Summary of uncertainty estimation approaches used in development and assessment of inverse optical models at SIO Ocean Optics Research Laboratory

Dariusz Stramski and Rick A. Reynolds
Scripps Institution of Oceanography (SIO), University of California San Diego
La Jolla, CA 92093-0238, USA

To provide an example of statistical metrics used in our work to develop inverse optical algorithms and assess and validate their performance (which include the semi-analytical algorithms and empirical algorithms for ocean color applications), we provide below a copy of Table 2 from our recent publication (Joshi et al., 2023). This publication is devoted to validation of new empirical POC algorithms that we developed for global ocean color satellite applications as described in another recent publication (Stramski et al., 2022). In Joshi et al. (2023), the validation analyses of new POC algorithms were conducted using two distinct types of validation datasets: an independent in situ dataset (i.e., in situ data independent of in situ algorithm development data) and satellite-in situ matchup datasets. These analyses provided the uncertainty statistics characterizing the performance of algorithms under two scenarios; (i) when the algorithm input of ocean remote-sensing reflectance, R_{rs}, originates from in situ measurements and therefore is unaffected by uncertainties in satellite observations, and (ii) when the input R_{rs} is estimated from satellite observations and therefore is additionally affected by multiple sources of uncertainty (e.g., satellite radiometry, atmospheric correction, satellite-in situ matchup spatial and temporal differences).

We note that in addition to statistical parameters shown in the table below, which mostly represent the aggregate statistics associated with systematic and random components of uncertainty, we also routinely analyze other statistics, for example the probability distributions and Bland-Altman-like plots of differences between the algorithm-derived and reference (usually measured) values; however, the length limit of publications typically prevents the presentation of all analyzed statistics in published papers. The uncertainty of reference measurements is typically reported (e.g., based on replicate measurements and knowledge associated with development and evaluation of a given measurement protocol) but can be also incorporated into assessment of final uncertainty of the algorithm-derived product.

Table 2 from Joshi et al. (2023). Statistical metrics that are used in validation and intercomparison of different POC algorithms.

Symbol	Description
N	Number of samples
x_i, y_i	Observed "x" and model-predicted (algorithm-derived) "y" value for sample i of N
Model evaluation metrics for log-transformed data	
R	Pearson's product moment correlation coefficient between $\log(y_i)$ and $\log(x_i)$
S and I	Slope and intercept of Model II linear regression of $\log(y_i)$ on $\log(x_i)$
$MdSA$	Median symmetric accuracy (in percent) calculated as $(10^{[\mathrm{median}(\lvert\log(yi) - \log(xi)\rvert]} - 1) \times 100$
MB_{log}	Mean bias calculated as $10^{[\Sigma(\log(yi) - \log(xi))/N]}$
Model evaluation metrics for untransformed data	
MdR	Median ratio of (y_i / x_i)
MdB	Median bias; median value of $(y_i - x_i)$
$MdAPD$	Median absolute percentage difference, median value of $100 \times [\lvert(y_i - x_i)/ x_i\rvert]$
$RMSD$	Root mean square deviation calculated as $[(1/N)\ \sum_{i=1}^{N}\left(y_i - x_i\right)^2\ ]^{0.5}$
% wins	Percentage wins in pairwise comparisons of closeness of x_i and y_i data for a given pair of compared algorithms

For PACE mission we are developing a multi-step inverse optical algorithm, called 4SAA for 4-step Semi-Analytical Algorithm, to estimate 10 hyperspectral ocean optical properties from PACE OCI observations of R_{rs}. The 4SAA consists of 4 independent component models operating in a stepwise fashion: (i) Kd model for estimating the spectral attenuation coefficient for downwelling plane irradiance averaged over the first attenuation depth, $\langle K_{\mathrm{d}} \rangle$, from input spectral R_{rs}; (ii) inverse AOP-IOP model (referred to as LS2) for estimating the total spectral absorption, a, and backscattering, b_{b}, coefficients from input spectral R_{rs} and $\langle K_{\mathrm{d}} \rangle$; (iii) ANW absorption partitioning model for estimating the spectral phytoplankton, a_{ph}, and non-phytoplankton, a_{dg}, absorption coefficients from input non-water absorption coefficient, a_{nw}; and (iv) ADG absorption partitioning model for estimating the spectral CDOM absorption, a_{g}, and "depigmented" (a proxy for non-algal) particulate absorption, a_{d}, coefficients from input a_{dg}. The development of four component models of 4SAA builds upon and enhances previous studies of Jamet et al. (2012) for Kd model, Loisel and Stramski (2000) and Loisel et al. (2018) for LS2 model, Zheng and Stramski (2013) for ANW model, and Stramski et al. (2019) for ADG model. These previous studies include the analysis to assess the model skills. For example, Loisel et al. (2018) report on several statistical metrics characterizing uncertainties in LS2-derived products as assessed through the analysis of three different types of datasets, the synthetic dataset, in situ dataset, and satellite-in situ matchup dataset.

