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Note

Verification of a simple band ratio algorithm for retrieving Great Lakes open water surface chlorophyll concentrations from satellite observations

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ABSTRACT

We compared *in situ* surface chlorophyll concentration values measured between 2012 and 2015 as part of the U.S. Environmental Protection Agency's Great Lakes National Program Office (GLNPO) annual monitoring program with corresponding concentration estimates obtained by applying our previously published (Lesht et al., 2013) Great Lakes Fit (GLF) band ratio algorithm to data from the Moderate-resolution Imaging Spectroradiometer (MODIS) sensor. Coefficients used in the original GLF algorithm were derived from similarly matched GLNPO and satellite observations collected between 2002 and 2011. The Model II linear relationship between the original GLF-predicted log-transformed values and the new set (2012–2015) of field observations yielded intercept = 0.036, slope = 1.063, and r^2 = 0.830. Residuals for modeled chlorophyll concentrations below ~8.0 mg m $^{-3}$ were unbiased and normally distributed, but positively biased at higher modeled concentrations. When applied to the entire dataset (2002–2015), the linear relationship between the GLF-modeled and the observed values had intercept = 0.000, slope = 0.999, and r^2 = 0.820. New model coefficients derived from the entire (2002–2015) dataset were very similar to those obtained from the 2002–2011 data. Continual testing and assessment of any empirical model are desirable especially when the model is designed to be employed by a broad community. We conclude that this comparison of the GLF algorithm with the additional four years of independent data further validates its use for estimating surface chlorophyll concentrations from satellite observations of the open waters of the Great Lakes.

Introduction

Several papers have described new algorithms for estimating chlorophyll concentrations in the Great Lakes from satellite observations (see Lesht et al., 2012 for a review of work prior to 2012 and more recently Lesht et al., 2013 and Shuchman et al., 2013). However, in contrast to the continual assessment of algorithms developed by the major space agencies (*e.g.*NASA and ESA) which are provided to users *via* the agencies' web sites, to our knowledge no work has been reported in which the performance of these Great Lakes-specific algorithms has been tested with new, independent observations. Because all empirical or semi-empirical algorithms depend on the data from which their numerical coefficients are derived, testing with new data is essential both to assess the models' success and to examine their limitations (Augusiak et al., 2014). In some cases it might be desirable simply to update the model coefficients as more data are acquired (Werdell et al., 2003), in other cases models may have to be discarded or structurally modified if systematic failure is observed.

In Lesht et al. (2013) we demonstrated that a simple band-ratio algorithm could be used to estimate surface chlorophyll values in the offshore waters of the Great Lakes from ocean color satellite observations (SeaWiFS from 1998 to 2010 and MODIS from 2002 to 2011). In that work we tuned the MODIS retrieval model to field data collected in all five lakes as part of the annual GLNPO monitoring program that we pooled across ten years (2002–2011). Although we presented an uncertainty analysis based on Monte-Carlo and sub-sampling methods in that paper, we were unable to test the algorithm with new, independent data. The primary purpose of this note is to report the results of our assessment of the GLF algorithm's performance based on comparison of its predictions with new MODIS observations collected from 2012 to 2015. Such a test is necessary to demonstrate that the algorithm is capable of representing data that were not available when it was developed and so could not have affected its structure or coefficients (Augusiak et al., 2014). For completeness, our secondary objective was to determine how much the original model coefficients change when the model is fit to the full (2002–2015) dataset.

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Methods

Matching field observations and satellite data

Our original methods for matching the GLNPO field measurements with the satellite observations (Lesht et al., 2013) were similar to the procedures described by Bailey and Werdell (2006). Field sampling and determinations of *in situ* chlorophyll concentrations followed standard GLNPO protocols (U.S.E.P.A., 2010) and were consistent throughout the study period. For the satellite data, we processed Level 1A (digital counts) data to Level 2 (geophysical values, L2) using the *l2gen* (v8.1.4) processing code in SeaDAS (Baith et al., 2001). We limited comparisons to satellite images that were collected within one day of the field sampling. This temporal window is larger than the ± 3-h window used by Bailey and Werdell (2006); inconsistencies in the recorded times of the GLNPO field sampling made it impossible for us to resolve them to intervals finer than one day. Images that satisfied the temporal matching criterion next were checked for viewing geometry and for overall cloud cover. Images for which the solar zenith angle at the scene center exceeded 70° were rejected as were those for which more than 20% of the pixels exceeded a satellite zenith angle of 60°. We also rejected images in which less than 20% of the lake surface was cloud free. For the images that passed this screening, we then checked the native-resolution L2 pixels within 5 × 5-pixel boxes centered on the field sampling locations to ensure that none of the NASA quality flags (http://oceancolor.gsfc.nasa.gov/VALIDATION/flags.html) we used (ATMFAIL, LAND, CLDICE, HIGLINT, HILIT, STRAYLIGHT, CHLFAIL, NAVFAIL) were set. This quality test is more stringent than the one used by Bailey and Werdell (2006) who accepted matches for which 50% of the pixels (rather than all) in the 5 × 5 box were unflagged. The CHLFAIL test, which checks the basic shape of the input reflectance spectrum, is based on the standard NASA OC3M wavelengths; because we used these same wavelengths in the GLF algorithm (described below) CHLFAIL also screened pixels for which the input spectra were inappropriate for use with the GLF algorithm. To further limit the sampling area, we used the arithmetic mean value of the retrieved values within a 3 × 3 pixel box centered on the sample location as the representative satellite value for that location. Finally, we rejected matches for which any of the values of remote sensing reflectance (*Rrs*) was less than zero, indicating possible overcorrection by the atmospheric radiation model used to remove the contributions of atmospheric scattering and reflectance from the signal received at the satellite. We used the same SeaDAS default2-bandNIR iteration model (Bailey et al., 2010) that Shuchman et al. (2013) showed performs well over the Great Lakes in our processing.

