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Interactive comment on "A Global End-Member Approach to Derive a_{CDOM}(440) from Near-Surface Optical Measurements" *by* Stanford B. Hooker et al.

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Overview

The manuscript is a fascinating and fun read. The authors present a robust dataset and thoroughly describe the methods used. However, significant revisions are suggested to more clearly link the author's subjective classification of environments to other literature discussing optical variability and the need to pre-screen for unique optical water types to effectively retrieve inherent optical properties from a given system. The authors would be well-served to present the full data set to display dynamic range across unique environments and graphically present the ability to measure radiometric variability at the millimeter scale – a fascinating accomplishment. A clearer link between this capability and the decision to treat certain environments as anomalous is also warranted.

General comments

It seems the author's treated any data that did not conform to the algorithm as anomalous or atypical. Is this the best treatment of the dataset? This manuscript effectively serves as a more complete validation of the original end-member approach presented in Hooker et al. (2013). The goal of algorithms is to observe the environment "as is", so such a subjective treatment of any water that does not conform to anticipated algorithm output doesn't seem to be appropriate. Discussions of the "parent watermass" suggest that harbors, creek/river inputs, etc. are oddities; in fact, these spatial gradients are what we are trying to retrieve accurately with algorithms, and was a highlight of why the C-OPS was such an important instrument in the coastal zone in Hooker et al. (2013). The dataset is quite good and the algorithm useful. I think the author's would be best served by exploring the data, presenting the dynamic range (with associated categories, if necessary) and relate to algorithm performance. Discussion of potential improvements is also warranted, particularly considering that upcoming sensors are expected to have advanced spectral capabilities that, hopefully, will make band ratios less relevant for estimating a final product.

Presenting noise in measurements, and the ability to observe millimeter scale variability, would be quite useful as an additional figure. This was shown in Hooker et al. (2013) and was quite useful to fully understand the concept in that paper. Perhaps the existing figures showing performance across subjectively classified environments could be reduced into subplots of a single figure, allowing for fuller presentation of the dataset, including CDOM spectra and the ability to observe such fine scale variability in radiometry.

Was there any consideration of using CDOM spectral slope as a proxy of conservative versus non-conservative water masses?

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A discussion of “anomalous” features is certainly warranted for radiometry measurements; however, it seems throughout that the author’s measured “anomalous” conditions with the assumption that the Kd(320)/Kd(780) relationship observed for conservative waters holds to a universal truth across environments. This seems to be a gross simplification of the complexity of radiometry and a weakness of the current manuscript. As stated by the authors:

Lines 16-19, page 27: “The validation approach was based on the concept that water masses evolving conservatively (i.e., free from stressors that might cause anomalies to the natural range in the gradient of a constituent) are suitable for validating the original Hooker et al. (2013) inversion algorithm for deriving aCDOM(440) from Kd(λ) spectral end members.”

Effectively, observations that did not conform to the algorithm are considered “anomalous” and subjectively classified. Why did the authors not use an objective clustering approach to classify different environments, and consider an effective algorithm for each of these water types?

The introduction is fascinating and an interesting discussion. However, consider that the last ~1 page of text does not have a single citation. It seems much more relevant to tie this work more clearly into existing literature considering optical water variability due to different environments and optical complexity within a specific environment. This would leave much of the introduction intact while more clearly linking to how this builds upon past efforts, which it certainly does.

Specific Comments

Lines 16-22, page 7: These are helpful

All preceding paragraphs of this section (2.1) seem more suitable for supplementary material. I understand the motivation to show and describe improvements to the instrument from that shown in Hooker et al. (2013), but this takes valuable space away from

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a more complete presentation of the dataset. Currently, all that is shown is the instrument, sampling locations and relationships with the empirical algorithm. Displaying the dynamic range of the data would be particularly useful.

Line 8, page 11: Why were only the Pacific Ocean and half of the Arctic Ocean samples baseline-corrected? Did use of 590-600 nm result in a significant offset for these spectra?

Lines 18-27, page 11: The section on western US coastal and inland water CDOM analysis is not clear. The two references to quantifying CDOM as the absorption coefficient at 440 nm and use of the Single Exponential Model make it seem that only CDOM at 440 nm was measured (there was no reference to quantifying CDOM at 440 nm for the other water samples). But, you also mention absorption spectra were measured – using Ultrapure water to dilute the signal? Were the samples optically thick and needed dilution? Please clarify this section, and to the extent possible, condense the sections on analysis of differently sourced water samples.

