Advanced guidance to bio-optical algorithms for use in coastal and inland waters

In order to estimate ecological response variables (Adrian et al., 2009; Dörnhöfer and Oppelt, 2016) linked to the biogeochemical state of aquatic ecosystems from remote-sensed images, we consider two types of algorithms: 1/ Atmospheric correction algorithms to remove the effect of the atmosphere from the top-of-the-atmosphere (TOA) signal recorded by the remote sensor, and 2/ Bio-optical algorithms to retrieve information about the biological and biogeochemical properties of water from such data. This section focuses on bio-optical algorithms and is directed towards an audience with experience in the use of satellite data products and interest in product development. Introductory guidance on algorithm selection, use of these products, and product development, intended for a less experienced audience, can be found in our companion document.

The development of new satellite data products commonly addresses the biophysical, biological, and biogeochemical state of aquatic ecosystems, and bio-optical algorithms are used to translate the optical signal recorded by the remote sensor to the bio-optical and biogeochemical variables of interest. The derived data products can include estimates of the inherent and apparent optical properties (IOPs and AOPs), associated constituent concentrations, and measures of transparency. Some of these algorithms might translate the optical signal recorded by the remote sensor without the removal of the contributions of the atmosphere and air-water interface, while most of them presume at least the effects of the scattering and absorption of sunlight by air molecules (Rayleigh scattering) were accounted for through the process of atmospheric correction. Details on atmospheric correction can be found in a future document.

Bio-optical algorithms use relationships of IOPs and constituent concentrations to interpret measurable, often unique, absorption and scattering signatures of optically-active constituents (IOCCG, 2018). These signatures (Fig. 1) are used implicitly, in empirical and semi-empirical algorithms, or explicitly, in semi-analytical and analytical algorithms, and form the basis of any subsequent constituent determination. The AOPs (e.g., remote sensing reflectance and diffuse attenuation coefficient) and associated measures of transparency (e.g., Secchi depth, euphotic depth, and turbidity) are directly measurable through remote sensors. From these AOPs, the IOPs (e.g., total absorption and backscattering coefficients) and associated constituent concentrations (e.g., chlorophyll-a, sediments, and dissolved organic carbon) can be inferred. Some desirable variables (e.g., trophic state index and primary productivity) are only indirectly measurable. This means additional calculation steps are needed to derive information on them.

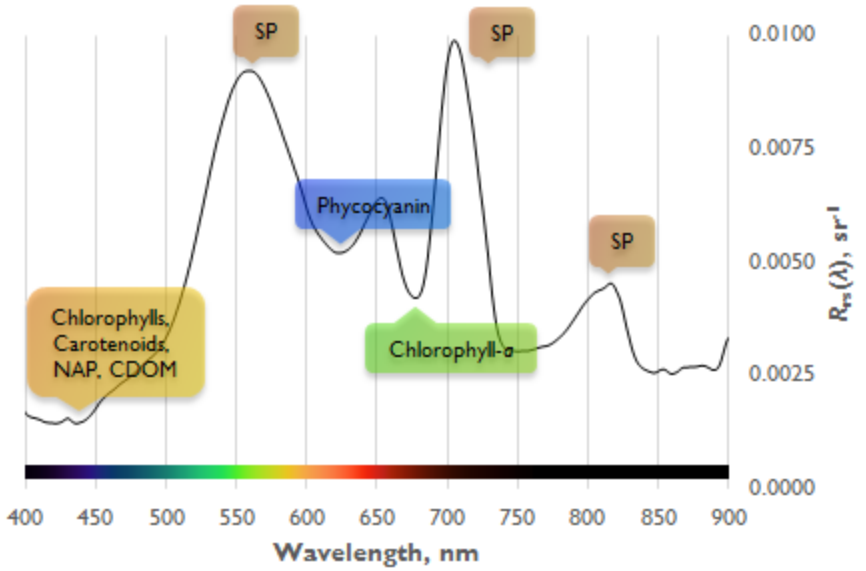

Figure 1. Remote sensing reflectance spectrum of a hypereutrophic lake (Chl*a* = 95.1 mg m^{-3}, TSM = 24.4 g m^{-3}) acquired on 21.09.2015 at Lake Winnebago, WI, USA. The absorption and scattering signatures of optically-active constituents are represented as troughs and peaks in spectral reflectance (e.g. chlorophyll-*a* absorption is depicted as a trough at 678 nm). Chlorophylls and carotenoids - Common algal pigments, NAP - Non-algal particles, CDOM - Coloured dissolved organic matter, SP - Suspended particles, Chl*a* - Chlorophyll-*a* concentration, TSM - Total suspended matter concentration

