Performance and uncertainty assessment of a novel multi-step semi-analytical algorithm for estimating seawater inherent optical properties from ocean reflectance

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1 Abstract

A current challenge of inversion models aiming to derive inherent optical properties (IOPs) of seawater constituents from radiometric measurements is that they often provide a limited number of IOPs or rely on highly restrictive assumptions about the spectral shapes of output variables. To alleviate these limitations, a novel multi-step (4-step) Semi-Analytical Algorithm (4SAA) has been developed that implements four independent component models to retrieve the hyperspectral diffuse attenuation coefficient for downwelling irradiance, K_d, and a suite of total and constituent IOPs from input remote-sensing reflectance, R_{rs}. This structure is advantageous as it enables independent optimization of each component model, in-depth characterization of uncertainties associated with each component model, and uncertainty propagation through the multi-step sequence of the algorithm. Here, we describe one approach to validate the first two steps of 4SAA utilizing a recently published synthetic optical database. The first two component models, referred to as KdNN (step 1) and LS2 (step 2), provide estimates of K_d and the total and non-water absorption (a, a_{nw}) and backscattering (b_b, b_{bp}) coefficients. To conduct our uncertainty analysis, we utilized an approach to perturb the input parameters of both KdNN and LS2. The performance and uncertainty assessment of both models are determined from 350 to 700 nm. Initial results suggest a satisfactory performance of the two models versus the synthetic database and provide insight into the propagation of uncertainty through the first two steps of 4SAA. We anticipate that this validation analysis will support the estimation of IOPs from ocean color measurements from the NASA PACE satellite mission.

