Proposal for an IOCCG Working Group

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Working Group Title: Classification of optical water types in aquatic radiometry

Scientific and programmatic background and rationale

Some 35 years ago Morel and Prieur (1977) introduced the concept of Case-1 and Case-2 waters to ocean colour research in order separate waters that are dominated by chlorophyll-a and those that are not. This separation aided the development of algorithms for each of the respective water types, as different underlying assumptions/generalisations could be made about the optical properties of the observed water bodies, but also created something of an artificial division in the aquatic optics community. At the global scale, most waters exist as part of a continuum of optical conditions, partially due to a continuum of physical and biological forcing factors and partially due to the fact that we are observing a fluid environment that can physically mix/blend.

It remains the case that no single 'perfect' algorithm works optimally across all optical conditions/water types and we should not expect to find such an algorithm in the near future. Instead, a promising development in recent years has been the move towards a broader optical water type classification and algorithm blending. This approach is founded on the premise that multiple optimal algorithms exist but for each we can define the most suitable optical environments. The strength of the 'optical water type' classification approach has seen its use grow in limnological and oceanographic remote sensing research (Moore et al. 2001, 2014, Jackson et al. 2017, Spyrakos et al. 2018). The utility of optical water classes has also grown beyond algorithm blending (Moore et al. 2001) to include product uncertainty estimation (Jackson et al. 2017), data quality flagging (Wei et al. 2016, Jiang et al 2023), water quality monitoring (Uudeberg et al. 2020) and environmental phenology studies (Trochta et al. 2015).

Unfortunately, although the limnology and ocean optics communities may agree that optical classification is useful, a harmonised approach to the creation and use of the classes has not yet emerged from the research community. Despite recent efforts to move to a unified fuzzy logic scheme (Jai et al. 2021), a diversity of distance metrics, data transformations and cluster optimisation schemes are applied at local scales (Bi et al. 2019, Botha et al. 2020, da Silva et al. 2020, Uudeberg et al. 2020). Though all these approaches provide interesting and useful results, the fragmented nature of the research makes the comparison of water types difficult, impeding collaboration and optimisation of methods. Also, as with most machine learning techniques, unsupervised clustering is susceptible to the problems of insufficient or biased training data, the 'central tendency' (Malik, 2020), and overtraining.

It is timely to convene and reconcile these growing issues under a common framework to unify and standardize definitions, interpretations, and uses to establish guidelines for a growing body of developers and users, as well as to close methodological gaps. This need is of particular urgency in light of new missions with hyperspectral capabilities. Where classification strategies most likely will have to be revised and expanded. We believe the IOCCG is the most appropriate forum to achieve these activities, as the user and development community is globally distributed across several continents, agencies and universities.

Terms of Reference

This working group on "Classification of waters through aquatic radiometry" aims to summarise the key principles, review the state of the art and provide recommendations for the future of classification schemes for the ocean colour community. This work shall be completed through the following activities:

- Perform a literature review and summary to feed into chapter 1.
- Review current approaches to optical clustering and class assignment from open ocean to coastal waters, including methods of comparing results from various clustering studies
- Recommend a common baseline and generalised approach from which ocean colour scientists can build.
- Identify needs and challenges for classification of hyperspectral data.

- Provide open code tools for users alongside reference datasets for algorithm testing and comparison.
- Convene a meeting/workshop on statistical approaches and metrics to discuss community approaches and feed into chapters 2,3 and 6.
- Summarise work and findings in an IOCCG report.

Draft timeline
Establishment of WG: April 2023
Draft working plan and distribution of work: June 2023
Collection of contributions September 2023
Meeting: November 2023
First draft version of report February 2024
Second draft version for review June 2024

Proposed Membership:
Jacob Bien, University of South Carolina
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Heidi Diersen, University of Connecticut / PACE team.
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Bror Jönsson, Plymouth Marine Laboratory / GLIMR team
Frédéric Mélin, Joint Research Centre
Tim Moore, Florida Atlantic University (**Co-Chair**)
Christian Müller, Helmholtz-Zentrum Hereon and LMU München.
Evangelos Spyrakos, University of Stirling

Proposed report Structure

1. Introduction:
Background/history
Recent growth a proliferation of approaches
Advances in machine learning and data driven approaches
Terminology

2. Underlying statistical principles and concepts:
Distance/similarity metrics
Clustering approaches
Requirements/limitations of use with ocean colour (data volumes etc)
Supervised vs unsupervised
Reproducible and invertible transformations

3. Comparing cluster sets:
How to compare cluster sets
Cluster merging approaches
Different data types (spatial, temporal, spectral resolutions, variables (SST, Rrs, etc))
Regional vs global importance.

4. Using classification schemes with combined in-situ and remote sensing data:
Enhancing the value of in-situ collection
Near real time targeting for sampling campaigns
Characterising clusters

5. Applications:
Algorithms (tailoring, blending, domain setting)
Data quality indicators
Province delineation
Water quality or climate monitoring

6. Recommendations for the community:

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