In open ocean waters, the optical properties vary predominantly with phytoplankton concentration, while coastal and inland waters are optically more complex and variantly dominated by the concentrations of multiple constituents. The optical complexity of these waters represents a challenge for the choice of appropriate algorithms for environmental monitoring applications as standard ocean color algorithms provide limited accuracy in these waters.

To overcome this challenge, many bio-optical algorithms (Giardino et al., 2019; Werdell et al., 2018) were developed in the past decades to address the transition from open ocean to coastal and inland waters. The following sections provide a classification of data-based empirical and semi-empirical methods, as well as physics-based semi-analytical and analytical methods, for some of the most commonly directly measured and derived variables.

Empirical and semi-empirical algorithms

This family of algorithms uses statistical relationships of the variables of interest to the optical signal recorded by the remote sensor (Tab. 1). Empirical algorithms use only statistical dependencies (Keller, 2001) and can take many different inversion approaches from univariate or multivariate linear regressions to spectral decomposition methods to estimate these variables (Werdell et al. 2018). Semi-empirical

algorithms use knowledge of the underlying physics to select the most appropriate single bands and/or band combinations for the determination of a model equation (Keller, 2001) whereas they use statistical methods to adjust the model and/or determine the model parameters.

Table 1. Overview of empirical and semi-empirical algorithms applied to retrieve bio-optical and biogeochemical variables from remote sensing data. DOC - Dissolved organic carbon, a_{cdom} - Coloured dissolved organic matter absorption coefficient, S_{cdom} - Slope of the CDOM absorption coefficient, K_d - Diffuse attenuation coefficient for downwelled light, PC and PE - Phycocyanin and phycoerythrin concentrations, FLH - Fluorescence line height, MPH - Maximum peak height

Family of algorithms	**Commonly estimated bio-optical and biogeochemical variables**	**Implementation**	**References**
Empirical and semi-empirical	DOC, a_{cdom} , and/or S_{cdom}	Blue to near-infrared based algorithms using single or multiple bands, band ratios and/or other band arithmetic operations	Brezonik et al., 2015; Cao and Tzortziou, 2021; Cao et al., 2018; Ficek et al., 2011; Kutser, 2012; Kutser et al., 2005; Mannino et al., 2008; Menken et al., 2006
	TSM	Red-near-infrared based algorithms using single bands, band ratios, and/or other band arithmetic operations	Doxaran et al. 2002, 2009; Feng et al., 2014; Knaeps et al., 2015; Kumar et al., 2016; Miller and McKee, 2004; Nechad et al., 2010; Novoa et al., 2017; Ondrusek et al. 2012; Petus et al., 2010
	Chl*a*, PC, PE, and/or algal biomass	Blue-green based algorithms using band ratios and/or other band arithmetic operations for Chl*a* retrievals in clear waters, red-near-infrared based algorithms in turbid waters, use of green to orange bands for PC and PE retrievals and detection of cyanobacterial blooms	Gitelson et al., 2007; Lunetta et al. 2015; Mishra and Mishra, 2012; Neil et al., 2021; 2019; O'Reilly and Werdell, 2019; O'Reilly et al., 1998
		Reflectance peak-height algorithms using FLH or MPH	Gower and King, 2012; Gower et al., 2005; Matthews and Odermatt, 2015; Matthews et al., 2012
	K_d, Secchi depth, and/or euphotic depth	Blue to near-infrared based algorithms using single bands, band ratios and/or other band arithmetic operations	Alikas and Kratzer, 2017; Binding et al. 2015; Chipman et al. 2004; McCullough et al. 2012; Olmanson et al. 2008; Zhao et al., 2011
	Turbidity	Red-near-infrared based algorithms using single bands, band ratios, and/or other band arithmetic operations	Binding et al. 2010; Dogliotti et al., 2015; Doxaran et al. 2009; Nechad et al., 2009; Vantrepotte et al., 2011
	Trophic state index	Inferred from Chl*a* as an indicator of algal biomass and/or Secchi depth as an indicator of water clarity	Binding et al. 2011; Carlson, 1977; Hu et al., 2021; Matthews et al. 2012; Olmanson et al. 2008

