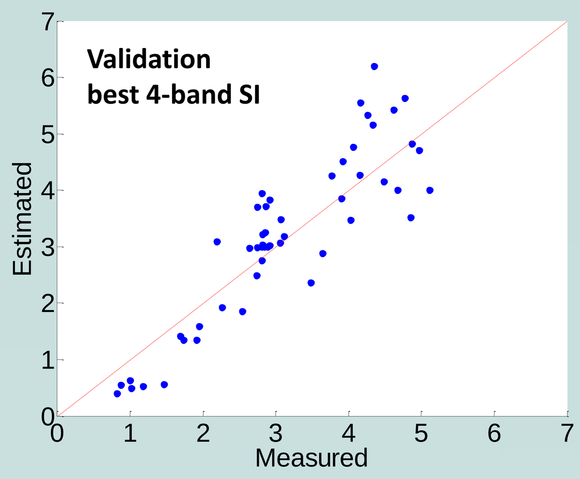
Very fast: **0.004 sec** per SI model (11200 SI models in 42.8 s.)

Best validated SIs (**50% validation data**) ranked according to R^2:

SI formulation	Best band combination (B1, B2, B3, B4)	RMSE	NRMSE	R^2
ND 4-bands: (b2-b1)/(b3+b4)	560, 2190, 1610, 1610	0.69	16.01	**0.79**
ND 3-bands: (b2-b1)/(b2+b3)	560, 2190, 740	0.70	16.74	**0.79**
ND 2-bands: (b2-b1)/(b2+b1)	665, 560	0.76	16.86	**0.74**
SR 2-bands: (b2/b1)	665, 560	0.77	20.36	**0.74**

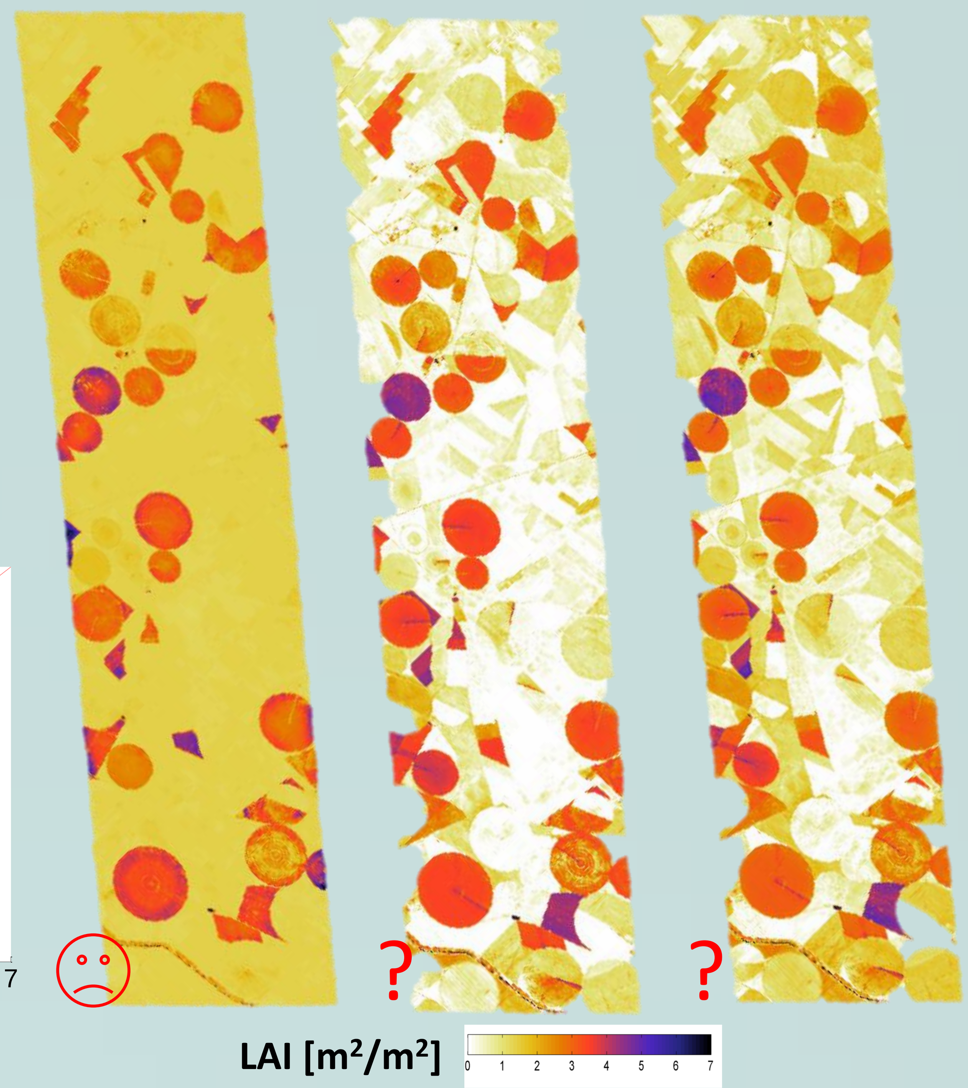
A 4-band SI with bands in green and SWIR best validated. Green and red led to best 2-band index.





