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A Machine Learning Approach to Estimate Surface Chlorophyll *a* Concentrations in Global Oceans From Satellite Measurements

Chuanmin Hu^{ID}, Lian Feng^{ID}, and Qi Guan^{ID}

Abstract—Various approaches have been proposed to estimate surface ocean chlorophyll *a* concentrations (Chl, mg m^{-3}) from spectral reflectance measured either in the field or from space, each with its own strengths and limitations. Here, we develop a machine learning approach to reduce the impact of spectral noise and improve algorithm performance at the global scale for multiple satellite sensors. Among several candidates, the support vector regression (SVR) approach was found to yield the best algorithm performance as gauged by several statistical measures against field-measured Chl. While statistically the performance of the SVR is slightly worse than the empirical color index (CI) algorithm proposed in Hu *et al.* (2012) for $\text{Chl} < 0.25 \text{ mg m}^{-3}$, its applicability to global waters is much extended, from the CIs $0.01\text{--}0.25 \text{ mg m}^{-3}$ (about 75% of the global oceans) to its $0.01\text{--}1 \text{ mg m}^{-3}$ [about 96% of global oceans according to Sea-viewing Wide Field-of-view Sensor (SeaWiFS) statistics]. Within this range, not only does the SVR show much improved performance over the traditional band-ratio OCx approaches, but the SVR leads to much reduced image noise and much improved cross-sensor consistency between SeaWiFS and Moderate Resolution Spectroradiometer (MODIS)/Aqua and between MODIS/Aqua and Visible Infrared Imaging Radiometer Suite (VIIRS). Furthermore, compared with the hybrid Ocean CI (OCI) algorithm currently used by the U.S. NASA as the default algorithm for all mainstream ocean color sensors, the SVR avoids the need to merge two different algorithms for intermediate Chl (band subtraction for CI and band ratio for OCx), thus may serve as an alternative approach for global data processing.

Index Terms—Algorithm, chlorophyll *a*, empirical, machine learning, Moderate Resolution Spectroradiometer (MODIS), ocean color, remote sensing, Sea-viewing Wide Field-of-view Sensor (SeaWiFS), support vector regression (SVR), Visible Infrared Imaging Radiometer Suite (VIIRS).

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I. INTRODUCTION

ONE of the primary ocean color data products from satellite measurements is the surface ocean chlorophyll *a* concentration (Chl, mg m^{-3}). This is usually through two steps (see review by Hu and Campbell [1]): atmospheric correction to derive the spectral surface remote-sensing reflectance ($R_{rs}(\lambda)$, sr^{-1}) from the calibrated at-sensor spectral radiance ($L_t(\lambda)$, $\text{mW cm}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$) [2]–[4], and bio-optical inversion to estimate Chl from $R_{rs}(\lambda)$ using an algorithm established from field measured Chl and $R_{rs}(\lambda)$. The latter is the subject of this study.

There are two general approaches to develop algorithms to estimate Chl from $R_{rs}(\lambda)$: empirical and semianalytical [1]. The former is based on the principle that, for most waters, R_{rs} in the blue decreases with increasing Chl while R_{rs} in the green is more stable, leading to algorithms to use R_{rs} band ratios (blue/green) or band subtractions (blue–green or blue–green–red) to estimate Chl [5]–[15]. Such empirical Chl algorithms do not distinguish Chl from other water constituents such as colored dissolved organic matter (CDOM) or suspended nonliving particles, and in waters where they do not covary the algorithms may lead to large uncertainties [16]–[18]. In contrast, semianalytical algorithms estimate Chl (or phytoplankton pigment absorption) and other water constituents at the same time, based on the spectral optical properties of these water constituents (e.g., [19]–[27]).

While both empirical and semianalytical approaches have their strengths and limitations, because empirical algorithms are simple to design and implement and generally more tolerant to spectral noise, they have been used widely, especially for regional studies where algorithm coefficients can be tuned with field data (e.g., [28]–[30]). For global applications, the blue/green band ratio algorithms (hereafter referred to OCx where *x* represents the number of spectral bands used in the algorithm [12], [31]) have been used by the U.S. NASA since the 1980s to process ocean color data collected by the Coastal Zone Color Scanner (1978–1986), Sea-viewing Wide Field-of-view Sensor (SeaWiFS, 1997–2010), Moderate Resolution Spectroradiometer (MODIS, 2000–present on Terra and 2002–present on Aqua), Medium Resolution Imaging Spectrometer (MERIS, 2002–2012), Visible Infrared Imaging Radiometer Suite (VIIRS, 2012–present), among others. Recently, the OCx algorithms have been updated to incorporate the advantage of the blue–green–red color index (CI) algorithm for low-Chl

TABLE I
CHL RANGES (IN mg m^{-3}) OF THE DATA FROM THE NOMAD2 AND SEABASS DATA SETS
USED FOR ALGORITHM DEVELOPMENT AND VALIDATION, RESPECTIVELY

	Min	Max	Mean	Median	STD	# of points
NOMAD2	0.03	77.86	2.89	0.90	6.29	638
SeaBASS for SeaWiFS	0.01	32.18	1.30	0.57	2.32	1145
SeaBASS for Aqua	0.03	29.00	1.49	0.72	2.71	331

waters [14], leading to a hybrid Ocean CI (OCI) algorithm as the default algorithm for all ocean color sensors [13], [14].

The success of the global empirical algorithms is mainly due to the fact that, for most waters, relative to R_{rs} in the green, R_{rs} in the blue decreases with increasing Chl. When other water constituents such as CDOM or suspended sediments overwhelm phytoplankton to dominate the R_{rs} changes, for example in CDOM-rich or sediment-rich coastal waters, the OCx or OCI algorithms often fail. In such cases, in addition to using semianalytical algorithms to separate the water constituents explicitly, machine learning empirical approaches such as neural networks (e.g., [32]–[37]) may be developed for regional applications. Indeed, numerous articles have used machine learning approaches to achieve improved retrievals of ocean color variables over other empirical algorithms that have explicit functional forms. Several common machine learning approaches, including multilayer perceptron (MLP), artificial neural network (ANN), and support vector machine (SVM), were used to derive Chl concentrations for Cases I and II waters on global and regional scales [32], [34], [38]–[42]. Similar approaches also performed well for retrieving diffuse attenuation coefficient (K_d) and inherent optical properties (IOPs) for both coastal and open oceanic waters [43]–[45]. Although the governing equations are not explicit in these approaches, the variable dependences of $R_{rs}(\lambda)$ on the different water constituents are taken care of by the internal functions of machine learning. As long as the training data set covers sufficient data range and variable proportions of the water constituents, these approaches appear to work well. However, machine learning approaches on global Chl retrievals have not been attempted, or at least have not been reported in the literature.

Recognizing the strengths and limitations of the three types of empirical approaches [OCx, CI, machine learning] and the lack of a global Chl algorithm based on machine learning, the objective of this article is to develop an optimal machine learning algorithm to estimate Chl for most waters in global oceans. Currently, although OCI is being used by NASA as the default algorithm for multiple sensors because of its tolerance to $R_{rs}(\lambda)$ errors for low-Chl waters and because of its improved cross-sensor consistency over the OCx algorithms, the algorithm switch from low- to higher-Chl waters leads to the question of whether there exists a machine learning approach to combine the advantages of the CI algorithm [for its tolerance to spectrally related $R_{rs}(\lambda)$ noise or errors], the OCx algorithm (for its simple blue/green principle), and the computer intelligence (for its implicit treatment of variable relationships among the water constituents). This article is to explore the various machine learning approaches, from which an optimal one is selected for global applications.

