Global Retrieval Algorithms for Phytoplankton Functional Types (PFTs): toward the Applications to OLCI and GlobColour Merged Products

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Objectives

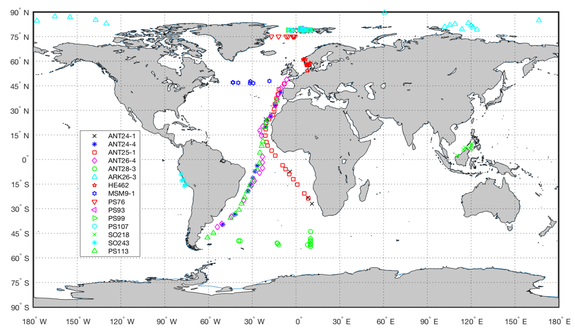
We focus on PFT retrieval algorithms that are then applied to Sentinel-3 (S3) OLCI data and merged ocean colour (OC) products from CMEMS GlobColour archive:

- Two algorithms were investigated for their capability in PFT retrievals, namely the adapted generalized IOP (AGIOP) and the empirical orthogonal function (EOF)-based algorithm, using in situ measurements, matchups between in situ and satellite data, and satellite OC products.
- The retrieved PFTs (mainly the diatoms, haptophytes, prokaryotic phytoplankton (cyanobacteria)) based on in situ data sets are compared with the in situ diagnostic pigment analysis (DPA) based PFTs.
- The two algorithms are also preliminarily applied to the GlobColour merged OC products and OLCI data.

Data sets

In-situ datasets

- 15 cruises from 2007 to 2018 worldwide
- 208 collocated R_{rs}, HPLC pigments and absorption



Campaigns and stations with collocated R_{rs}, HPLC pigments and absorption data.

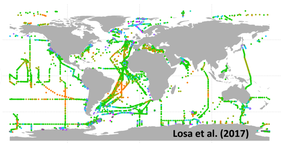
Satellite data and matchups

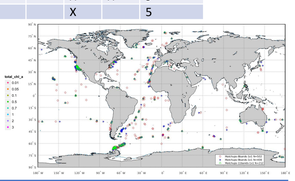
- GlobColour merged ocean colour (OC) R_{rs} products
- Sentinel 3A OLCI L3 R_{rs} product
- Matchups between GlobColour merged R_{rs} and in situ global HPLC data collected in 1997–2012

Numbers of available matchups between HPLC pigments and R_s (1x1 pixel, 3x3 and 5x5 pixels) with different band combinations from the merged OC products$_r$. Blue highlights the matchups used in the EOF based algorithm (SeaW = SeaWiFS, MO = MODIS, ME = MERIS, V = VIIRS).

Sensors	Number of Matchups		Available Wavebands (nm)											Number of bands
	1x1	3x3 5x5	412	443	490	510	531	547	551	555	560	620	670	678	
SeaW	1223	609	X	X	X	X				X			X		6
SeaW+MO+ME	408	266	X	X	X	X	X			X			X	X	9
SeaW+ME	502	129	X	X	X	X				X	X	X	X		8
SeaW+MO+ME	212	64	X	X	X	X	X			X	X	X	X	X	11
MO+ME+V	3	2	X	X	X	X	X	X	X	X	X	X	X	X	12
SeaW+MO+ME	766	516	X	X	X		X	X		X			X	X	8
MO+V	25	27	X	X	X		X	X	X	X			X	X	9
SeaW	1596	880	X	X	X					X			X		5