Map (1 layer) generated in 1.1 s.

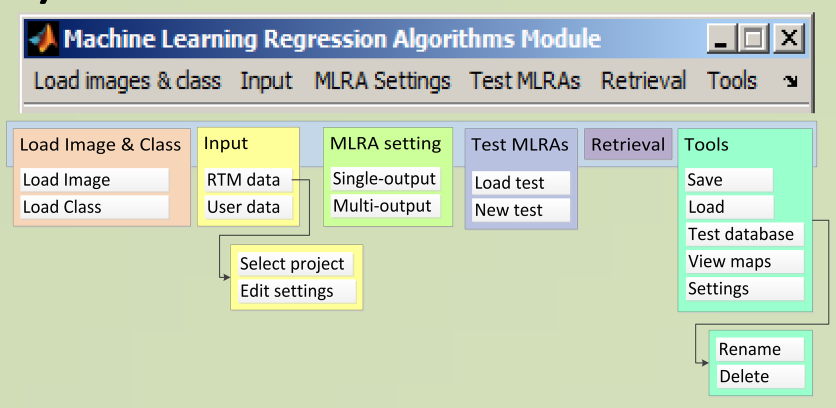
ND 2-band ND 3-band ND 4-band



LAI [m²/m²]

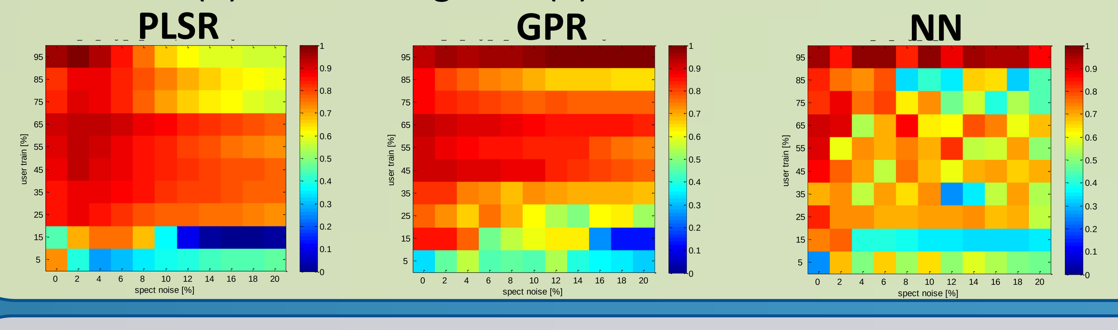
4. (*ii*) Nonparameteric regression: Machine learning regression algorithms (MLRAs) - LAI

ARTMO's *Machine Learning Regression Algorithms (MLRA)* module:



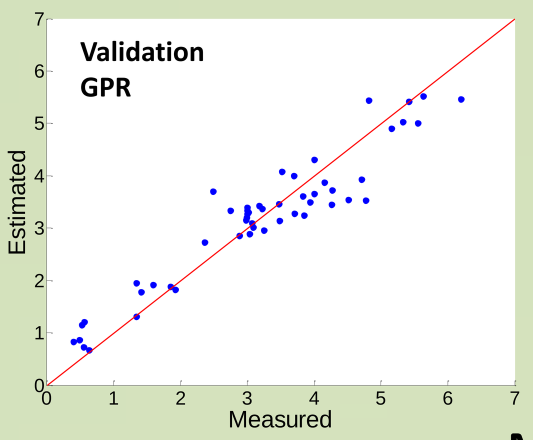
- **More than 10 MLRAs** have been implemented, e.g. neural nets (NN), kernel ridge regression (KRR) , Gaussian Processes regression (GPR), principal component regression (PCR), partial least squares regression (PLSR) , regression trees (RT) - (http://www.uv.es/gcamps/code/simpleR.html).
- Options to add noise and partitionate training- validation are provided.

