Algorithm uncertainties information for the Uncertainties Working Group

Project title: Going beyond chlorophyll-a: Developing phytoplankton community composition algorithms from hyperspectral remote sensing reflectance

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Project overview

Our project consists of 1) adapting and implementing the Gaussian decomposition method to estimate chlorophylls a, b, c, and photoprotective carotenoids from hyperspectral remote-sensing reflectance observations, and 2) using these estimates of phytoplankton pigments, in addition to other bio-optical and physical measurements, as inputs to an algorithm that estimates diatom biomass (carbon) concentrations across a wide range of oceanic regions and conditions, and where plankton cell imagery data are used as algorithm target quantities. The pigment algorithm is currently in the process of being implemented and uncertainties are described here. The diatom algorithm is still in development; some information is provided here and more will be available upon algorithm completion.

Phytoplankton accessory pigment algorithm via Gaussian decomposition of Rrs (a.k.a. “GPIG”)

*Algorithm uncertainty estimation*

Pigments are estimated from hyperspectral Rrs via a combined inversion and Gaussian decomposition method, and the magnitude of Gaussian functions is regressed against phytoplankton pigment concentrations determined using HPLC analysis. The coefficients determined from these regressions are thus able to be used to estimate pigments from subsequent hyperspectral Rrs measurements. To determine uncertainties in the coefficients, a bootstrapping method iteratively subsamples all data (with replacement; n = 10,000 iterations) during the fitting between Gaussian magnitudes and HPLC pigment concentrations. Following this, we calculated the standard deviation of all iterations for each coefficient and results are provided as coefficient uncertainty values. The uncertainties of the coefficients can then be used during the estimation of pigment concentrations from Rrs (for example, via a Monte Carlo approach, where coefficients are multiplied by a random number from a standard normal distribution over thousands of simulations).

This approach is detailed in:

Chase, A. P., Boss, E., Cetinic ́, I., & Slade, W. (2017). Estimation of phytoplankton accessory pigments from hyperspectral reflectance spectra: Toward a global algorithm. Journal of Geophysical Research: Oceans, 122. <https://doi.org/10.1002/2017JC012859>

*Validation plan for implemented pigment algorithm*

The GPIG algorithm will be validated against coincident measurements of hyperspectral Rrs and phytoplankton accessory pigment collected as a part of the PACE validation efforts. Challenges include spatial resolution of match-ups between in situ data and PACE-based Rrs measurements. This will be addressed by comparing sub-pixel variability of ship-based Rrs with PACE OCI-derived Rrs, to assess whether increased sub-pixel variability also leads to increased uncertainties in pigments estimated from Rrs.

Diatom carbon algorithm

*Algorithm uncertainty estimation*

Diatom carbon concentrations are estimated using an algorithm that includes environmental and optical input parameters. There are several sources of uncertainty in the algorithm: uncertainties in the input parameters, uncertainty/accuracy in the machine learning algorithm itself, and uncertainty in the target parameters (plankton cell imagery data in this case). We propagate all uncertainties and errors such that the end product (diatom carbon concentration) has an average uncertainty associated with the concentration value. A demonstration of this approach can be found in the supporting information of:

Chase, A. P., Boss, E. S., Haëntjens, N., Culhane, E., Roesler, C., & Karp- Boss, L. (2022). Plankton imagery data inform satellite-based estimates of diatom carbon. *Geophysical Research Letters*, *49*, e2022GL098076. <https://doi>. org/10.1029/2022GL098076

*Validation plan for implemented pigment algorithm*

Following the completion and implementation of the diatom carbon algorithm planned during 2024, plankton cell imagery data collected during PACE mission validation efforts will be used to compare to diatom carbon concentrations estimated from PACE data. A notable challenge with this effort is the need to account for the sources of uncertainty in the input parameters that are derived from other satellite measurements (not PACE), including ocean SST and SSS. Uncertainties in these products will need to be combined with the uncertainties in the phytoplankton pigments (determined as described above in this document) that will be derived from PACE OCI. Additionally, there is also the challenge of spatial resolution differences between in situ data and satellite match-ups. These uncertainties will be assessed during algorithm product validation.