Band-ratio or spectral-curvature algorithms for satellite remote sensing?

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For the retrieval of chlorophyll concentrations or the total absorption coefficients of oceanic waters based on water color, there are algorithms that use either band ratios or spectral curvatures of remote-sensing reflectance or water leaving radiance. We show that band-ratio algorithms have the potential to be applied to a wider dynamic range of oceanic waters, whereas spectral-curvature algorithms show stable performance as long as the data set falls within the appropriate range.

1. Introduction

For the retrieval of chlorophyll concentrations or the total absorption coefficient for oceanic waters based on water color, there are algorithms that use either band ratios or spectral curvatures1–8 of remote-sensing reflectance or water leaving radiance. Although band-ratio algorithms are popular and widely used, there are few comparisons about their performance, and the advantages and drawbacks of the two kinds of algorithm have not been clearly delineated. By comparing the sensitivity and performance of absorption algorithms using a two-band ratio and a spectral-curvature approach, we show that two-band-ratio algorithms remain sensitive over a wider dynamic range of absorption values and perform better at low- and high-absorption values.

To evaluate the sensitivity and performance of a two-band-ratio algorithm and a spectral-curvature algorithm to variations in the absorption coefficient, we created a data set including both case-1 and case-2 waters3 by using a remote-sensing reflectance model for deep waters.11 In this data set, we varied the pigment concentration $C$ and other bio-optical parameters in a way that closely mimics the natural field. The following provides details of the data creation.

For homogeneous, optically deep waters, subsurface remote-sensing reflectance is a function of in-water absorption and scattering coefficients.11–13 Generally,

$$r_{rs} = g(b_b/a),$$

where $g$ is a weak function of $b_b/a$ with a typical value of approximately 0.09. $a$ and $b_b$ are the total absorption and backscattering coefficients, respectively, and,

$$a(\lambda) = a_w(\lambda) + a_p(\lambda) + a_g(\lambda),$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda),$$

where $a_w$, $a_p$, and $a_g$ are the absorption coefficients for water molecules, pigments, and gelbstoff–detritus, respectively, and $b_{bw}$ and $b_{bp}$ are the backscattering coefficients for water molecules and suspended particles. Values for $a_w$ and $b_{bw}$ are already known.15,16 We used the following bio-optical models12,13 to create optical data that simulates ocean waters:

$$a_p(440) = 0.06 C^{0.65},$$

$$a_p(440) = p_1^* a_p(440),$$

$$b_{bp}(550) = (0.002 + 0.02[0.5 - 0.25 \log(C)])^* p_2^* C^{0.62},$$

Further,

$$a_p(\lambda) = [a_0(\lambda) + a_1(\lambda) \ln[a_p(440)]a_p(440)],$$

$$b_{bp}(\lambda) = b_{bp}(550) \left( \frac{550}{\lambda} \right),$$

$$a_g(\lambda) = a_g(440) \exp[-0.015(\lambda - 440)].$$

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where values for $a_0(\lambda)$ and $a_1(\lambda)$ are known. Note that $C$ is used only as a free parameter for the designation of a wide range of absorption values.

For case-1 waters, $p_1 \approx 0.8$, $p_2 \approx 0.3$, and $n \approx 1.0$, and all the optical parameters covary with $C$ values. Since many natural waters are not case 1, we perturbed the case-1 parameters as follows:

$$p_1 = 0.5 + \frac{3.5 R_1 a_0(440)}{0.02 + a_0(440)},$$

$$p_2 = 0.1 + 0.5 R_2,$$

$$n = 0.2 + \frac{1.5 + R_3}{1 + C},$$  \hspace{1cm} (5)

where $R_1$, $R_2$, and $R_3$ are random values between 0 and 1. These kinds of perturbation result in $p_1$, $p_2$, and $n$ random values for each $C$ value, but fall within a range that is consistent with field observations. For example, $p_1$ ranges between 0.5 and 4.0 in general, $p_2$ between 0.1 and 0.6, and $n$ between 0.2 and 2.5. Also, to be consistent with field observations, the range for $p_1$ is narrower for low $C$ values (open ocean), wider for high $C$ values (coastal), and $n$ decreases when $C$ values increase, but in a random way for both $p_1$ and $n$.

Thus, for each $C$ value, there is a range of simulated $r_{rs}$ spectra that is not just a function of $C$, but is also a function of the random values of $R_1$, $R_2$, and $R_3$. For a $C$ range of from 0.05 to 30 mg/m$^3$, 480 $r_{rs}$ spectra were simulated.