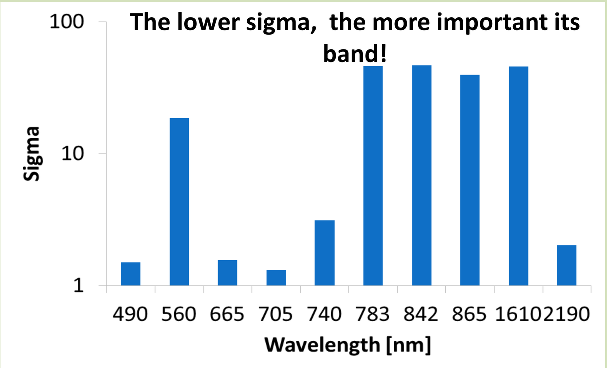
Examples of **robustness**: validation results (R^2) along increasing noise levels (X) and training data (Y):



50% validation results ranked according to R^2:

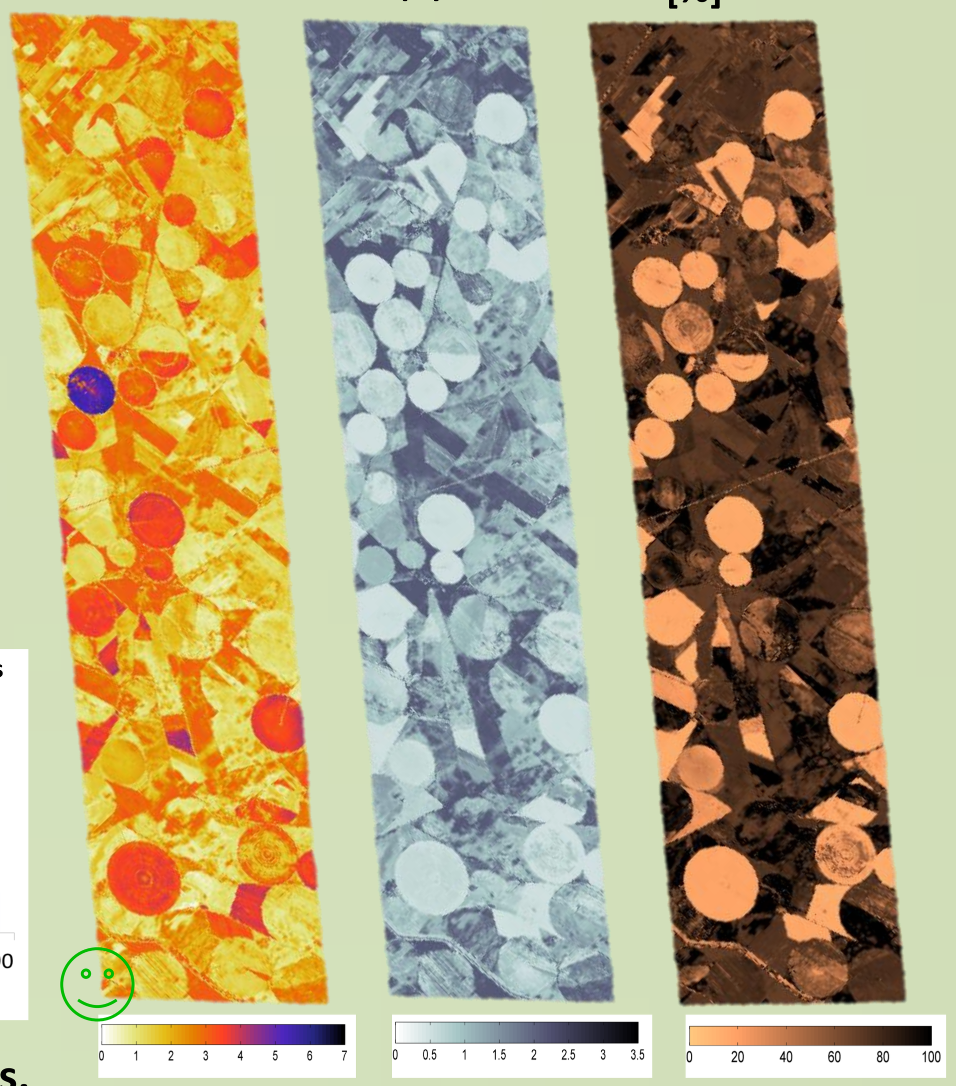
MLRA	RMSE	NRMSE	R^2	Time (s.)
Kernel ridge Regression	0.41	7.04	0.93	0.063
Gaussian Processes Regression	**0.47**	**8.17**	**0.91**	0.788
Neural Network	0.46	7.99	0.91	6.069
VH. Gaussians Processes Regression	0.48	8.30	0.90	2.473
Extreme Learning Machine	0.48	8.26	0.89	0.061
Bagging trees	0.58	10.03	0.87	1.296
Relevance vector Marchine	0.59	10.20	0.86	16.501
Least squares linear regression	0.56	9.62	0.86	0.002
Boosting trees	0.70	12.10	0.79	1.100
Partial least squares regression	0.71	12.16	0.78	0.008
Regression tree	0.78	13.46	0.72	0.006
Principal components regression	0.79	13.70	0.71	0.002