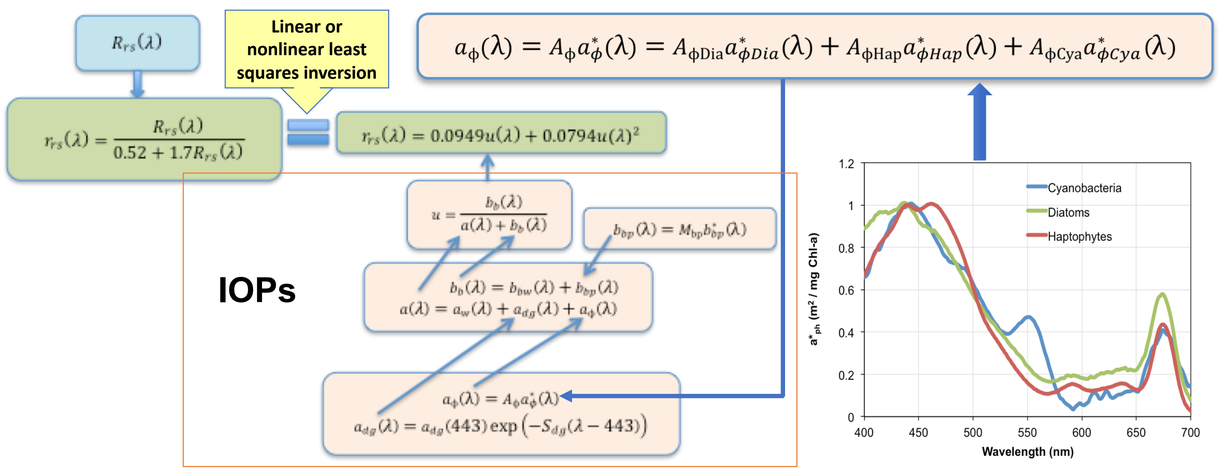
- Global in situ HPLC data 1988-2012 (left)
- R_{rs} Matchups (right)





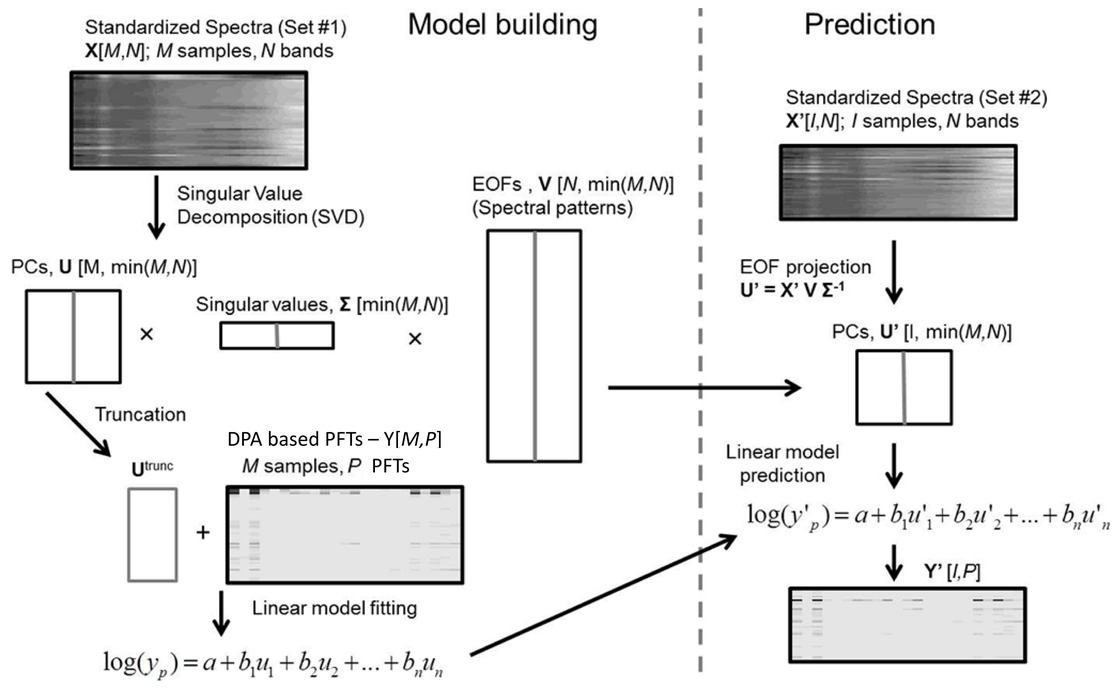
Methods

Adapted Generalized IOP (AGIOP)



- Adapted from GIOP by **Werdell et al. (2013)**, assuming that $a_\phi(\lambda)$ is a linear sum of subcomponents with unique spectral dependencies.
- $a_\phi(\lambda)$ is decomposed into absorption by 3 PFTs – diatoms, haptophytes, and cyanobacteria. Specific absorption of the three PFTs were obtained from natural waters where one PFT was dominating.
- Using R_{rs} at different wavebands and the spectral shapes of the IOPs as input, eigenvalues (the Chl-a concentrations of the 3 PFTs, $a_{dg}(440)$, and $b_{bp}(440)$) can be derived via linear or nonlinear least squares inversions.