2 Multi-Step Inverse Algorithm

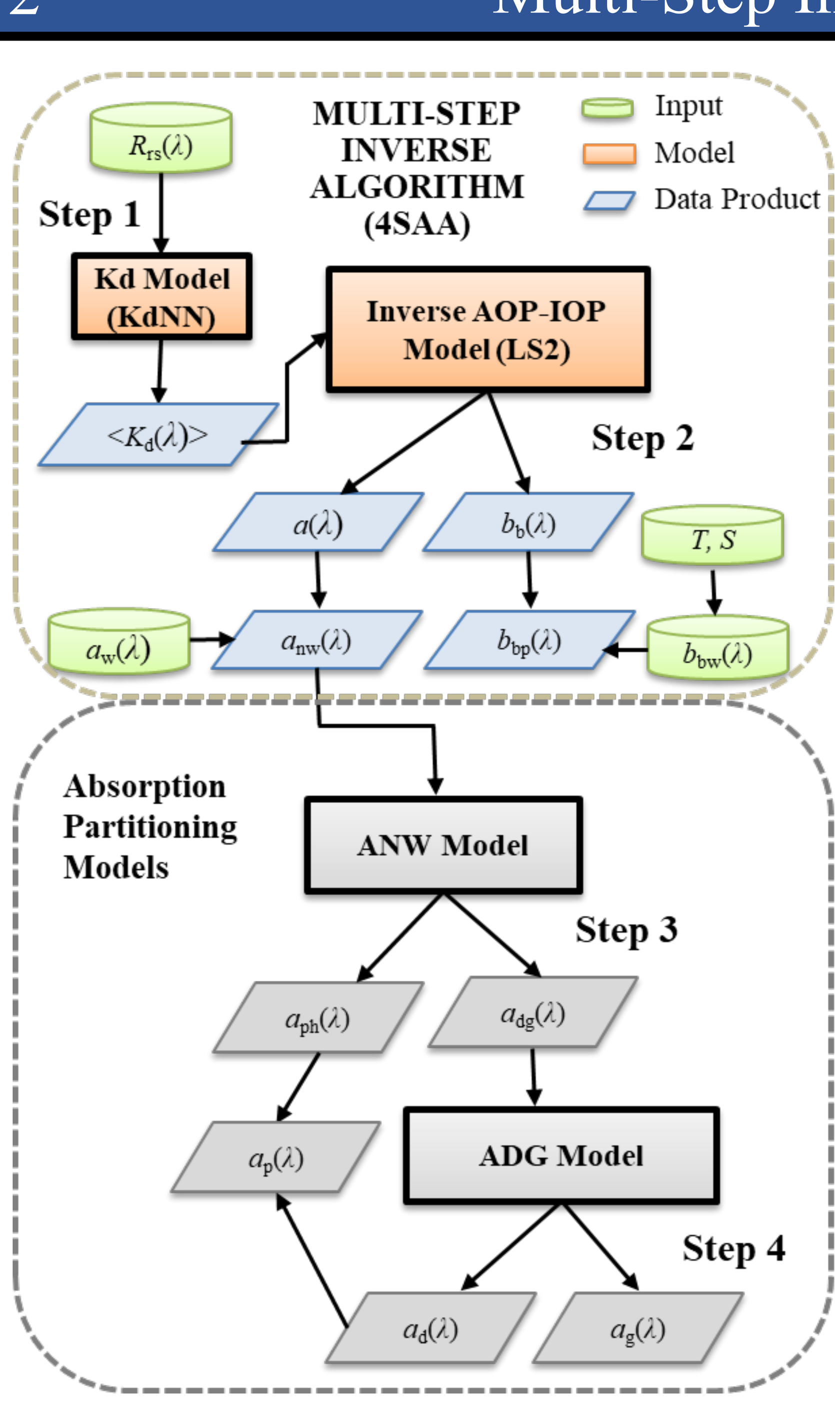

Fig. 1 Flowchart of the 4-step Semi-Analytical Algorithm (4SSA). The first two component models, KdNN and LS2, are highlighted in color and the absorption partitioning models are gray.

Multi-Step Inverse Algorithm:

- Semi-analytical
- Multiple *independent* component models
- Derives 1 AOP and 9 IOPs from input $R_{rs}(\lambda)$

Four Steps:

Step 1: $K_d(\lambda)$ Neural Network[1] (KdNN)

- Trained on wavelengths 400–700 nm
- Input: $R_{rs}(\lambda)$ – 12 specified wavelengths
- Output: $K_d(\lambda)$ – hyperspectral (1 nm)

Step 2: Inverse AOP-IOP Model[2] (LS2)

- Input: $R_{rs}(\lambda)$, $K_d(\lambda)$ – arbitrary wavelength (350–700 nm)
- Output: $a(\lambda)$, $a_{nw}(\lambda)$, $b_b(\lambda)$, $b_{bp}(\lambda)$ – arbitrary wavelength

Steps 3 & 4: Absorption Partitioning Models

- Input: $a_{nw}(\lambda)$ or $a_{dg}(\lambda)$ – arbitrary wavelength
- Output: $a_{ph}(\lambda)$, $a_{dg}(\lambda)$, $a_d(\lambda)$, and $a_g(\lambda)$ – arbitrary wavelength or 1 nm

Objectives:

1. Assess the performance of the KdNN and LS2 independently as well as the performance when combining KdNN & LS2
2. Quantify the uncertainties associated with the KdNN and the coupled KdNN & LS2 models

3 Synthetic Optical Database

Synthetic Optical Database[3]:

- Distribution of IOPs for RTE simulations are consistent with global distributions
- RTE simulations of AOPs
- Selected simulation for analysis accounts for Raman scattering and chlorophyll-a fluorescence at 0° solar zenith angle ($N = 3320$)

Significance:

Database covers a wide range of IOPs and can be used to assess 4SAA

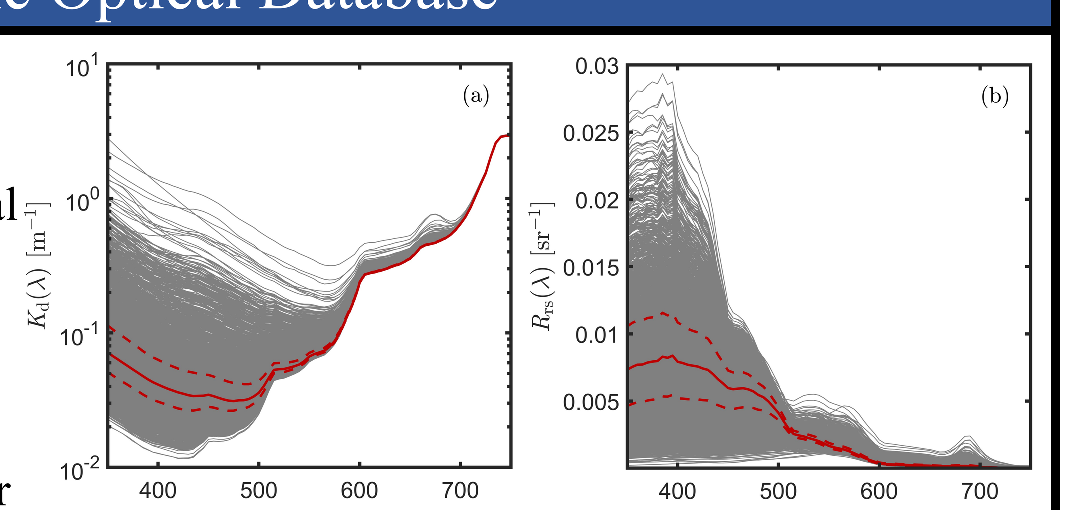

Fig. 2 Database of 3320 simulations of (a) the average diffuse attenuation coefficient for downwelling irradiance over the first attenuation depth, $K_d(\lambda)$, and (b) remote sensing reflectance $R_{rs}(\lambda)$. Gray lines form all available AOP spectra within the dataset. Solid red lines denote the median and dashed red lines depict the interquartile range for a given AOP from the database.

4 Monte Carlo Uncertainty Assessment

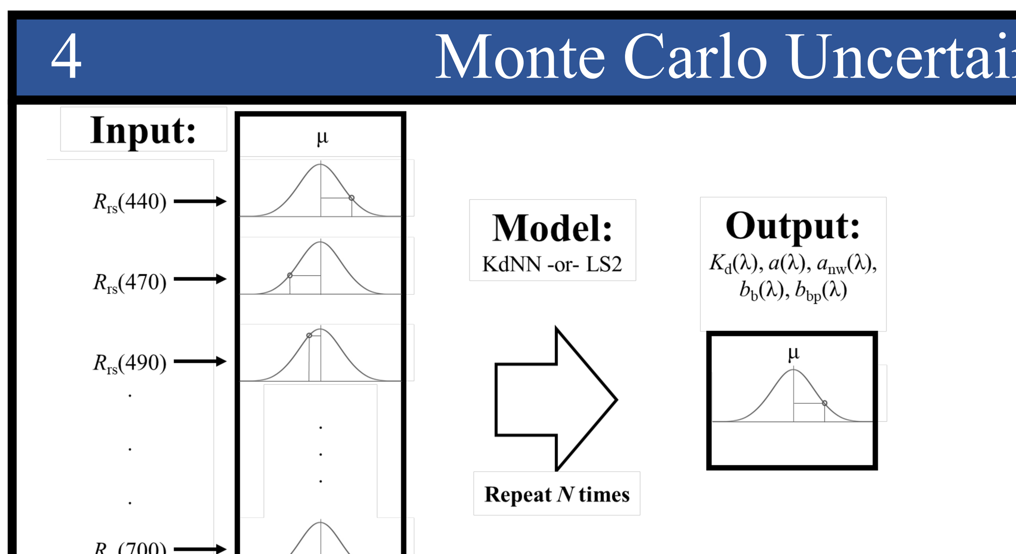

Fig. 3 Schematic of the Monte Carlo method applied to KdNN or LS2.* Input parameters, $R_{rs}(\lambda)$ & $K_d(\lambda)$, are randomly perturbed assuming a normal distribution, with the mean (μ) equal to the original input value. Points highlighted in the distribution correspond to the randomly selected error for a given iteration. This process generates a distribution of model output. *The input parameters in the example correspond to KdNN.