Machine learning algorithms represent a computationally more complex subset of empirical methods. They can comprise physics-based and/or empirical elements and are addressed in the next section. Readers are referred to the academic literature for information on the full range of empirical and semi-empirical methods. Empirical and semi-empirical algorithms are often easily interpretable without the need to understand the underlying physical relationships, and are computationally less expensive than other methods. Semi-empirical algorithms can partly annul some of the contributions of the atmosphere and air-water interface if band arithmetic operations are applied to bands in which these contributions are comparable.

Empirical and semi-empirical algorithms are associated with the need for coincident field measurements to calibrate and validate the algorithms either for global-scale applications (e.g., NASA chlor_a standard product for Chla retrievals in clear oceanic and coastal waters) or for specific locations and timeframes. The algorithms can provide accurate constituent retrievals although their accuracy depends on the range of conditions included in the dataset upon which the pertinent statistical relationship was built. Thus, empirical algorithms developed for specific regions or specific sensors are often difficult to adapt to new locations and sensors. Similarly, empirical algorithms tuned on spatiotemporally restricted datasets may provide less reliability in retrospective data analysis compared to other methods. The direct estimation of the variables of interest without the consideration of the IOPs can result in untraceable uncertainties. Moreover, the use of the same spectral band combinations for different variables (e.g. the use of a red-NIR ratio for Chla and the same NIR band for TSM and/or turbidity) can affect the ability to disentangle the contributions of individual constituents as the IOPs of these constituents vary independently of each other. Nevertheless, empirical and semi-empirical algorithm performances have been assessed over a large range of optical conditions and some band ratios and line-height approaches, which are less sensitive to interference from the atmosphere and air-water interface, have found practical use in standard image processing software packages (e.g. ESA SNAP MPH/CHL product).

Machine learning algorithms

Most of the empirical and semi-empirical algorithms outlined in the section above estimate the variables of interest as a relatively simple function of the water-leaving radiance or reflectance, typically using univariate or multivariate linear regressions. On one hand, these algorithms are easily interpretable and implementable, but they have a limited ability to model the more complex relationships found in the data. On the other hand, machine learning algorithms, such as artificial neural networks (ANN), tree-based models, such as Random Forests (RF), or support vector machines (SVM), can overcome this limitation through their ability to model complex relationships, but they are less easily interpretable, i.e. most are effectively 'black box' algorithms (Tab. 2). In general, machine learning algorithms tend to be 'data hungry' and their development can require larger calibration data sets compared to the ones used in linear regression approaches.

Table 2. Examples of machine learning algorithms applied to retrieve bio-optical and biogeochemical variables from remote sensing data. RLR - Regularized linear regression, RFR - Random forest regression, KRR - Kernel ridge regression, GPR - Gaussian process regression, SVR - Support vector regression, MDN - Mixture density network, BPNN - Back-propagation neural network, BST - eXtreme gradient boosting tree, XGBoost and LightGBM - Specific types of gradient boosting frameworks

Family of algorithms	Commonly estimated bio-optical and biogeochemical variables	Implementation	References
Machine learning	DOC, a_{cdom} , and/or S_{cdom}	RLR, RFR, KRR, GPR, and SVR	Ruescas et al. 2018
Single-parameter output	TSM	MDN or ANN	Balasubramanian et al., 2020; Chen et al. 2015
	Chl*a*, PC, PE, and/or algal biomass	BST, MDN, or ANN	Cao et al., 2020; Pahlevan et al., 2020; Vilas et al. 2011
	K_d, Secchi depth, and/or euphotic depth	RFR	Jamet et al., 2012; Rubin et al. 2021
	Turbidity	ANN	Wang et al., 2019
	Trophic state index	ANN, RFR, and SVR or meta-classification using XGBoost, LightGBM, NB, and ANN base-classifiers	Watanabe et al. 2020; Werther et al., 2021
Multi-parameter output	Chl*a* and TSM	ANN, RFR, Cubist, or SVR	Keiner and Yan, 1998; Kim et al. 2014
	Chl*a*, TSM, and a_{cdom}	ANN	Alikas et al., 2008; Brockmann et al., 2016; Doerffer and Schiller, 2007; Philipson et al., 2016; Schroeder et al., 2007; Toming et al., 2017
	Chl*a*, TSM, a_{cdom}, and Secchi depth	ANN	Kallio et al. 2015; Soomets et al., 2020
	Chl*a*, TSM, and turbidity	ANN, RFR, CBR, and SVR	Hafeez et al., 2019