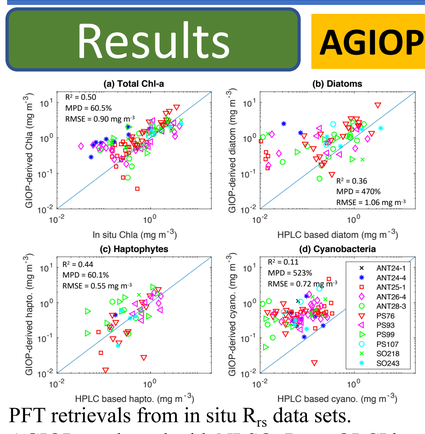
Empirical Orthogonal Functions (EOF) based algorithm



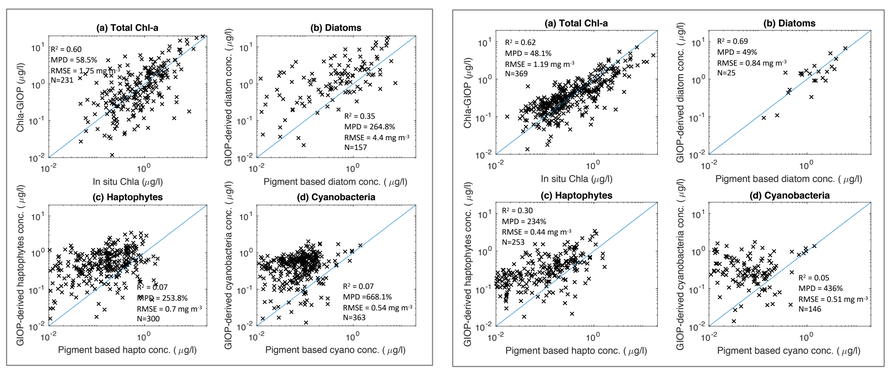
Schematic overview of EOF steps in model building and prediction. Multiple linear regression models are fit to log-transformed pigment concentrations, yp, as the response variable and EOFs derived from a spectral (reflectance) data set, X, as predictor variables. Model building (left) is used for "full-fit" models to all data samples (M) or to a training subset of samples for cross-validation. Prediction (right) is used for the assessment of the model error on a validation subset of samples (I) for cross-validation or in the extrapolation of model predictions to GlobColour merged R_{rs} data sets (adapted from **Bracher et al. 2015**).

Results

AGIOP

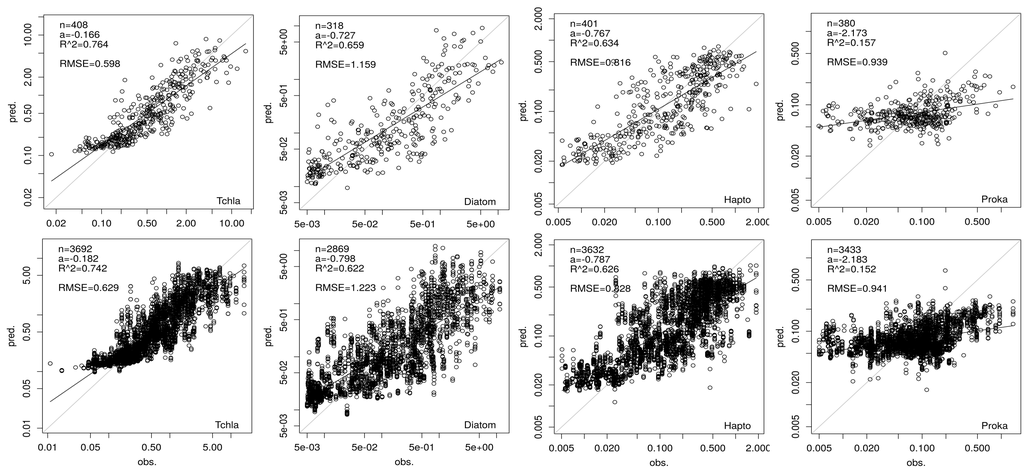


PFT retrievals from in situ R_{rs} data sets.
AGIOP conducted with NLSQ, R_{rs} at OLCI bands