Fig. 1. Relative frequency distributions of Chl for NOMAD data set (training data set for SVR algorithm in this study) and global SeaWiFS images derived from OC4, OCI, and SVR in January and June 2010.

II. DATA AND METHODS

A. Field Data for Algorithm Development: NASA Bio-Optical Marine Algorithm Data Set Version 2

For consistency, the same data set used in previous algorithm developments, namely the NASA bio-Optical Marine Algorithm Data set (NOMAD) (version 2) containing field measured $R_{rs}(\lambda)$ and Chl data [46] (Table I and Fig. 1), was used for algorithm development. These $R_{rs}(\lambda)$ and Chl data were collected by many research groups around the world, and they covered large dynamic ranges and variable oceanic environments, thus forming appropriate data pairs for algorithm development. Most Chl data were determined fluorometrically from water samples, and $R_{rs}(\lambda)$ data have been collected in the field following NASA-recommended Ocean Optics protocols.

B. Algorithm Development

There are different types of machine learning, which have all been considered or tested.

First, deep learning was considered but not tested because 1) only 638 data pairs (i.e., R_{rs} and Chl) from NOMAD could be found and 2) only six bands could be used if a sensor-specific algorithm were to be applied to both SeaWiFS and MODIS (MODIS/Aqua). The limited data volume makes it impractical to involve deep learning.

Second, of other machine learning approaches, several popular approaches have been tested with various R_{rs} input forms (see below). These include Gaussian Process (GP), Random Forest (RF), MLP, and support vector regression (SVR). Through extensive tests, it was found that SVR yielded the best algorithm performance in terms of uncertainty statistics. For reference, results from these approaches are presented in Supplementary Table S1. For illustration purpose,

Fig. 2. Flowchart to show the development of the SVR algorithm and its application to satellite data to derive the Chl data product. For brevity, VIIRS is not included in the flowchart, but was used in the application.

Fig. 2 shows a flowchart of how the SVR algorithm is developed from the NOMAD data, applied to satellite data, and then evaluated within SeaWiFS Bio-optical Archive and Storage System (SeaBASS) data (see Section II-C).

Finally, the optimal way on how to use $R_{rs}(\lambda)$ as the SVR model inputs was determined from trial and error. Originally, $R_{rs}(\lambda)$ values at 443, 490, 555, and 670 nm were as the inputs, yet the performance was not satisfactory (Supplementary Table S2). Then, various forms of $R_{rs}(\lambda)$ band combinations were tried, including band ratios and band differences (e.g., CI defined in [14]). After extensive tests, it was determined that the following R_{rs} combinations would yield the best algorithm performance, therefore used to train the SVR algorithm used in this study to derive global Chl maps

$$\begin{aligned} & (R_{rs}(490) - R_{rs}(443)) / (490 - 443) \\ & (R_{rs}(555) - R_{rs}(510)) / (555 - 510) \\ & R_{rs}(555) - (R_{rs}(670) - R_{rs}(443)) * (555 - 443) / (670 - 443) \\ & R_{rs}(555) - (R_{rs}(670) - R_{rs}(490)) * (555 - 490) / (670 - 490). \end{aligned}$$

Note that the first group defines the spectral slope at 490 and 555 nm, respectively, while the second group defines the spectral curvature at 555 nm relative to the two neighboring wavelengths. In particular, the first curvature (i.e., relative to 443 and 670 nm) is defined by Hu *et al.* [14] as the CI, which was used to estimate clear-water Chl through nonlinear regression. In the algorithm testing and evaluation, the kernel function of SVR was selected to be the radial basis function (RBF). There are two main reasons behind this choice. One is that the RBF kernel function required relatively fewer preassigned parameters than other kernel functions, which also performed generally well with relatively a small data set (i.e., 638 pairs of R_{rs} and Chl from the NOMAD data set). Two is that the RBF kernel function led to a better performance than those from the linear, polynomial, and sigmoid kernel functions.

Because Chl distribution in nature tends to be log normal [47] for either the NOMAD data set or satellite-derived global Chl data (see Fig. 1), it is natural to perform the model training using log-transformed Chl (i.e., $\text{Chl}_{\log}$) instead of Chl. However, the analysis of the correlation between various R_{rs} combinations and $\text{Chl}_{\log}$ indicated higher correlation with

$1/\text{Chl}_{\log}$ than with $\text{Chl}_{\log}$. Then, $1/\text{Chl}_{\log}$ was used as the dependent variable to train the SVR model. To avoid infinite $1/\text{Chl}_{\log}$ when Chl approaches 1.0 mg m^{-3} , the range of the log-transformed Chl was used to “normalize” $1/\text{Chl}_{\log}$ as

$$\text{Chl}'_{\log} = 1 / (\text{Chl}_{\log} + \text{Chl}_{\log, \max}^{\text{Train}} - \text{Chl}_{\log, \min}^{\text{Train}})$$

where $\text{Chl}_{\log}$ is the log-transformed Chl, and $\text{Chl}_{\log, \max}^{\text{Train}}$ and $\text{Chl}_{\log, \min}^{\text{Train}}$ are the maximum and minimum log-transformed Chl in the training data set. In order to improve the SVR performance, $\text{Chl}'_{\log}$ was further normalized as

$$\text{Chl}''_{\log} = \frac{\text{Chl}'_{\log} - \mu}{\sigma}$$

where μ and σ are the mean and standard deviation of the log-transformed Chl, respectively. In the SVR training, the data pairs of $\text{Chl}''_{\log}$ and its corresponding spectral R_{rs} were used. In application of the trained SVR algorithm to satellite-derived spectral R_{rs} , the output was $\text{Chl}''_{\log}$, which was converted to Chl using the above equations.

The training used wavelengths of 443, 490, 555, and 670 nm because most ocean color sensors have these four bands. When the wavelengths of a specific sensor are slightly different from the above (e.g., MODIS band is at 547 instead of 555 nm), a conversion factor, based on field measured R_{rs} from the NOMAD data set, is applied to satellite-retrieved R_{rs} to convert to one of the four wavelengths above. Such a conversion follows the same approach of [14], which is also currently used as the standard practice in the NASA software package SeaDAS (Jeremy Werdell, NASA GSFC, personal communication). Comparison between sensor-specific SVR algorithms and such a “unified” algorithm indicated that although the former led to slightly lower uncertainties (see below), the latter led to much better cross-sensor consistency, therefore was selected in this study.

To put the SVR algorithm in the context of the mainstream algorithms, two other algorithms are used here as the references. One is the traditional blue/green band ratio algorithm [31], with recent updates by O'Reilly and Werdell [12]. The algorithm estimates Chl from R_{rs} ratios between blue bands and a green band. For SeaWiFS, the algorithm takes the form of

$$\begin{aligned} R &= \max(R_{rs, 443}, R_{rs, 490}, R_{rs, 510}) / R_{rs, 555} \\ \chi &= \log_{10}(R) \\ y &= a_0 + a_1 \cdot \chi + a_2 \cdot \chi^2 + a_3 \cdot \chi^3 + a_4 \cdot \chi^4 \\ \text{Chl} &= 10^y. \end{aligned} \quad (1)$$

In the above equations, a_0 – a_4 are the algorithm coefficients determined through nonlinear regression between field-measured Chl and R_{rs} in the NOMAD data set. In the version 6 algorithm (OC4v6), the regression coefficients are a_0 – $a_4 = 0.3272, -2.9940, 2.7218, -1.2259, \text{ and } -0.5683$, respectively. Because of a lack of the 510-nm band, MODIS uses 443, 488, and 547 nm to form a similar OC3v6 algorithm with coefficients determined using the same approach. Collectively, they are called OCx algorithms.