For application of 4SAA to PACE mission, quantification and understanding of uncertainty estimates and uncertainty budget of satellite-derived 4SAA products will require characterization of all main sources of uncertainties within the 4SAA structure and propagation of uncertainties through multiple steps of 4SAA as appropriate to a specific data product under consideration. We envision a need for a multi-level approach in the process of validation and uncertainty characterization of 4SAA products. It is noteworthy that in this multi-level approach not every component of validation analysis will require all quantities involved in 4SAA to be measured together, and not every component of uncertainty characterization will require the use of R_{rs}. For example, for characterization of intrinsic uncertainties of ANW and ADG absorption partitioning models, high-quality measurements of constituent absorption coefficients will be sufficient. Other levels of uncertainty characterization will involve the use of in situ R_{rs} as input to Kd and LS2 models and the use of PACE OCI-derived R_{rs} as input to Kd and LS2 models in conjunction with matchup in situ measurements of data products. The multi-level uncertainty characterization of 4SAA products will provide information on individual contribution of every step of 4SAA starting with satellite-derived R_{rs} and progressing to combined uncertainty of different products derived downstream within the multi-step structure of 4SAA. A combined uncertainty of the result will be generated from the identified uncertainties using statistical principles of forward uncertainty propagation, with simulation-based Monte Carlo approach providing likely the most appropriate approach given the formulation and structure of 4SAA.

References

Jamet, C., H. Loisel, and D. Dessailly. 2012. Retrieval of the spectral diffuse attenuation coefficient Kd(λ) in open and coastal ocean waters using a neural network inversion. *J. Geophys. Res. Oceans*, 117, C10023.

Joshi, I. D., D. Stramski, R. A. Reynolds, and D. H. Robinson. 2023. Performance assessment and validation of ocean color sensor-specific algorithms for estimating the concentration of particulate organic carbon in oceanic surface waters from satellite observations. *Remote Sens. Environ.*, 286, 113417. https://doi.org/10.1016/j.rse.2022.113417

Loisel, H., and D. Stramski. 2000. Estimation of the inherent optical properties of natural waters from irradiance attenuation coefficient and reflectance in the presence of Raman scattering. *Appl. Opt.*, 39, 3001–3011.

Loisel, H., D. Stramski, D. Dessailly, C. Jamet, L. Li, and R. A. Reynolds. 2018. An inverse model for estimating the optical absorption and backscattering coefficients of seawater from remote-sensing reflectance over a broad range of oceanic and coastal marine environments. *J. Geophys. Res. Oceans*, 123, 2141–2171.

Stramski, D., I. Joshi, and R. A. Reynolds. 2022. Ocean color algorithms to estimate the concentration of particulate organic carbon in surface waters of the global ocean in support of a long-term data record from multiple satellite missions. *Remote Sens. Environ.*, 269, 112776. https://doi.org/10.1016/j.rse.2021.112776

Stramski, D., L. Li, and R. A. Reynolds. 2019. Model for separating the contributions of non-algal particles and colored dissolved organic matter to light absorption by seawater. *Appl. Opt*., 58, 3790–3806.

Zheng G. and D. Stramski. 2013. A model based on stacked-constraints approach for partitioning the light absorption coefficient of seawater into phytoplankton and non-phytoplankton components. *J. Geophys. Res. Oceans*, 118, 2155–2174.