Machine learning algorithms can take many different forms (Fig. 2). Artificial Neural Networks (Fig. 2a) use one or more layers of nodes, where each node contains a value determined as a weighted sum of the inputs. In the first layer of nodes (left column of green points) these inputs are the input data, while in the second layer of nodes (right column of green points) the input is the first layer of nodes. Weights (the lines connecting the points) are iteratively modified to minimize a cost function, such as the sum-of-squares or cross-entropy error between predictions (blue point) and the data used for model calibration. Support Vector Machines (Fig. 2b) are more akin to standard regression models, but with a cost function that incorporates tolerance of errors within a set threshold. Models based on decision trees, such as Random Forest (Fig. 2c), iteratively split the input data (yellow point) using thresholds that optimize a given criterion (e.g. minimizing heterogeneity of each data subset), until a stopping criterion is met (all data contained in blue 'terminal node' points) and a prediction is made as the mean value of each subset. In Random Forest, this process is repeated using bootstrap samples of the original data to generate multiple trees, whose predictions are then averaged. The Cubist model (Fig. 2d) is similar to Random

Forest, except the predictions for terminal nodes are made with a local linear regression model instead of the mean value of the subset. Readers are referred to the academic literature for more detailed descriptions of these and many other types of machine learning models.

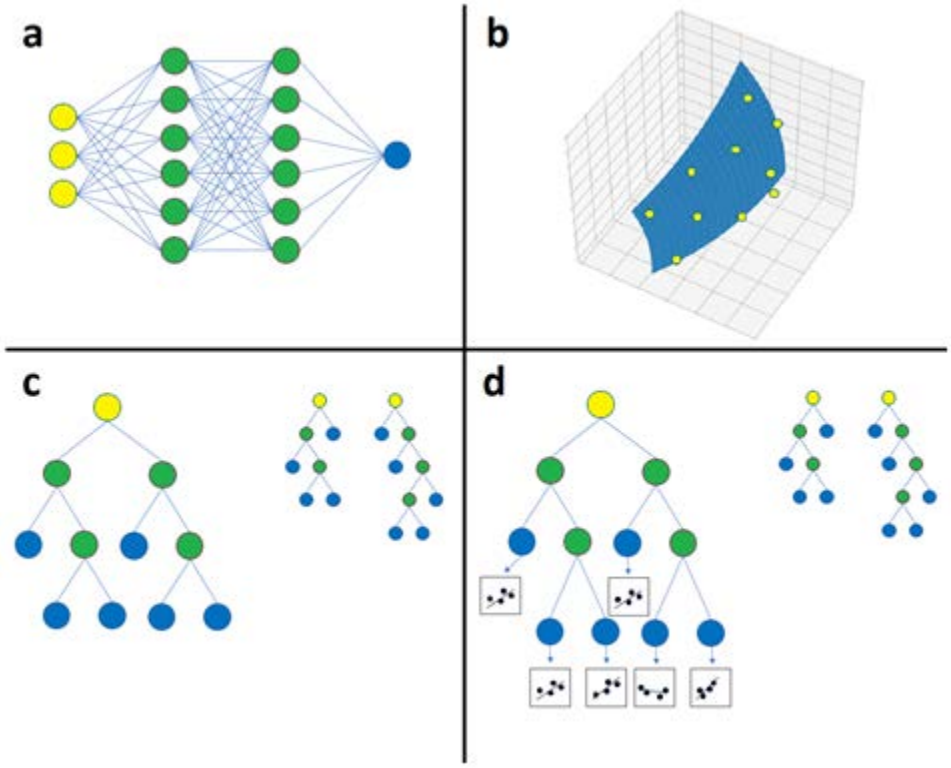

Figure 2. Concept maps for commonly-used machine learning algorithms. a: Artificial Neural Network. b: Support Vector Machine. c: Random Forest. d: Cubist. Yellow points indicate inputs, green points indicate internal calculations, blue points indicate outputs/predictions.