Another algorithm is the OCI algorithm [14], which is a hybrid between the OCx algorithm and a CI algorithm. The CI algorithm takes the following form:

$$CI = R_{rs,555} - [R_{rs,443} + (555 - 443)/(670 - 443) \times (R_{rs,670} - R_{rs,443})]$$

$$\text{Log}_{10}(\text{Chl}) = a_0 + a_1 \times CI \quad [\text{for } CI \leq -0.0005]. \quad (2)$$

In the above equation, a_0 and a_1 are the algorithm coefficients determined through nonlinear regression between field-measured Chl and R_{rs} in the NOMAD data set. In [14], they were determined to be $a_0 = -0.4909$ and $a_1 = 191.6590$. The CI algorithm is only applicable for clear waters ($\text{Chl} < 0.25 \text{ mg m}^{-3}$). The OCx algorithm is used for more productive waters ($\text{Chl} > 0.4 \text{ mg m}^{-3}$) when applied to satellite data processing. For intermediate Chl (between 0.25 and 0.4), a weighted average is used. Collectively, the algorithm is termed as OCI.

C. Algorithm Evaluation: SeaBASS and Satellite Data

All algorithms were evaluated using the same data sets, from both *in situ* and satellite measurements. As in previous works [13], [14], the field-collected Chl data available from the NASA SeaBASS ([48], Table I) were used to evaluate the satellite-derived Chl, where the latter was obtained after applying the Chl algorithms to the satellite-derived $R_{rs}(\lambda)$. The flowchart in Fig. 2 shows how SeaDASS data are used to evaluate the algorithm performance after application to satellite data.

Following the community standard, the following NASA recommended criteria, were used to find the satellite-*in situ* matching pairs: sensor zenith angle $< 56^\circ$; solar zenith angle $< 70^\circ$; bathymetry $> 30 \text{ m}$; $< 3\text{-h}$ time difference between *in situ* and satellite measurements; median value of coefficients of variation (CV, calculated as standard deviation divided by mean) of several products (R_{rs} of 412–555 nm, aerosol optical thickness at 865 nm) $< 15\%$ for the 5×5 -pixel window centered at the *in situ* station; difference between simulated and measured surface irradiance $< 100\%$; and $> 50\%$ pixels in the 5×5 box must be valid (i.e., not associated with any of the standard quality-control flags such as stray light, high glint, and so on) [49]. A total of 1145 matching pairs were obtained for SeaWiFS between 1998 and 2010, and 331 matching pairs were obtained for MODIS Aqua between 2002 and 2010, respectively. These are basically the same data sets as used in [13] and [14].

From the matching pairs, several statistical measures were used to gauge the similarity (or difference) between the satellite (y'_i) and *in situ* (y_i) Chl data, among which are

Median absolute difference (MRD)

$$= 10 \left(\frac{1}{n} \sum_{i=1}^n |\log y'_i - \log y_i| \right)$$

$$\text{Bias} = 10 \left(\frac{1}{n} \sum_{i=1}^n (\log y'_i - \log y_i) \right)$$

Mean relative difference (MRD)

$$= \frac{1}{n} \sum_{i=1}^n \left| \frac{y'_i - y_i}{y_i} \right|$$

Root-mean-square difference (RMSD)

$$= \sqrt{\frac{1}{n} \sum_{i=1}^n \left(\frac{y'_i - y_i}{y_i} \right)^2}$$

Unbiased MRD (UMRD)

$$= \frac{1}{n} \sum_{i=1}^n \left| \frac{2(y'_i - y_i)}{y'_i + y_i} \right|$$

Unbiased RMSD (URMSD)

$$= \sqrt{\frac{1}{n} \sum_{i=1}^n \left(\frac{2(y'_i - y_i)}{y'_i + y_i} \right)^2}$$

$$\text{Mean ratio} = \frac{1}{n} \sum_{i=1}^n \frac{y'_i}{y_i}$$

$$\text{Median ratio} = \text{median} \left(\frac{y'_i}{y_i} \right).$$

In the current literature, various forms of the above statistical measures have been used to gauge algorithm performance. The use of all these forms is to put our results in the context of the published works. Also note that we use the term “difference” (D) instead of “error” (E) in these statistical measures because *in situ* data also contain some degrees of uncertainties. The use of the “unbiased” terms is to account for the fact that even though *in situ* measurements are usually considered as the “truth,” these measurements in reality may also contain large uncertainties. When the *in situ* Chl are very small and are biased low, the use of them in the denominator may yield unrealistic large error terms. Therefore, instead of having the *in situ* data in the denominator, the satellite data are also used in the denominator in the “unbiased” measures above. For the same reason, the statistical measures are termed as “differences” rather than “errors.”

In addition to algorithm evaluations using satellite-*in situ* matching pairs, the algorithms were also evaluated in their ability to yield consistent data products from two different sensors (e.g., SeaWiFS versus MODISA and MODISA versus VIIRS), and in their tolerance to noise. In the cross-sensor consistency evaluation, global daily R_{rs} data at 9-km resolution from the three sensors for selected months were obtained from the NASA GSFC (<https://oceancolor.gsfc.nasa.gov>, data accessed in June 2018). The SVR algorithm was applied to the global daily R_{rs} data from each of the three sensors to estimate global daily Chl distributions, and compare with the global Chl data derived from the OCI and OCx algorithms. The global daily Chl distributions from the three algorithms (SVR, OCI, and OCx) and three sensors were then used to estimate monthly Chl distributions. In the noise tolerance evaluation, daily snapshot data of selected data granules over ocean gyres were obtained, where Chl distributions were derived in a similar fashion as above. Then, the snapshot Chl images were first inspected visually, and then analyzed for image noise following the approach of [14]. The assumption behind the noise evaluation is simple: in an ocean gyre away from major nutrient sources, Chl should be stable in both space and time (i.e., minimal pixel-to-pixel variations and day-to-day variations). Then, the standard deviation of

TABLE II
EVALUATION OF SeaWiFS-DERIVED CHL USING SeaBASS *In Situ* CHL AND THREE ALGORITHMS: OC4, SVR (THIS STUDY), AND OCI.
NOTE THAT OCI SWITCHES TO CI FOR CHL < 0.25 mg m⁻³. GRAPHICAL FORM IS PRESENTED IN FIGS. 3 AND 4

	SVR	OC4	OCI	<i>in-situ</i> Chl < 1 mg/m ³			<i>in-situ</i> Chl < 0.25 mg/m ³		
				SVR	OC4	OCI	SVR	OC4	OCI
MAD	1.57	1.59	1.59	1.51	1.54	1.54	1.53	1.55	1.46
Bias	0.95	0.97	0.96	1.15	1.15	1.13	1.24	1.29	1.24
MRD	51.9%	56.8%	56.2%	59.2%	66.2%	65.2%	75.2%	87.4%	53.1%
RMSD	173.7%	261.3%	260.7%	211.8%	321.0%	320.3%	299.7%	459.2%	90.7%
UMRD	42.1%	42.6%	42.9%	39.2%	40.5%	40.8%	39.5%	40.5%	36.3%
URMSD	54.2%	55.2%	55.3%	50.0%	51.8%	51.8%	52.0%	53.3%	46.6%
Mean ratio	1.17	1.24	1.22	1.38	1.45	1.43	1.58	1.72	1.39
Median ratio	0.96	1.00	1.00	1.14	1.15	1.15	1.12	1.15	1.16
R ² linear	0.51	0.49	0.49	0.48	0.34	0.34	0.05	0.02	0.32
R ² log	0.79	0.78	0.78	0.70	0.67	0.67	0.36	0.34	0.40
N	1145	1145	1145	748	748	748	357	357	357