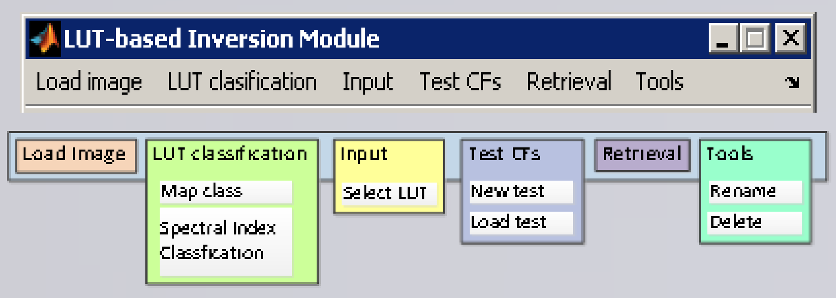
Map (3 layers) generated in 7.5 s.

LAI Mean prediction (μ) | GPR Uncertainty (σ) | Relative uncertainty [%]



5. (*iii*) Inversion of canopy RTM through cost functions - LAI

ARTMO's *Inversion* module:



Retrieval of biophysical parameters through LUT-based inversion.

- LUTs prepared in ARTMO and loaded in ***Inversion*** module
- **More than 60 cost functions** have been implemented.
- Various **regularization options**: **adding noise, mean of multiple solutions, data normalization**.

PROSAIL LUT (sub-selection 100000):

Model Parameters		Units	Range	Distribution
***Leaf variables:* PROSPECT-4**				
N	Leaf structure index	unitless	1.1	-
LCC	Leaf chlorophyll content	(μg/cm²)	5–75	Gaussian ($\dot{x}$ 35, SD: 30)
C_m	Leaf dry matter content	(g/cm²)	0.001–0.03	Uniform
C_w	Leaf water content	(cm)	0.002–0.05	Uniform
***Canopy variables:* 4SAIL**				
LAI	Leaf area index	(m²/m²)	0.1–7	Gaussian ($\dot{x}$: 3, SD: 2)
α_{soil}	Soil scaling factor	unitless	0	-
ALA	Average leaf angle	(º)	40–70	Uniform
HotS	Hot spot parameter	(m/m)	0.05–0.5	Uniform
skyl	Diffuse incoming solar radiation	(fraction)	0.05	-
θ_s	Sun zenith angle	(º)	22.3	-
θ_v	View zenith angle	(º)	0	-
φ	Sun-sensor azimuth angle	(º)	0	-

Examples of cost functions:

Shannon (1948):

$$D(P,Q) = -\sum_{\lambda_1=1}^{\lambda_n} \left(\frac{p(\lambda_l)+q(\lambda_l)}{2}\right) log\left(\frac{p(\lambda_l)+q(\lambda_l)}{2}\right) + \frac{1}{2}\left(\sum_{\lambda_1=1}^{\lambda_n} p(\lambda_l)log(p(\lambda_l)) + \sum_{\lambda_1=1}^{\lambda_n} q(\lambda_l)log(q(\lambda_l))\right)$$

Laplace distribution:

$$D(P,Q) = \sum_{\lambda_1=1}^{\lambda_n} |p(\lambda_l) - q(\lambda_l)|$$

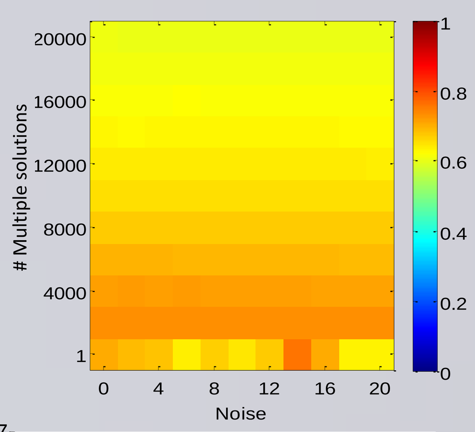
Pearson chi-square:

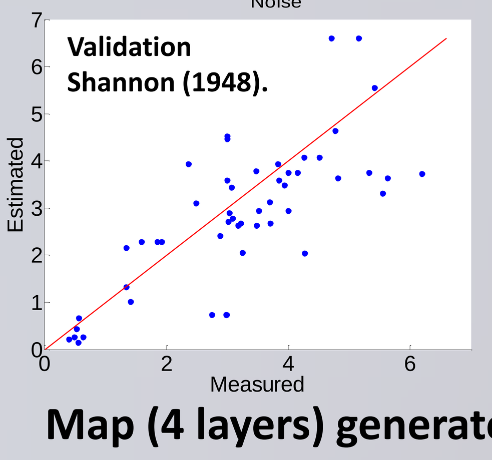
$$D[P,Q] = \sum_{\lambda_1=1}^{\lambda_n} \frac{(q(\lambda_l)-p(\lambda_l))^2}{p(\lambda_l)}$$

In total 5508 inversion strategies analyzed. **50% validation results** for best noise & multiple samples ranked according to R^2:

Cost function	% Noise	% multiple samples	RMSE	NRMSE	R^2	time (s.)
Shannon (1948)	**14**	**single best**	**0.96**	**16.56**	**0.76**	0.027
Laplace distribution	6	single best	0.86	14.74	0.74	0.021
Neyman chi-square	0	single best	0.89	15.31	0.74	0.005
Pearson chi-square	16	single best	1.03	17.74	0.73	0.005
Least absolute error	6	single best	0.89	15.28	0.72	0.005
Geman and McClure	16	2	0.83	14.36	0.71	0.007
RMSE	16	2	0.83	14.37	0.71	0.006
Exponential	16	2	0.85	14.66	0.71	0.008
K(x)=x(log(x))-x	20	single best	1.06	18.25	0.70	0.009
K(x)=(log(x))^ 2	0	2	1.01	17.40	0.69	0.012
K-divergence Lin	4	single best	2.60	44.84	0.64	0.009
Shannon entropy	6	2	1.15	19.82	0.60	0.013
Gen. Kullback-Leibler	10	2	1.20	20.63	0.58	0.013
Neg. Exp. disparity	0	4	1.04	17.96	0.58	0.007
Kullback-leibler	4	18	1.66	28.62	0.57	0.009
K(x)=log(x)+1/x	2	single best	2.07	35.65	0.55	0.012
Harmonique Toussaint	2	20	1.57	27.04	0.54	0.005
K(x)=-log(x)+x	2	2	1.77	30.52	0.49	0.012

Example of **robustness** (R^2) along increasing noise levels (X) and mean of multiple solutions (Y) in the Shannon (1948) Cost Function inversion:





LAI Mean prediction (μ)

Map (4 layers) generated in 90925.9 s. (> 25 hours)