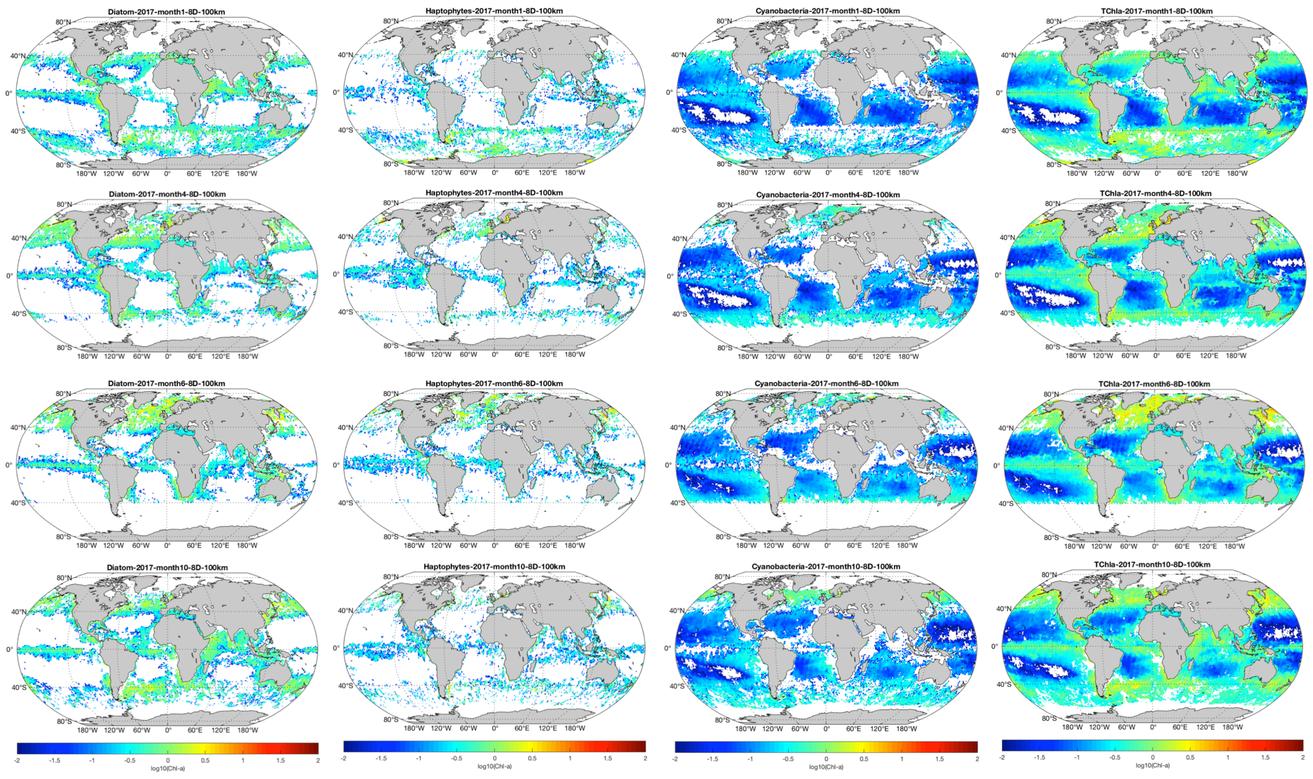


PFT retrievals from matchups between GlobColour merged OC R_{rs} at 8 bands and in situ HPLC data.
Left: Nonlinear least squares (NLSQ); Right : Non-negative linear matrix inversion (Nonneg-LMI).