Fig. 3. Evaluation of SeaWiFS-derived Chl using SeaBASS *in situ* Chl and three algorithms: OC4, SVR (this study), and OCI. (a) Visual comparison between OC4 and SVR. (b) Visual comparison between OCI and SVR. Algorithm performance statistics are listed in Table II.

a 3×3 pixel window is regarded as the noise, whose magnitude is referenced against the mean value of the 3×3 pixel window. This calculation was repeated for each 3×3 pixel window in the individual images, with results partitioned according to the mean Chl values of the 3×3 pixel windows.

III. RESULTS

A. Algorithm Performance Evaluation With Field Data

1) *SeaWiFS*: Table II shows the statistical measures of the SVR algorithm when applied to SeaWiFS R_{rs} data, when the concurrent and collocated field-measured Chl were used as the reference for the evaluation (see Section II-C). The graphical forms of the evaluation are presented in Fig. 3 for the entire data set and Fig. 4 for the major oceans. In Table II, the statistical measures are listed separately for the 1) entire data set; 2) data with Chl < 1 mg m⁻³; and 3) data with Chl < 0.25 mg m⁻³. For comparison, the performance of the

OCx and OCI algorithms is also presented in Table II and Figs. 3 and 4.

From Table II, when all data are used in the evaluation, the SVR algorithm shows slightly better performance than OCx and OCI, as indicated by all but the “median ratio” statistical measures. When the data are restricted to Chl < 1 mg m⁻³, the improvement of SVR over OCx and OCI appears to increase, but the increase is small. When the data are restricted to Chl < 0.25 mg m⁻³ (for this range, the OCI algorithm switches to the CI algorithm), SVR performance is still better than OCx, but worse than OCI (except for the median ratio values).

The algorithm differences can also be examined graphically in Fig. 3(a) for SVR versus OCx and in Fig. 3(b) for SVR versus OCI. In Fig. 3(a), SVR resulted in a narrower data spread around the 1:1 line when compared with OCx, especially for those extreme outliers. However, for Chl > 2 mg m⁻³, SVR Chl is biased low and the bias appears to be more

Fig. 4. Same as Fig. 3, but only SeaWiFS SVR Chl is compared with SeaDAS *in situ* Chl here, with data partitioned to the Atlantic Ocean, Pacific Ocean, Southern Ocean, and Indian Ocean, respectively.

severe than OCx. In Fig. 3(b), the data spread in SVR Chl is lower than in OCI for $\text{Chl} > 1 \text{ mg m}^{-3}$ but the difference for $\text{Chl} < 0.25 \text{ mg m}^{-3}$ is not clear. The visual inspection results are consistent with those listed in Table II.

Similar to other empirical algorithms, the performance of the SVR algorithm may be different across major ocean basins (see Fig. 4). This effect has been demonstrated for the OCx algorithm in [17] and for the OCI algorithm in [50], as a result of different proportions of CDOM and detrital particles relative to phytoplankton pigment absorption in different oceans. For extremely clear waters ($< 0.1 \text{ mg m}^{-3}$) in the Pacific, the SVR Chl may be biased low [see Fig. 4(b)], but for most waters in the Indian Ocean, the SVR Chl may be biased high [see Fig. 4(d)]. However, the number of matching pairs under these circumstances is too low to make a solid conclusion, suggesting the necessity of collecting more field data in these regions.

2) *MODISA*: The same observations from SeaWiFS can be extended to MODISA for the three algorithms. From all statistical measures, Table III shows that the

SVR algorithm performs better than OCx and OCI for either all data or data restricted to $\text{Chl} < 1 \text{ mg m}^{-3}$. For data with $\text{Chl} < 0.25 \text{ mg m}^{-3}$, SVR performance is still better than OCx, but becomes worse than OCI.

The graphical form of these algorithm comparisons in Fig. 5 reveals the performance difference visually. For most data range, SVR resulted in a tighter relationship than OCx and OCI between MODISA Chl and *in situ* Chl. Only when Chl is $< 0.25 \text{ m}^{-3}$ does SVR appear to be slightly worse than OCI. Similar to the SeaWiFS evaluation results, the MODISA results suggest that when Chl is $> 2 \text{ mg m}^{-3}$, SVR Chl appears to be biased low.

When partitioned to different major ocean basins, the SVR shows similar performance for MODISA (see Fig. 6) as for SeaWiFS (see Fig. 4). For extremely clear waters ($< 0.1 \text{ mg m}^{-3}$) in the Pacific the SVR Chl appears to be biased low [see Fig. 6(b)], but for the Indian Ocean the SVR Chl appears to be biased high [see Fig. 6(d)]. However, there are only four matching pairs for the former and two matching pairs for the latter, making these observations statistically

TABLE III
EVALUATION OF MODISA-DERIVED CHL USING SEABASS *In Situ* CHL AND THREE ALGORITHMS: OC4, SVR (THIS STUDY), AND OCI.
NOTE THAT OCI SWITCHES TO CI FOR CHL < 0.25 mg m⁻³. GRAPHICAL FORM IS PRESENTED IN FIGS. 5 AND 6

	SVR	OC3	OCI	<i>in-situ</i> Chl < 1 mg/m ³			<i>in-situ</i> Chl < 0.25 mg/m ³		
				SVR	OC3	OCI	SVR	OC3	OCI
MAD	1.52	1.62	1.62	1.43	1.61	1.62	1.35	1.41	1.32
Bias	0.98	1.16	1.18	1.23	1.35	1.38	1.19	1.21	1.19
MRD	43.4%	67.3%	68.8%	46.8%	77.9%	80.2%	40.5%	47.0%	34.6%
RMSD	63.5%	159.1%	161.3%	71.5%	188.6%	191.5%	68.5%	81.2%	50.9%
UMRD	39.6%	44.6%	44.7%	34.4%	44.7%	44.8%	29.1%	32.9%	27.0%
URMSD	51.7%	57.1%	57.4%	44.0%	56.2%	56.5%	39.5%	44.3%	35.0%
Mean ratio	1.14	1.44	1.46	1.35	1.64	1.67	1.30	1.35	1.26
Median ratio	1.04	1.18	1.18	1.20	1.32	1.33	1.11	1.14	1.10
R^2 linear	0.40	0.37	0.37	0.57	0.13	0.13	0.52	0.42	0.63
R^2 log	0.78	0.75	0.75	0.75	0.74	0.74	0.71	0.65	0.71
N	331	331	331	212	212	221	63	63	63

Fig. 5. Evaluation of MODISA-derived Chl using SeaBASS *in situ* Chl and three algorithms: OC3, SVR (this study), and OCI. (a) Visual comparison between OC3 and SVR. (b) Visual comparison between OCI and SVR. Algorithm performance statistics are listed in Table III.

meaningless. Therefore, to make a solid conclusion, more field data are required for these regions.