Section 2.5 The categorization of optical variability across water bodies is interesting, and the details are certainly relevant. However, it seems that the categorizations are rather subjective, and effectively used to explain outliers in the algorithm relationship. In the present state of the manuscript, this seems quite subjective. For a universal algorithm, it seems highly relevant to look for underlying means for deviations in the relationship that would aid in how the algorithm is applied. Effectively, you have categorized the environment that results in deviating optical properties that do not perform well within the algorithm; however, you haven't utilized the dataset to hypothesize on specific, only general, mechanisms (e.g., minerogenic content of particles and refractive index, spectrally different CDOM, dominance of phytoplankton absorption and scattering on Kd relationships rather than a relatively generic "sediment resuspension"). While quite difficult, the level of detail for the other sections seems to warrant this consideration. You have attempted to bypass this variability by using the end-member approach, targeting the wavelengths most and least influenced by aCDOM; other optical parameters significantly impacting the signal suggests a more detailed explanation, outside of categories, is warranted.

Lines 6-7, page 16: "…the new acreage is a source of atypical constituents, either in composition or concentration."

Really, this is the challenge of creating flexible, accurate algorithms that work across a variety of water types, either due to spatial, temporal or extreme event variability. It seems rather than addressing how to accurately estimate CDOM by modifying the algorithm, the authors highlight what is "abnormal" about these environments. There is certainly room for this, but I think the authors would be better served by focusing on how their algorithm could be adapted for these environments, rather than subjectively classifying environments where the algorithm does not perform well. The authors emphasize how the sensitivity of the instruments used detects these changes, but there is no analysis for how this increased sensitivity can be used to develop more capable algorithms.

Line 27-28, page 18: "For example, local wind conditions could elevate the values associated with a typical bloom into atypical concentrations"

Doesn't this call into question the purpose of classifications? These are conditions that will be observed, either through in situ or satellite observations. Could the algorithm be improved by factoring in wind conditions?

Lines 22-24, page 20: "As end members are brought spectrally closer together, the range of expression available to distinguish two similar but optically different water masses decreases."

Perhaps the mechanics of this could be explored and explained?

Lines 16-17, page 21: "Application of Λ412 670 data to the corresponding algorithm in Fig. 8 results in 13 observations with negative (predicted) aCDOM(440) values, which are removed to leave 212 unique stations. This process demonstrates how end-member algorithms can be used to quality assure optical data in archives (Sect. 3.7).”

Lines 2-4, page 23: “With respect to the algorithm, the increased bias, variance, and 13 negative derived values obtained with NOMAD data (which is a small, quality controlled subset of the larger NASA SeaBASS archive) in clearer waters suggests the legacy data are degraded by sampling artifacts.”

Is this an issue with the algorithm or the measurements?

Lines 14-15, page 23: “The data set established herein has an extensive number of observations directly suitable for validation exercises (Figs. 3 and 9) plus 15 subcategories (Sect. 2.5) of potentially (but not automatically) problematic water bodies (Figs. 4–7), with the latter determined subjectively.”

The authors acknowledge that “problematic” water bodies were determined subjectively, and these observations do not agree well with the algorithm. Yet, don’t these observations span natural environmental variability that can be observed? Outside of directly observing human structures (e.g., reflectance of a shipwreck visible from surface waters), why did the authors not consider how to retrieve valid aCDOM(440) values for these waters, and rather chose to assume the algorithm works very well and these waters are problematic? Further, it isn’t clear how the algorithm can be used to determine whether legacy data is valid or not, as its performance is based on these subjective classifications, no?

Lines 7-8, page 24: “Consequently, a subcategorization scheme based on the optical measurements alone might be advantageous to the validation process, particularly for archival data.”

This is assuming that CDOM should behave conservatively across water masses? It seems the very point the paper is making is that “abnormal” environments produce CDOM of a different spectral nature. This is important. Why have the authors not attempted to accurately estimate this variability?

Line 18-24, page 23: The author's reference clustering analysis, particularly fuzzy clustering presented by Moore et al. (various years) – why were subjective categorizations used rather than an objective approach such as that of Moore et al.? It would also be useful to reference this work earlier, perhaps in the introduction. Discussing the need for classifications to build effective algorithms could also be elaborated.

Lines 11-14, page 26: "The decrease in the percent composition of the validation quality data as a function of increasing class number (N1–N5) is an indicator of the difficulty of validating an algorithm within increasingly complex waters. The recurring contribution of a relatively small number of principal subjective subcategories to the gradient in optical complexity starting with N2 and then continuing for N3–N5 confirms the original subcategory approach has merit."

Conversely, the end member approach only performs well in bodies of water with little optical variability. It isn't clear why a subjective deconstruction of water bodies was used versus a fuzzy clustering approach where alternate relationships between Kd and aCDOM(440) were explored. Fuzzy clustering approaches use an objective classification scheme to separate out waters with the intention of providing a framework where different algorithms can be applied. Why was that not explored here?

Line 28, page 26: "evolving conservatively" – is this being used to represent anything that is a natural process within the water column, with no added optical constituents? Is photo- and microbial degradation of CDOM considered a conservative process? Perhaps a clearer discussion of Case 1 and Case 2 waters and how that classification relates to the classification used here would clarify this?

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