The use of Mixture Density Networks (MDNs) has attracted increased attention in water quality applications (Balasubramanian et al., 2020; Pahlevan et al., 2020; Smith et al., 2021). MDNs represent a combination of a conventional neural network with a mixture density model and address limitations in the prediction of continuous variables where the conditional averages of traditional neural networks provide only a very limited representation of the statistical properties of the target variables. This problem particularly arises in multi-valued situations where MDNs model the conditional probabilities of the target variables for the provided input data through a combination of mixing coefficients and conditional density functions to provide a more accurate characterization of the target space (Bishop, 1994). MDNs were part of a recent performance assessment of atmospheric correction processors and downstream data products (Pahlevan et al., 2021).

Semi-analytical and analytical algorithms

This family of algorithms is based on the spectral inversion of radiative transfer and bio-optical models and attempts to retrieve the IOPs from the water-leaving radiance or reflectance (Tab. 3). The concentrations of the associated constituents are then related to the IOPs using empirical relations specific to each location and water type.

The estimation of IOPs from these radiometric quantities is inherently an inverse problem where a forward model relating the spectral reflectance to the IOPs is often required. In the most rigorous sense, the forward model is a radiative transfer code (RTC) such as HydroLight (Sequoia Scientific, Inc.). However, a full-fledged RTC is computationally more expensive than other methods and is not practical for routine operations. A more practical and popular approach is to use a simple analytical equation to relate the spectral reflectance to the IOPs and then tune the coefficients of this equation by running an RTC (Lee et al., 2002; Zhu et al., 2011; Xue et al., 2019).

The inputs to the forward model to compute the spectral reflectance are the total absorption and backscattering coefficients. Optically-active constituents considered in this approach include phytoplankton pigments, suspended particles, and CDOM. Besides the water molecules themselves, phytoplankton pigments, suspended particles, and CDOM contribute to total absorption in natural waters while the suspended particles account for most of the backscattering. Each absorption and backscattering term is modeled as the product of a constant coefficient, which is the value of the IOP at a specific reference wavelength, multiplied by a wavelength dependent function, which is the specific IOP (SIOP). The approach to model inversion typically takes the shape of curve fitting, matrix inversion, look-up table, or neural network techniques (Keller, 2001). Readers are referred to the academic literature for more detailed descriptions of these and other inversion techniques.

This approach provides a robust mechanism to spectral inversion where the consideration of the underlying physics results in more reliability in retrospective data analysis and under varying recording conditions compared to other methods, and an improved accuracy for the range of environmental impacts accounted. The physics-based stepwise retrieval of the IOPs and variables of interest results in traceable uncertainties and mechanistic transparency. Challenges to the use of semi-analytical and analytical algorithms include the availability of representative SIOPs and their ranges needed to develop and run most algorithms. Moreover, it often represents a challenge to apply semi-analytical and analytical algorithms to satellite sensors with a limited number of spectral bands (e.g. it is very difficult to retrieve all constituents and spectral slopes from Landsat 8/9 OLI). The interpretation of the physical relationships requires a robust physical knowledge and can make the algorithms less easily interpretable for less experienced users.