Overall, the algorithm evaluations of both SeaWiFS and MODISA data yielded consistent results. These results suggest that for most waters (<1–2 mg m⁻³) SVR may yield slightly more accurate Chl retrievals than both OCx and OCI, but for clear waters (<0.25 mg m⁻³) SVR may yield slightly worse retrievals than OCI.

B. Algorithm Performance Evaluation Without Field Data

1) *Individual Sensors*: Regardless of how much field data is available, they may never be enough to evaluate satellite data as a whole. This is because the global oceans are not sampled proportionally in either time or space, and each point in the field-based evaluation may carry a different weight when ocean waters corresponding to the point are considered in global validations. Such a mismatch between field data distributions and satellite data distributions is clearly shown

in Fig. 1. Consequently, a perfect match between field and satellite data (i.e., no bias, mean ratio = 1.0, very low RMSD values) may actually lead to much higher uncertainties when global satellite data are used for the same evaluation. Vice versa is also true—a poor performance in field-based evaluation does not necessarily lead to bad performance when global satellite data are used. Furthermore, cross-sensor consistency and image artifacts are difficult to reveal in field-based evaluations, making it necessary to evaluate algorithms using global satellite images.

Fig. 7 shows the mean SeaWiFS global Chl distributions in January and June 2010 derived from the OCx, OCI, and SVR algorithms. Their spatial patterns are very similar, with all major oceanographic features (equatorial upwelling, ocean gyres, high Chl in high-latitude seas, and coastal waters) revealed clearly. These results suggest that while slight differences exist in the algorithms when field data are used in the evaluations (Table II and Figs. 3–4), such differences are

Fig. 6. Same as Fig. 5, but only MODISA SVR Chl is compared with SeaDAS *in situ* Chl here, with data partitioned to the Atlantic Ocean, Pacific Ocean, Southern Ocean, and Indian Ocean, respectively.

difficult to visualize when examining large-scale Chl patterns, indicating that they may perform equally well.

Global means may hide some subtle differences due to, for example, image noise or small artifacts that can only be revealed in snapshot daily images. Fig. 8 shows an example of such cases, where image noise and other artifacts are clearly visible in the OCx Chl image, but not as apparent in the OCI or SVR Chl image. Although the ability of SVR in revealing the ocean eddy features and other small patterns is not as good as the OCI, its improvement over OCx is significant. Such a tolerance to noise has significant impact on not only image quality, but also on data product consistency across different sensors, as revealed below.

Similar to the SeaWiFS observations, MODISA global monthly mean Chl data products show similar distributions from the three algorithms (see Fig. 9). All major features, including equatorial upwelling, ocean gyres, and high-latitude productive waters, are revealed clearly in all three products for both winter (January 2010) and summer (June 2010).

When evaluated using daily snapshot images, both OCI and SVR show significant noise reduction over the OCx algorithm, especially near clouds and sun glint (see Fig. 10).

The noise reduction from the SVR algorithm is quantified from SeaWiFS and MODISA measurements over ocean gyres, in reference against the OCx algorithm and OCI algorithm (see Fig. 11). For simplicity, the errors are termed as “pixelization” errors or speckling noises. Fig. 11(a) shows that for SeaWiFS measurements, pixelization errors for Chl $< 0.1 \text{ mg m}^{-3}$ are $> 10\%$ from the OCx algorithm, which also increase sharply with decreasing Chl. In contrast, both SVR and OCI show much reduced pixelization errors, usually $< 5\%$. Furthermore, both algorithms show relatively stable errors independent of Chl values. For Chl $> 0.2 \text{ mg m}^{-3}$, all these algorithms approach 7% pixelization errors. Because $\sim 38\%$ of the global oceans have Chl $< 0.1 \text{ mg m}^{-3}$ according to SeaWiFS statistics, the reduction in pixelization error appears to be significant. Similar observations are obtained from MODISA images [see Fig. 11(b)]. Although pixelization errors from the

Fig. 7. SeaWiFS global Chl distributions in (a), (c), and (e) January 2010 and (b), (d), and (f) June 2010 derived from three algorithms: (a) and (b) OC4, (c) and (d) OCI, and (e) and (f) SVR.

Fig. 8. Comparison between SeaWiFS Level-2 Chl distribution off the U.S. east coast on June 1, 2004, derived from three algorithms: (a) OC4, (b) OCI, and (c) SVR. The images cover a region of 28.5° – 36.5° N and 76.5° – 70.5° W, the same region used in [14] when the OCI algorithm was proposed. The Level-2 quality control flags were turned off to show the eddy features.

MODISA data are much reduced from SeaWiFS data in all three algorithms due to significantly improved signal-to-noise ratios of the MODISA sensor over SeaWiFS [51], the trend among the three algorithms is the same: for $\text{Chl} < 0.1 \text{ mg m}^{-3}$, OCx algorithm leads to much higher pixelization errors than the OCI and SVR algorithms, while all three algorithms approach the same value of 4% for $\text{Chl} > 0.2 \text{ mg m}^{-3}$.

2) *Cross-Sensor Consistency*: The SVR algorithm tolerance to noise is also revealed from simulations, where different levels of noise (0%, 5%, 10%, and 15%) were added to the

input R_{rs} . Results in Supplementary Table S3 indicate that the algorithm performance is similar at different noise levels, suggesting the tolerance of the SVR algorithm to input R_{rs} noise.

For long-term studies of ocean changes in response to climate variability or human activities, cross-sensor consistency is perhaps more important than data product accuracy, as most sensors are designed to have a five-year mission life, and multidecadal data from multiple sensors are therefore required to observe long-term changes. Indeed, one of the

Fig. 9. MODISA global Chl distributions in (a), (c), and (e) January 2010 and (b), (d), and (f) June 2010 derived from three algorithms: (a) and (b) OC3, (c) and (d) OCI, and (e) and (f) SVR.

Fig. 10. Comparison between MODISA Level-2 Chl distribution in the South Pacific gyre (approximately 2200×440 km centered at 25.2°S , 110.8°W) on (a)–(c) March 4, 2003, and (d)–(f) July 27, 2003, derived from three algorithms: (a) and (d) OC3, (b) and (e) OCI, and (c) and (f) SVR. The Level-2 quality control flags were turned off to show color features and noise.

significant advantages of the OCI algorithm over the OCx algorithm is its ability to bring multiple sensors much closer for low-Chl waters [13], [14]. Figs. 12 and 13 show that the SVR algorithm has similar advantage to assure cross-sensor consistency.

In Fig. 12, global distributions of Chl ratios between SeaWiFS and MODISA are illustrated, where Chl was derived from both OCI and SVR algorithms (for brevity, results from the OCx algorithms are not shown here as they show worse cross-sensor consistency, see [14]). For each algorithm,

Fig. 11. Pixelization noise, estimated as the average ratio between the rms Chl and mean Chl of 3×3 pixels for each Chl range from multiple (a) SeaWiFS images and (b) MODISA images. The total number of pixels for each Chl range is also plotted (red colored, right y-axis). The results indicate that both OCI and SVR yielded much “cleaner” images than OCx for oligotrophic oceans ($\text{Chl} < 0.1 \text{ mg m}^{-3}$).

there are differences between SeaWiFS and MODISA Chl, and these differences appear to be spatially coherent. For example, Fig. 12(a) from the OCI algorithm shows the ratios of < 1.0 in the northern hemisphere gyre but > 1.0 in the southern hemisphere gyre in January 2010, while Fig. 12(c) from the SVR algorithm for the same month shows the ratios of < 1.0 in the gyres of both hemispheres. However, these differences are mostly small (within -10% to 10% , or the ratio is between 0.9 and 1.1). When viewed in data histogram statistics (Fig. 12, bottom panels), similar consistency is obtained between SeaWiFS and MODISA Chl from both OCI and SVR algorithms. However, for the same sensor, there are noticeable differences between the algorithms. For example, for January 2010, there is only one mode in the histogram ($\sim 0.12 \text{ mg m}^{-3}$) from the OCI algorithm, but there appear two modes (~ 0.07 and 0.15 mg m^{-3}) from the SVR algorithm. For this analysis, it is impossible to determine which algorithm is closer to the “truth” due to lack of sufficient field data.