Monte Carlo Uncertainty Assessment:

- Randomly perturb input parameters
  - Normally distributed
  - Spectrally independent
  - Perturb input $R_{rs}(\lambda)$ for KdNN
  - Perturb input $R_{rs}(\lambda)$ & $K_d(\lambda)$ for LS2
- $N = 100$ iterations
- Input $R_{rs}(\lambda)$ uncertainty from NASA PACE science data product goals
- Model uncertainty quantified as the median relative standard deviation of the output distribution expressed as a percentage (rel. unc.)

5 Performance Assessment of KdNN & LS2

Performance Assessment of KdNN & LS2:

Scenario 1: KdNN – synthetic $R_{rs}(\lambda) \rightarrow K_d(\lambda)$

Scenario 2: LS2 – synthetic $R_{rs}(\lambda)$ & $K_d(\lambda) \rightarrow a(\lambda)$, $a_{nw}(\lambda)$, $b_b(\lambda)$, $b_{bp}(\lambda)$

Scenario 3: Coupled KdNN & LS2 – synthetic $R_{rs}(\lambda)$ & algorithm-derived $K_d(\lambda)$ $\rightarrow K_d(\lambda)$, $a(\lambda)$, $a_{nw}(\lambda)$, $b_b(\lambda)$, $b_{bp}(\lambda)$

Key Results:

- Retrievals of $K_d(\lambda)$, $a(\lambda)$, and $b_b(\lambda)$ generally show agreement with reference values
- Satisfactory retrievals of $a_{nw}(\lambda)$ and $b_{bp}(\lambda)$ from LS2 over significant portions of the spectrum
- LS2 estimations of IOPs are clearly influenced by $K_d(\lambda)$ input
- Challenge retrieving non-water absorption >550nm
- Chlorophyll-a fluorescence in red is seen in LS2-derived backscattering