Table 3. Examples of semi-analytical and analytical algorithms applied to retrieve bio-optical and biogeochemical variables from remote sensing data. a - Total absorption coefficient, a_{ph}, a_{dg}, a_g, and a_{cdm} - Phytoplankton, detrital and dissolved (gelbstoff) matter, dissolved matter, and coloured detrital matter absorption coefficients, b_b - Total backscattering coefficient, b_{bp} - Particulate backscattering coefficient, CF - Curve fitting, LLS - Linear least squares, LMI - Linear matrix inversion, LUT - Look-up table, QAA - Quasi-analytical algorithm, QAA-E - Extended quasi-analytical algorithm, 3SAA - Three-step semi analytical algorithm

Family of algorithms	**Commonly estimated bio-optical and biogeochemical variables**	**Implementation**	**References**
Semi-analytical and analytical	TSM	Three-step algorithm for water type classification, semi-analytical b_{bp} retrieval, and empirical TSM retrieval	Jiang et al., 2021
Single-parameter output	Chl*a*, PC, PE, and/or algal biomass	Red-near-infrared based algorithms using band ratios for a_{chl} and Chl*a* retrieval, use of nested band ratios for a_{pc} and PC retrieval	Gilerson et al., 2010; Gons et al., 2005; Simis et al., 2005; Simis et al., 2007
Multi-parameter output	Chl*a*, TSM, and a_{cdom}	CF and LLS	Keller 2001; Knaeps et al., 2010
	Chl*a*, TSM, and a_{cdom}	LMI	Brando and Dekker, 2003; Brando et al., 2012; Campbell and Phinn, 2010; Campbell et al., 2011; Hoogenboom et al., 1998
	Chl*a*	LUT	Salem et al., 2017
	a_{ph}, a_{dg}, b_b, and/or a_g	QAA and QAA-E	Lee et al. 2002; Zhu et al., 2011
	Chl*a*, a_{cdm}, and b_{bp}	GSM	Maritorena et al., 2002
	a, a_{ph}, a_{cdm}, b_b, and b_{bp}	3SAA	Jorge et al., 2021

Considerations for algorithm choice

Constituent retrieval approaches typically range from data-based empirical and semi-empirical to physics-based semi-analytical and analytical methods (IOCCG, 2018). Optical water type classifications (Moore et al., 2014; Spyrakos et al., 2017) can represent a practical tool to support algorithm selection in water quality studies as some algorithms are more adapted to certain optical conditions and constituent concentration ranges (Neil et al., 2019). Especially empirical, semi-empirical, and machine-learning algorithms tend to struggle when measurements lie outside the range upon which the algorithm was built. Optical water type classifications to select the most appropriate algorithm on a per-pixel basis and develop merged data products can provide improved accuracy in scenarios with little information on the level of optical complexity of the waters studied.

The choice of appropriate algorithms for environmental monitoring applications requires the consideration of their needs for field measurements for calibration and validation efforts, as well as their accuracy, reliability, maturity, and complexity. It should reflect the level of optical complexity of the

waters under consideration, the optically-active constituent concentration ranges, the spectral characteristics of the sensor to which they will be applied, the availability of representative specific inherent optical properties and their ranges needed to develop and run algorithms, and computation time/resources (IOCCG, 2018).

Remote sensors used for the development of new satellite data products (Fig. 3) range from traditional ocean colour sensors, such as the Terra and Aqua Moderate Resolution Imaging Spectroradiometer (MODIS) and Sentinel-3 Ocean and Land Colour Instrument (OLCI), to land monitoring sensors, such as the Landsat 8 Operational Land Imager (OLI) and Sentinel-2 MultiSpectral Instrument (MSI). Past hyperspectral missions, such as the Hyperspectral Imager for the Coastal Ocean (HICO), and their data archives remain valuable assets in proof-of-concept studies, while present and future hyperspectral missions, such as the PRecursore IperSpettrale della Missione Applicativa (PRISMA), Plankton, Aerosol, Cloud, and ocean Ecosystem (PACE), and Geostationary Littoral Imaging and Monitoring Radiometer (GLIMR) and their targeted data products can provide new insights on aquatic ecology and biogeochemistry and their sensitivity to environmental change in large water bodies (Giardino et al., 2020; Loizzo et al., 2018; Werdell et al., 2019). The choice of appropriate datasets for a study might result in a compromise in terms of the spatial, spectral, radiometric, and temporal resolution needed to accommodate the waters studied.