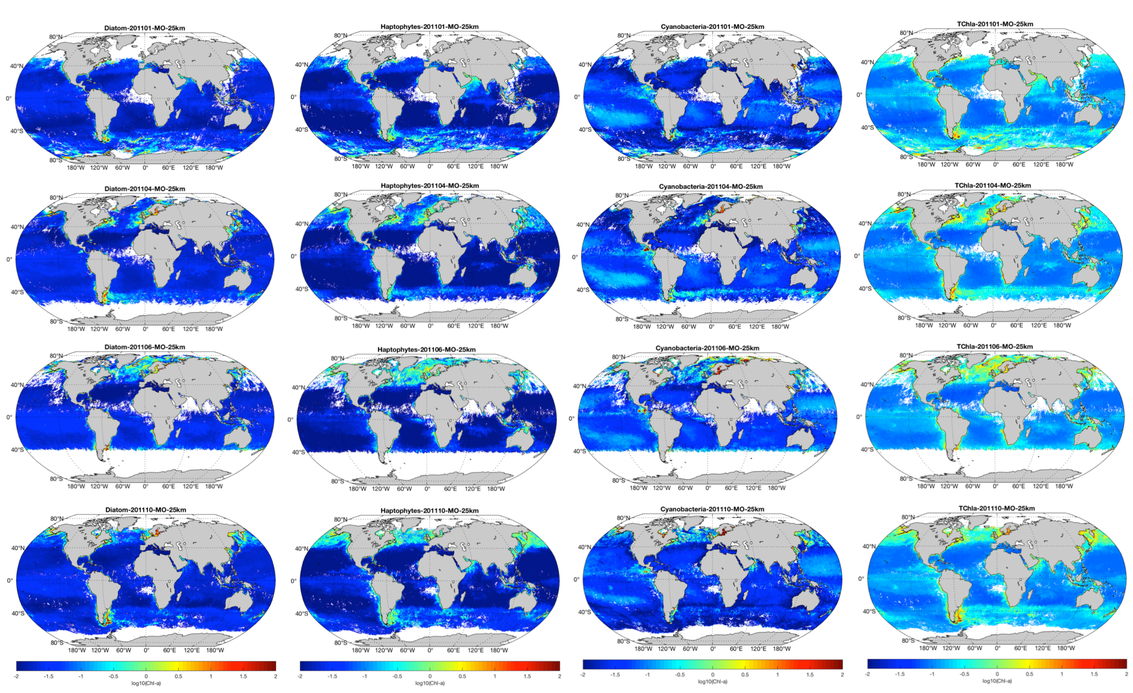
EOF-based algorithm



Regressions between observed (obs.) based on DPA and predicted (pred.) PFTs using EOF modes derived from GlobColour merged R_{rs} products at 9 bands. Top panel: using R_{rs} 1x1 pixel, bottom panel: R_{rs} 3x3 pixels.



Global PFTs retrieved by AGIOP applied to monthly OLCI R_{rs} data (GlobColour level 3 product) in January, April, June and October 2017. Panels from left to right: diatoms, haptophytes, cyanobacteria, and total Chl-a.



Global PFTs retrieved by EOF-based algorithm (9 bands) applied to GlobColour merged monthly R_{rs} products in January, April, June and October 2011.
Panels from left to right: diatoms, haptophytes, cyanobacteria, and total Chl-a.

Conclusions

- Both AGIOP and EOF based PFT retrieval algorithms can well retrieve diatoms and haptophytes but perform less accurate for cyanobacteria mainly due to their general low concentration resulting weak signal in the reflectance spectra.
- By both algorithms (especially EOF) total Chl-a were generally overestimated typically at small values therefore in oligotrophic regions for global retrievals.
- AGIOP generally works but is unstable when using different minimization inversion methods. Inversion by LMI is robust for global data but less coverage of valid retrievals.
- EOF outperformed the AGIOP from both prediction accuracy of in-situ matchups and valid retrieval coverage for global data.

Acknowledgements

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Key References

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