Similar cross-sensor consistency is obtained between VIIRS and MODISA from both OCI and SVR algorithms (see Fig. 13). From each algorithm, although there are some spatially coherent differences between the two sensors, these differences are mostly small (within -10% to 10% , or the ratio is between 0.9 and 1.1). Data statistics shown in the histograms (Fig. 13, bottom panels) also suggest cross-sensor consistency when either OCI or SVR algorithm is applied to the two

sensors. Although the data statistics are pulled from a different year (2012) for VIIRS/MODISA than in Fig. 12 (2010) for SeaWiFS/MODISA, the histogram patterns for either January or June are similar in different years, indicating temporal stability of the algorithms.

IV. DISCUSSION

A. Unified Algorithm or Sensor-Specific Algorithm?

In the past, because of the different band settings among sensors, sensor-specific algorithms have been developed to account for the differences in the number of bands, band-center wavelengths, and band passes. For example, SeaWiFS used a four-band band-ratio (OC4) algorithm but MODISA and VIIRS used a three-band band-ratio (OC3) algorithm. The most recent effort by O'Reilly and Werdell [12] further developed this concept to five-band (OC5) and six-band (OC6) band-ratio algorithms, with improved performance over the original OC4 or OC3 algorithms.

The question is why not use all six SeaWiFS bands and six MODISA bands to develop sensor-specific SVR algorithms here. After all, the sensor-unique bands (i.e., 510 nm on SeaWiFS and 531 nm on MODISA) may carry independent information from other bands, and the inclusion of the 412-nm band may account for some of the variability induced by CDOM. Indeed, our initial attempt was to use all bands from individual sensors to develop sensor-specific SVR algorithms, which did lead to slightly better performance over the sensor-independent (i.e., unified) SVR algorithm (Supplementary Tables S4 and S5 and Supplementary Figs. S1 and S2). However, two problems were encountered.

First, after the addition of the 412-nm band, although statistical measures were improved when field data were used to evaluate the algorithm performance, the algorithm generated unrealistic spatial patterns in the South Pacific and South Atlantic Gyres (Chl values are unrealistically high) when applied to SeaWiFS global data. Although the reasons are still not fully understood, we speculate that it is because most NOMAD data points are from the northern hemisphere, and lack of training data in the southern gyres may confuse the SVR algorithm when applied to these gyres because CDOM proportion in total absorption is different between the two hemispheres [50]. Second, even without the use of the 412-nm band, when the 510-nm band was used to develop a SeaWiFS-specific SVR algorithm and the 531-nm band was used to develop a MODISA-specific SVR algorithm, it is impossible to achieve similar cross-sensor consistency as shown in Fig. 12. Supplementary Fig. S3 shows the comparison between sensor-specific SVR and sensor-independent SVR for their cross-sensor consistency between SeaWiFS and MODISA. For most oceans (e.g., the Southern Ocean and Equatorial zones), the departure from 1.0 is more severe from the sensor-specific SVR, which further justifies the use of a sensor-independent (i.e., unified) SVR in this study. Similar to the SeaWiFS 510-nm and MODISA 531-nm bands, MODISA is equipped with a unique 678 nm to estimate solar stimulated fluorescence that is useful to assess phytoplankton physiology in open ocean waters [52] and Chl in optically complex coastal

Fig. 12. Evaluation of cross-sensor consistency between SeaWiFS and MODISA using the OCI algorithm and SVR algorithm. (a) and (b) Ratio of MODISA/SeaWiFS OCI Chl for January and June 2010, respectively. (c) and (d) Ratio of MODISA/SeaWiFS SVR Chl for January and June 2010, respectively. A ratio of 1.0 indicates perfect consistency. The bottom panels show their histogram distributions. Chl data were derived from the 9-km daily global R_{rs} data using the two algorithms.

waters [53]. However, the problem with this band is that it is very easy to saturate [51, Fig. 2(b)] or get contaminated by straylight, leading to 33% reduced data as compared with Chl ([54, Fig. 1] 3.29% for fluorescence line height (nFLH) versus 4.91% for Chl).

Therefore, with a slight tradeoff, only four common bands (443, 490, 555, and 670 nm) were used to develop a unified, sensor-independent SVR algorithm, which shows significant advantage in cross-sensor consistency when compared with a

sensor-specific approach. In the unified approach, the slight differences in band centers and band passes across different sensors are taken care of by converting the satellite-retrieved R_{rs} to these wavelengths, and such conversions are currently available in NASA's software package (SeaDAS) [Jeremy Werdell, NASA/Ocean Biology Processing Group (OBPG), personal communication], which are also applied to the sensor-independent OCI algorithm as the default option by NASA.

Fig. 13. Evaluation of cross-sensor consistency between VIIRS and MODISA using the OCI algorithm and SVR algorithm. (a) and (b) Ratio of MODISA/VIIRS OCI Chl for January and June 2010, respectively. (c) and (d) Ratio of MODISA/VIIRS SVR Chl for January and June 2010, respectively. A ratio of 1.0 indicates perfect consistency. The bottom panels show their histogram distributions. Chl data were derived from the 9-km daily global R_{rs} data using the two algorithms.

B. Algorithm Applicability

Because SVR by nature is still an empirical algorithm, all pros and cons of empirical algorithms are applicable to the SVR algorithm developed here. Specifically, the algorithm is only applicable to the same data range and environmental conditions that were used in the algorithm training. In particular, unlike the band-ratio or band-subtraction algorithms (OCx and OCI) where the functional forms between Chl and R_{rs} are

explicit and physically meaningful (e.g., blue–green band ratio increases with decreasing Chl in a monotonic way), the SVR algorithm does not have an explicit function form. Therefore, greater caution should be paid to regions where Chl values are either outside the training data range or collected under different conditions (e.g., under moderate sun glint), as these regions may show unexpected errors. This is also why in addition to field-based evaluations, image-based evaluations

TABLE IV
COMPARISON OF ALGORITHM PERFORMANCE BETWEEN SVR (THIS STUDY) AND THE MOST RECENT BAND-RATIO ALGORITHMS (OC5 AND OC6 [12]) USING CONCURRENT SEAWIFS AND SEABASS DATA. HERE, THE OC5 AND OC6 ALGORITHM COEFFICIENTS ARE APPLIED TO SEAWIFS R_{rs} DATA TO ESTIMATE CHL