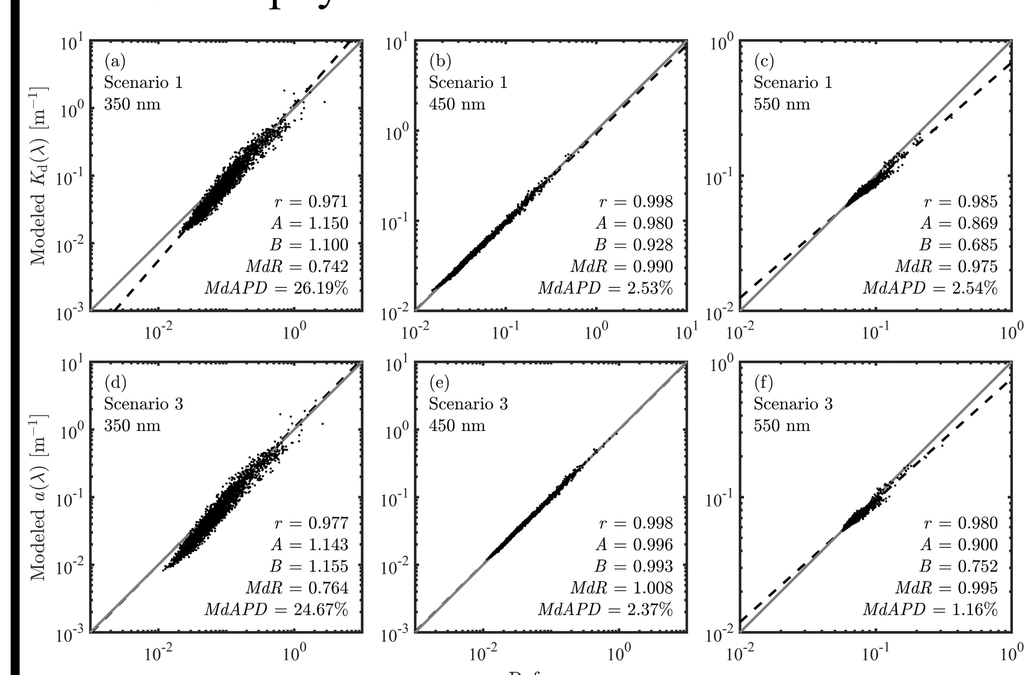

Fig. 4 Assessment of (a)–(c) KdNN (Scenario 1) and (d)–(f) LS2 (Scenario 3) as scatter plots of modeled versus reference $K_d(\lambda)$ or $a(\lambda)$. The 1:1 line and best-fit line derived from the Model II linear regression to $\log_{10}$-transformed dataset are represented by the solid gray and dashed black lines, respectively.

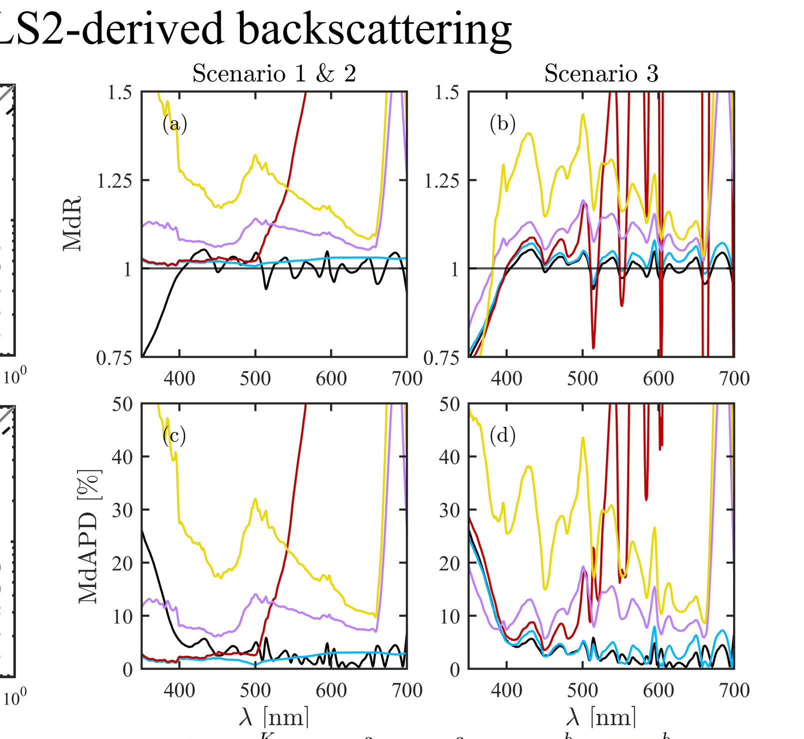

Fig. 5 Spectral values of (a, b) median ratio, MdR, and (c, d) median absolute percent difference, MdAPD, calculated from model-derived and reference values for each scenario. (a, c) Error statistics of Scenario 1 and 2, and (b, d) error statistics of Scenario 3.

6 Uncertainty Assessment using Monte Carlo Perturbations

Uncertainty Assessment of KdNN & LS2:

Scenario 1: KdNN

Perturb synthetic $R_{rs}(\lambda) \rightarrow K_d(\lambda)$

Scenario 3: Coupled KdNN & LS2

Perturb synthetic $R_{rs}(\lambda)$ & algorithm-derived $K_d(\lambda) \rightarrow a(\lambda)$, $a_{nw}(\lambda)$, $b_b(\lambda)$, $b_{bp}(\lambda)$

Key Results:

- $K_d(\lambda)$ retrieval errors directly impact $a(\lambda)$ and $b_b(\lambda)$
- Rel. unc. for $K_d(\lambda)$, $a(\lambda)$, and $b_b(\lambda)$ remains generally below 30%
- Rel unc. for LS2-derived $a_{nw}(\lambda)$ and $b_b(\lambda)$ <40%

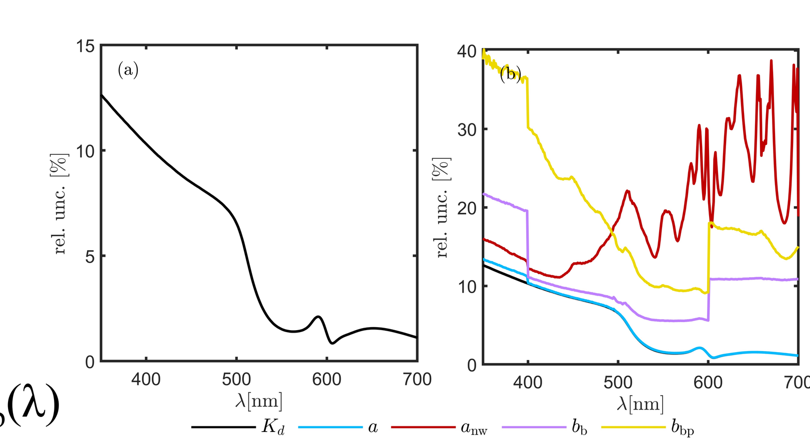

Fig. 7 Spectral relative uncertainty obtained from Monte Carlo uncertainty analysis of (a) Scenario 1 and (b) Scenario 3.

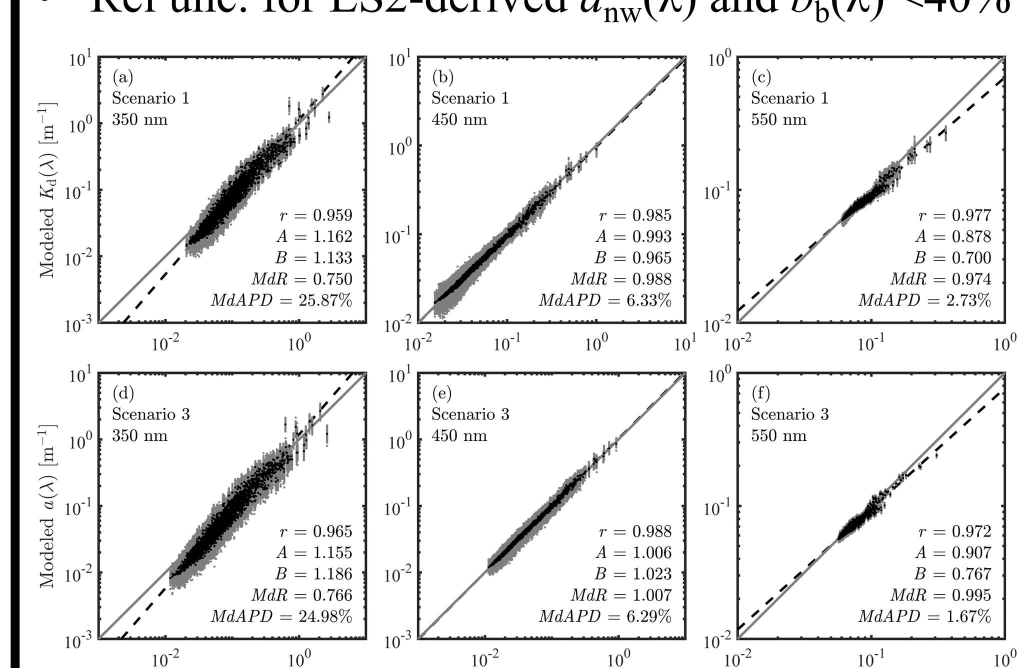

Fig. 6 Similar to Fig. 4. Black points show model output. Gray points denote retrievals of optical properties from Monte Carlo analysis.