We did not include either a check for spatial homogeneity or a pixel-by-pixel check of the satellite viewing angle in our original (Lesht et al., 2013) analysis; both were used by Bailey and Werdell (2006) in their study. To make our approach in the present work even more comparable to theirs, we added the pixel-based validation flag HISATZEN to the suite of flags checked in the 5 × 5 pixel box and also used a spatial homogeneity test, similar to that presented by Kahru et al. (2014) in the new calculations presented here. For the homogeneity test we rejected matches if the retrieved chlorophyll concentration (C) values in the 5 × 5 pixel region surrounding the sampling location were such that $(C_{\max} - C_{\min})/C_{\min} > 1$. We include comparisons between the results of the original analysis (Lesht et al., 2013) and of the updated analysis where appropriate below.

Chlorophyll retrieval

The general form of the band-ratio retrieval algorithm is $log_{10}(Chl_{mod}) = c_0 + \sum_{i=1}^{n} c_i X^i$, in which X is $log_{10}(MBR)$, the c_i are the model coefficients, and *MBR* represents the maximum band ratio, which for MODIS is calculated as $Max\{Rrs_{443}, Rrs_{488}\}/Rrs_{547}$ in which Rrs_{nnn} is the remote sensing reflectance at nominal wavelength *nnn*. In our original investigation of the GLF we found that a third-order polynomial was adequate for use in the Great Lakes and noted that the primary effect of adding the fourth-order term to the polynomial was to change the shape of the relationship at larger values of $log_{10}(MBR)$ (smaller values of chlorophyll). The fourth-order term is used in the standard NASA band-ratio algorithms because it is necessary for retrievals in the ocean where the lowest chlorophyll concentrations can be over an order of magnitude smaller than they are in the Great Lakes (Lesht et al., 2013). Although we did test a fourth-order version of the GLF as part of this work, we noted only a slight improvement over the third-order model and report only the most basic results of this test.

The coefficients used in the original GLF model were obtained by using an iterative method based on successive applications of a reduced major axis (Model II) regression, the appropriate regression approach when both variables are uncertain (Press and Teukolsky, 1992). This procedure, which yields the model coefficients that result in a 1:1 relationship between the retrieved and observed log-transformed chlorophyll values, is the same method used by NASA in their development of the standard SeaWiFS and MODIS retrieval algorithms (O'Reilly et al., 2000). In the present study, we used a maximum likelihood fitting method based on direct minimization of the chi-square function appropriate when both variables are subject to experimental error to determine the GLF coefficients. The chi-square function is written as Press and Teukolsky (1992)

$$\chi^2(a,b) = \sum_{i=1}^{N} \frac{(y_i - a - bx_i)^2}{\sigma_y^2 + b^2\sigma_x^2} \qquad (1)$$

in which y is $\log_{10}(C_{\text{mod}})$ and x is $\log_{10}(C_{obs})$. Because the retrieval algorithm is in the form of a polynomial $\log_{10}(C_{mod}) = c_0 + \sum_{j=1}^{n} c_j X^j$, in which X is $log_{10}(MBR)$, n is the degree of the polynomial ($n = 3$ in the original GLF and $n = 4$ in the standard NASA retrieval models) and the c_j values are the model coefficients, we can substitute this polynomial for y_i, apply the desired constraints that the intercept (a) equals zero and slope (b) equals 1, and re-write Eq. (1) as a function only of the model coefficients (c_j).

$$X^2(c) = \sum_{i=1}^{N} \frac{\left(\left(c_0 + \sum_{j=1}^{n} c_j X_i^j\right) - x_i\right)^2}{\sigma^2_{\left(c_{0+\sum_{j=1}^{n} c_j X_i^j}\right)} + \sigma_x^2} \qquad (2)$$

We used the R (R Core Team, 2014) package optimx (Nash and Varadhan, 2011) to minimize Eq. (2) with respect to the parameter vector c. The initial parameter vector needed to begin the minimization was obtained by using the function *monpol* from R package MonoPoly (Murray et al., 2013) for the third-order model and with the *lm* function from the R base stats package (R Core Team, 2014) for the fourth-order model (fourth-order models are not necessarily monotone). Our experience comparing the original and the maximum likelihood fit methods showed that the maximum likelihood method yields nearly identical results to the original method (see Table 2) but is more intuitive and computationally efficient.

Comparison statistics

Our analysis generally follows the procedures outlined by Bailey and Werdell (2006) and Campbell and O'Reilly (2006) both of which were developed specifically for evaluation of satellite retrieval algorithms. To provide measures of the overall bias and uncertainty associated with the GLF, we calculated both the ratio of satellite to *in situ* chlorophyll and the absolute percent difference for each matched pair of