	SVR	OC5	OC6	<i>in-situ</i> Chl < 1 mg/m ³			<i>in-situ</i> Chl < 0.25 mg/m ³		
				SVR	OC5	OC6	SVR	OC5	OC6
MAD	1.57	1.62	1.63	1.51	1.58	1.58	1.53	1.60	1.62
Bias	0.95	0.96	0.97	1.15	1.14	1.18	1.24	1.25	1.30
MRD	51.9%	59.6%	57.5%	59.2%	69.7%	67.5%	75.2%	92.9%	87.6%
RMSD	173.7%	292.8%	189.9%	211.8%	360.0%	232.1%	299.7%	515.9%	328.1%
UMRD	42.1%	44.3%	44.7%	39.2%	42.6%	43.1%	39.5%	43.3%	44.5%
URMSD	54.2%	56.9%	56.9%	50.0%	53.6%	54.0%	52.0%	55.3%	57.1%
Mean ratio	1.17	1.25	1.2	1.38	1.46	1.46	1.58	1.74	1.70
Med ratio	0.96	1.01	1.00	1.14	1.16	1.19	1.12	1.15	1.16
R^2 linear	0.51	0.47	0.50	0.48	0.30	0.44	0.05	0.02	0.05
R^2 log	0.79	0.76	0.76	0.70	0.66	0.66	0.36	0.33	0.31
<i>N</i>	1145	1145	1145	748	748	748	357	357	357

are performed here. To determine whether and where there might be data points from satellite measurements outside the algorithm training range, $R_{rs}(\lambda)$ statistics from both SeaWiFS and MODISA measurements were analyzed in their spectral slopes and curvatures (Supplementary Figs. S4 and S5) and band ratios (Supplementary Figs. S6 and S7) for the SVR algorithm and OC x algorithm, respectively. The statistics were used to compare with the $R_{rs}(\lambda)$ statistics used in the algorithm trainings (i.e., NOMAD data). Supplementary Fig. S4 shows that, for the SVR algorithm, there are indeed satellite data points outside the algorithm training range, and these data are mostly located in ocean gyres (extremely clear waters) with some scattered points near land (extremely turbid waters) (Supplementary Fig. S5). Likewise, Supplementary Fig. S6 shows that, for the OC x algorithm, there are also satellite data points outside the algorithm training range, and these data are also located in ocean gyres or near land (Supplementary Fig. S7).

Chl data statistics and histograms suggest that, for the clearest ocean gyres where Chl is $< \sim 0.02$ mg m⁻³ (Supplementary Fig. S5), even though nearly no NOMAD data point used in the SVR training is in this Chl range, the SVR algorithm still yielded reasonable and consistent results among different sensors, suggesting that the SVR algorithm may be applicable to even the clearest waters in the ocean. For the same reason, the same can be said for the OC x algorithm (Supplementary Fig. S7).

On the other hand, field-based algorithm evaluations suggest that the SVR algorithm may yield negatively biased Chl for Chl > 1.0 mg m⁻³. This is possibly due to lack of sufficient data points in the algorithm training. Although there appear many data points in this range from the NOMAD data (see Fig. 1), they come from different coastal waters with different optical complexity (e.g., dominated by CDOM absorption or particle scattering), thus may not be sufficient to represent global coastal waters. This reason can also explain the relative large difference between SVR and OCI Chl in several marginal seas such as the Arabian Sea and the Sea of Okhotsk. Without sufficient field data to evaluate algorithm in these regions, it is currently difficult to verify which

algorithm is better. However, considering that 1) 96% of the global oceans have Chl < 1.0 mg m⁻³ according to SeaWiFS data statistics, 2) cross-sensor consistency is not affected by the negative bias, and 3) nearly all empirical algorithms for waters with Chl > 1.0 mg m⁻³ require local algorithm tuning anyway (e.g., [29], [30], [55]–[59]), this shortcoming may not represent a significant drawback on the algorithm applicability. On the other hand, both empirical and semi-analytical algorithms using the red and near infrared (NIR) bands have been developed to specifically target turbid coastal waters for Chl estimates [56]–[59], suggesting that for waters with Chl > 1 mg m⁻³ where the SVR algorithm performs poorly, localized approaches should be developed. Indeed, the improvement of algorithm performance from band-ratio OC x to SVR does not appear to be algorithm specific, but may be conceptual. For example, even after algorithm tuning using other bands, the most recent algorithm updates in the band-ratio approach [12] did not result in lower uncertainties than the SVR algorithm developed here. Tables IV and V show the comparison of algorithm performance between SVR and OC5 and OC6 using common SeaBASS and satellite data. The OC5 and OC6 Chl values were derived after applying the algorithms (together with their parameterization) to the satellite-derived $R_{rs}(\lambda)$. It is clear that regardless of the data range (entire data set, < 1 mg m⁻³ or < 0.25 m⁻³), the SVR algorithm always shows the lowest data spread as measured by the MAD, MRD, UMRD, RMSD, and URMSD statistical measures. When measured by the mean ratio and median ratio, the results are mixed. Therefore, considering the additional advantage of the SVR approach in noise reduction, the SVR approach appears to be a feasible way to develop robust empirical algorithms to account for both known and unknown errors, and the current SVR Chl algorithm may serve as an alternative algorithm to the NASA's operational OCI algorithm.

The argument above is reinforced by applications of the SVR approach to other ocean color sensors, for example, MERIS. Results shown in Supplementary Figs. S8–S10 indicate that after appropriate training, the same SVR approach can successfully retrieve Chl over both global and local scales,

TABLE V
COMPARISON OF ALGORITHM PERFORMANCE BETWEEN SVR (THIS STUDY) AND THE MOST RECENT BAND-RATIO ALGORITHMS (OC5 AND OC6 [12]) USING CONCURRENT MODISA AND SEABASS DATA. HERE, THE OC5 AND OC6 ALGORITHM COEFFICIENTS ARE APPLIED TO MODISA R_{rs} DATA TO ESTIMATE CHL

	SVR	OC5	OC6	<i>in-situ</i> Chl < 1 mg/m ³			<i>in-situ</i> Chl < 0.25 mg/m ³		
				SVR	OC5	OC6	SVR	OC5	OC6
MAD	1.52	1.61	1.58	1.43	1.50	1.49	1.35	1.41	1.37
Bias	0.98	0.91	0.95	1.23	1.16	1.20	1.19	1.12	1.14
MRD	43.4%	47.0%	47.1%	46.8%	51.1%	52.0%	40.5%	41.9%	40.7%
RMSD	63.50%	67.4%	69.6%	71.5%	76.1%	79.6%	68.5%	66.9%	70.8%
UMRD	39.55%	44.3%	42.8%	34.4%	39.0%	38.1%	29.1%	32.7%	29.9%
URMSD	51.66%	56.6%	55.1%	44.0%	48.6%	48.3%	39.5%	43.8%	41.4%
Mean ratio	1.14	1.09	1.12	1.35	1.31	1.36	1.30	1.25	1.26
Med ratio	1.04	0.98	0.99	1.20	1.14	1.18	1.11	1.09	1.06
R^2 linear	0.40	0.46	0.52	0.57	0.47	0.49	0.52	0.53	0.50
R^2 log	0.78	0.74	0.75	0.75	0.76	0.77	0.71	0.72	0.71
N	331	331	331	212	212	212	63	63	63

with algorithm performance slightly improved over the OCx band ratio algorithm, especially for Chl < 1 mg m⁻³.