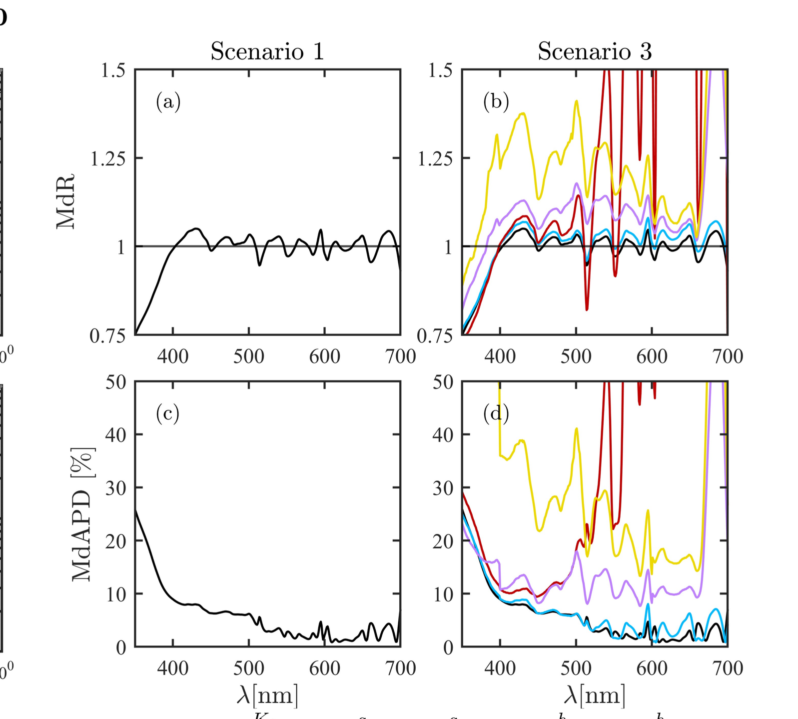

Fig. 8 Similar to Fig. 5. (a, c) Error statistics of Scenario 1 and (b, d) error statistics of Scenario 3.

7 Conclusions & Future Work

1. KdNN and LS2 yield generally satisfactory retrievals of $K_d(\lambda)$, $a(\lambda)$, $a_{nw}(\lambda)$, $b_b(\lambda)$, and $b_{bp}(\lambda)$ using inputs from the synthetic optical database. Notable exceptions are observed for $a_{nw}(\lambda)$ and $b_{bp}(\lambda)$ at wavelengths and/or environmental conditions where pure water is a significant contributor.
2. The Monte Carlo perturbations of input $R_{rs}(\lambda)$ provide a means to quantify the sensitivity of KdNN and LS2 to uncertainty in $R_{rs}(\lambda)$.
3. Application of similar uncertainty analysis to downstream absorption partitioning models.
4. Perform further performance assessment and validation analysis with in situ and satellite data.

8 References & Acknowledgements

[1]Jorge, D. S. F., Jamet, C., Loisel, H., Kehrli, M. D., Reynolds, R. A., Stramski, D., Retrieval of hyperspectral Kd from ocean color remote sensing measurements in support of PACE satellite mission. Poster for Ocean Optics XXVI, Oct 6-11, 2024. Las Palmas de Gran Canaria, Spain. (Poster M-061)

[2]Loisel, H., Stramski, D., Dessailly, D., Jamet, C., Li, L., & Reynolds, R. A. (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. Journal of Geophysical Research: Oceans, 123(3), 2141–2171. https://doi.org/10.1002/2017JC013632

[3]Loisel, H., Jorge, D. S. F., Reynolds, R. A., & Stramski, D. (2023). A synthetic optical database generated by radiative transfer simulations in support of studies in ocean optics and optical remote sensing of the global ocean. Earth System Science Data, 15(8), 3711–3731. https://doi.org/10.5194/essd-15-3711-2023

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