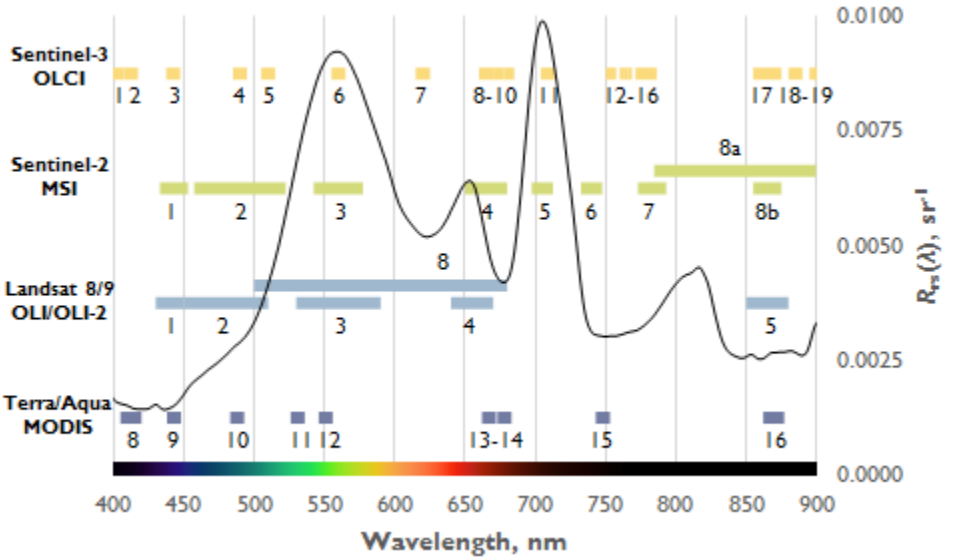

Figure 3. Remote sensing reflectance spectrum of a hypereutrophic lake (Chl*a* = 95.1 mg m^{-3}, TSM = 24.4 g m^{-3}) acquired on 21.09.2015 at Lake Winnebago, WI, USA overlaid with the spectral bands of four satellite sensors with relevance for the remote sensing of water quality.

Datasets and data access

Datasets are accessible through download and cloud access options. Information on downloads through graphical user and application programming interfaces for the aforementioned sensors is provided through the NASA OceanColor Web (https://oceancolor.gsfc.nasa.gov/), USGS Landsat Missions webpages (https://www.usgs.gov/core-science-systems/nli/landsat), ESA Sentinel webpages (https://sentinel.esa.int/web/sentinel/home), and PRISMA webpages (http://prisma-i.it/index.php/en/). Cloud access options primarily include the Copernicus Data and Information Access Service cloud environments and Amazon Web Services at commercial conditions. Google Earth Engine (https://earthengine.google.com/) provides free cloud access to selected datasets for research, education, and nonprofit uses while commercial or operational applications are possible at commercial conditions. Common software packages to process satellite data and retrieve constituent concentrations in a desktop setting include SeaDAS (https://seadas.gsfc.nasa.gov/), SNAP (https://step.esa.int/main/download/snap-download/), and ACOLITE (https://odnature.naturalsciences.be/remsem/software-and-data/acolite).

Recommendations for algorithm choice

Given the complex interactions in the atmosphere, at the water surface, and in the water column, the identification of universally applicable solutions to the monitoring of key ecological response variables in coastal and inland waters from remote-sensed images remains an elusive target, although significant progress has been made to address the challenges of optical complexity encountered in these waters, and a deeper knowledge of the IOPs and range and variability of water types are being obtained (IOCCG, 2018). The choice of algorithm through optical water type classifications and water type class dependent algorithm selection schemes can represent a pragmatic approach to constituent retrieval attempts in coastal and inland waters, as in the absence of a comprehensive knowledge of water and atmospheric constituent optical properties, the requirements remain unmet to satisfy a fully reductionist bio-optical modelling approach leading to quantitative water quality estimates (IOCCG, 2018). Many algorithms can provide overall information on the biogeochemical state of aquatic ecosystems while caution is advised and additional algorithm validation efforts are needed if information is intended for scientific studies and regulatory decisions where a high degree of data accuracy is required. Empirical and semi-empirical algorithms can provide a first approach to exploratory data analysis as less experienced users might want to explore if these algorithms can meet their monitoring needs while more advanced users are encouraged to explore machine learning or semi-analytical inversion methods.

Authorship information

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Date

2021-09-27

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