Finally, although SVR shows improved performance over OCx (for Chl < 1.0 mg m⁻³) and OCI (for Chl between 0.25 and 1.0 mg m⁻³), and improved cross-sensor consistency over OCx, there are relatively large differences between the histogram distributions when the algorithm changes from OCI to SVR (see Figs. 12 and 13). Such differences will inevitably lead to changes in global Chl time-series analysis. Actually, there have been several rounds of global data reprocessing (<https://oceancolor.gsfc.nasa.gov/reprocessing/>), and each time an algorithm is changed (e.g., from the earlier OC2 to OC4, and then to the recent OCI), global histograms and basin-wide averages are also changed. The question is which algorithm (OCx, OCI, and SVR) leads to more accurate results in time-series analysis and what are the implications on studies of climate variability when global processing switches from one algorithm to another. We feel that the question can be addressed with the following considerations.

One, statistics from field-data validations indicate that new algorithms are always more accurate than old ones (see tables and scatter plots in this article as well as in statistics from each historical reprocessing), otherwise there is no point to use the new algorithms. Two, statistically, it is nearly impossible to know which histogram distributions are closer to the “truth” because there is no way to collect field data even from an ocean basin (not to mention the global ocean) within a short period (e.g., one month). Three, however, it is possible to evaluate the algorithm performance in cross-sensor consistency. This is especially important for studies of climate variability because of the multiple sensors involved. This is why NASA adopted OCI as the default algorithm to bring all SeaWiFS, MODIS, and VIIRS to form a seamless multisensor data record (e.g., [60, Fig. 3.26]), even if OCI Chl histograms are different from OCx Chl histograms (see [14, Fig. 20]). In this regard, both OCI and SVR appear better than OCx, and they may both generate improved time-series for global-scale or basin-scale studies regardless of their differences in histogram distributions.

C. Extension to Other Data Products

The robustness of the SVR Chl algorithm suggests that it might be possible to extend the concept to other ocean color data products. As a test, we used the NOMAD data set to train an SVR algorithm to estimate the diffuse attenuation coefficient at 490 nm, $K_d(490)$ (m⁻¹). While there are several forms of empirical and semianalytical algorithms proposed by the community [61]–[63], the current standard (or default) algorithm used by NASA to produce global $K_d(490)$ data products is adopted from the blue–green band ratio algorithm [63] with algorithm coefficients tuned from the NOMAD data set. This algorithm is used here as the reference to evaluate the SVR algorithm.

Using the same methodology development approach as outlined in Section II-B, R_{rs} data from the NOMAD data set at the same four wavelengths (443, 490, 555, and 670 nm) were used to train the SVR algorithm for $K_d(490)$. The algorithm was then applied to satellite data, where colocated and concurrent field-measured $K_d(490)$ from the SeaBASS data set were used to evaluate the algorithm performance.

Fig. 14 and Table VI show that for the entire $K_d(490)$ range, the SVR $K_d(490)$ algorithm yielded better performance than the band-ratio algorithm. The scatter plots show tighter relationships between SVR $K_d(490)$ and *in situ* $K_d(490)$ than between band-ratio $K_d(490)$ and *in situ* $K_d(490)$ for both SeaWiFS and MODISA. In particular, the significant overestimates in the band-ratio $K_d(490)$ for $K_d(490) > 0.2$ m⁻¹ are much reduced. We attribute this improvement to the tolerance of the SVR algorithm to some unknown errors in the satellite-derived $R_{rs}(\lambda)$.

Indeed, machine learning approaches have been demonstrated to be effective in estimating bio-optical properties from satellite measurements for regional studies. For example, a self-organizing neural network was developed to estimate sea surface pCO_2 over the Atlantic subpolar gyre and North Atlantic, which performed much better than multiple linear regressions [64], [65]. Improved performance was also found in retrieval of IOPs for open oceans by using neural network [45]. Similarly, a neural network inversion algorithm

Fig. 14. Application of the SVR approach to estimate K_d_{490} from (a) SeaWiFS and (b) MODISA. The approach was tuned using NOMAD2 data, and then applied to SeaWiFS and MODISA R_{rs} data from the SeaBASS archive to estimate K_d_{490} (green dots). For comparison, the default SeaWiFS and MODISA K_d_{490} data (empty circles) are also plotted.

TABLE VI
COMPARISON OF SEAWIFS- AND MODISA-DERIVED K_d_{490} DATA USING TWO ALGORITHMS: THE NASA DEFAULT EMPIRICAL ALGORITHM (“DEFAULT”) AND THE SVR ALGORITHM DEVELOPED IN THIS STUDY (“SVR”). BOTH ALGORITHMS WERE APPLIED TO SATELLITE-DERIVED R_{rs} AND EVALUATED USING *In Situ* K_d_{490} OBTAINED FROM SEABASS

		MAD	Bias	MRD	RMSD	UMRD	URMSD	Mean ratio	Median ratio	R^2 linear	R^2 log	N
SeaWiFS	Default	1.35	1.13	59.5%	276.5%	27.6%	40.8%	1.45	1.06	0.28	0.80	651
	SVR	1.27	1.00	29.2%	104.3%	23.1%	33.1%	1.10	0.98	0.89	0.87	651
MODISA	Default	1.37	1.13	67.8%	311.3%	28.0%	42.3%	1.53	1.08	0.01	0.57	389
	SVR	1.35	0.97	25.0%	35.9%	24.1%	32.4%	1.03	0.99	0.02	0.70	389

was also developed to estimate $K_d(490)$ for coastal and open water and compared it with other published algorithms, which had higher accuracy for derived $K_d(490)$ than other algorithms [44]. Chen *et al.* [66] developed a neural net algorithm to estimate $K_d(490)$ from MODISA measurements over the East China Sea and Yellow Sea, which showed improvements over the band-ratio algorithms. Chen *et al.* [67] developed an approach to use a RF-based regression ensemble (RFRE) to estimate sea surface pCO_2 in the Gulf of Mexico and Gulf of Maine. Even if the explicit functional forms between sea surface pCO_2 and MODIS-derived $R_{rs}(\lambda)$ are unknown, the RFRE approach can successfully retrieve the former from the latter as long as there are sufficient field data to train the algorithm. Clearly, although caution is required when considering the applicability ranges, machine learning approaches may lead to robust algorithms to serve as alternatives of the current standard algorithms. For the same reason, although this study tested several popular machine learning approaches (e.g., GP, RF, MLP, and SVR) from which SVR was selected, there might be other machine learning approaches, after proper tuning and parameterization, that could yield equally well or even better performance than the SVR presented here. This is perhaps a subject of further research through more extensive tests in the future.

Finally, because of the lack of explicit functional expressions between R_{rs} and Chl in the SVR algorithm, it may be difficult for others to implement and test the algorithm for other sensors or for regional applications. To overcome this difficulty, the computer codes together with a README file are provided in the Supplementary Materials.

V. CONCLUSION

A SVR algorithm has been developed from the NOMAD data set to estimate Chl in surface waters of the global oceans. Evaluation of its application to SeaWiFS, MODISA, and MERIS measurements shows improvements over the traditional band-ratio OCx algorithms for the entire data range, and particularly for $Chl < 1 \text{ mg m}^{-3}$. Although its performance is slightly worse than the band-subtraction OCI algorithm for $Chl < 0.25 \text{ mg m}^{-3}$, it avoids the algorithm transition from band subtraction to band ratio in the OCI algorithm design, thus assuring internal algorithm consistency for the entire range. Furthermore, the SVR algorithm is tolerant to image noise and artifacts, and its application to SeaWiFS, MODISA, and VIIRS leads to consistent results across different sensors. Application of the same approach also leads to similar improvements in the satellite-derived diffuse attenuation coefficient. Machine learning approaches may therefore serve as alternative ways

to develop robust empirical algorithms for global oceans to estimate various bio-optical properties.

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