We calculated the following ratio and curvature values from the simulated data set:

$$\rho_{2B} = \frac{r_{rs}(555)}{r_{rs}(490)},$$

$$\rho_{\text{curv}} = \frac{r_{rs}(443)}{r_{rs}(490)} \cdot \frac{r_{rs}(490)}{r_{rs}(555)},$$  \hspace{1cm} (6)

Figure 1 shows how $\rho_{2B}$ and $\rho_{\text{curv}}$ relate to $a(443)$. In the log–log coordinates between $a(443)$ and $\rho_{2B}$ and $\rho_{\text{curv}}$, $\rho_{2B}$ increases with $a(443)$ in a linear manner for $a(443)$ values less than 0.2 m$^{-1}$, and then increases at a reduced rate. $\rho_{\text{curv}}$ approaches asymptotic values for both high and low $a(443)$ values. In terms of the dynamic range, for the entire $a(443)$ range (from $\sim 0.02$ to $\sim 2.4$ m$^{-1}$), $\rho_{2B}$ falls within the range from $\sim 0.23$ to $\sim 2.16$, but $\rho_{\text{curv}}$ ranges from $\sim 0.37$ to $\sim 1.28$, or half of the dynamic range of $\rho_{2B}$. For $a(443)$ greater than 0.4 m$^{-1}$ (typical for near-shore coastal waters), $\rho_{2B}$ varies from $\sim 1.47$ to $\sim 2.16$, whereas $\rho_{\text{curv}}$ varies from $\sim 1.07$ to $\sim 1.28$, or one third of the dynamic range. For $a(443)$ less than 0.07 m$^{-1}$ (equivalent to a pigment concentration of $\sim 0.4$ mg/m$^3$ for case-1 waters, and greater than 50% of the Sea-viewing Wide Field-of-view Sensor Bio-optical Algorithm Mini-workshop (SeaBAM) data have a pigment concentration of less than 0.4 mg/m$^3$), $\rho_{2B}$ varies from $\sim 0.23$ to $\sim 0.54$, whereas $\rho_{\text{curv}}$ varies from $\sim 0.38$ to $\sim 0.50$, again a factor of 2 smaller. These results suggest that the 555–490 band ratio is more sensitive to $a(443)$ than the 555–490–443 curvature approach. In other words, because of the narrow range in $\rho_{\text{curv}}$, much more precise measurements of remote-sensing reflectance are required if $\rho_{\text{curv}}$-based algorithms are applied to coastal waters. This is consistent with the analysis of Campbell and Esaaias with regard to spectral-curvature algorithms for chlorophyll concentration.

The reduction in sensitivity of $\rho_{\text{curv}}$ can be explained as follows. For a two-band $r_{rs}$ ratio between 555 and 490,

$$\rho_{2B} = \frac{r_{rs}(555)}{r_{rs}(490)} = \frac{g(555) b_3(555) a(490)}{g(490) b_3(490) a(555)}.$$  \hspace{1cm} (7)

As $g$ is only a weak function of wavelength for oceanic waters,

$$\rho_{2B} = \frac{b_3(555) a(490)}{b_3(490) a(555)} = \beta_{2B} a(490).$$  \hspace{1cm} (8)

Using a spectral curvature among 443, 490, and 555 nm, we have

$$\rho_{\text{curv}} = \frac{r_{rs}(555)}{r_{rs}(490)} \cdot \frac{r_{rs}(490)}{r_{rs}(443)} = \frac{b_3(555)b_3(490)}{b_3(490)^2} \frac{a(490)^2}{a(555) a(443)}.$$  \hspace{1cm} (9)

or

$$\rho_{\text{curv}} = \beta_{3B} \frac{a(490) a(555)}{a(443) a(490)} = \beta_{3B} \frac{a_{12}}{a_{23}},$$  \hspace{1cm} (10)

where $\beta_{3B}$ is the three-band ratio of backscattering coefficient, $a_{12}$ is the ratio of $a(555)/a(490)$, and $a_{23}$ is the ratio of $a(490)/a(443)$.

For oceanic waters, the quantities of $a$ or $b_3$ can vary by orders of magnitude from place to place. As $a$ and $b_3$ are sums of in-water components, all $a(\lambda)$ and $b_3(\lambda)$ values increase with an increase of in-water constituents, but at different rates for dif-
different wavelengths. Because of this feature, the ratio $a(555)/a(490)$ or $b_y(555)/b_y(490)$ is less sensitive than the individual $a(555)$ or $a(490)$ or $b_y(555)$ or $b_y(490)$ to the change of in-water constituents. In addition, a ratio of those ratios, e.g., $\alpha_{2a}/\alpha_{12}$, further reduces this sensitivity, resulting in $\alpha_{2a}/\alpha_{12}$ that is more insensitive than $a(443), a(490), or a(555)$ to the change of in-water constituents.

To test the above analysis, we applied a band-ratio algorithm and a spectral-curvature algorithm to the above simulated case-2 data set. Both algorithms were independently developed based on specific field data sets. The band-ratio algorithm is a recent update of the Lee et al.\textsuperscript{9} empirical algorithm with additional data. This updated algorithm is

\[
a(443) = \exp[-1.752 + 1.326 \gamma + 0.118(\exp(\gamma))^3],
\]

where $\gamma = \ln(r_{555}/r_{490})$.

Applying this two-band-ratio algorithm to the simulated data set, yields a root-mean-square error\textsuperscript{6} (rmse) of approximately 13\% for the entire $a(443)$ range (see Fig. 2). For three separate $a(443)$ ranges, rmse values are $\sim 11\% (N = 137)$ for $a(443)$ less than 0.07 m\(^{-1}\), $\sim 11\% (N = 193)$ for $a(443)$ between 0.07 and 0.4 m\(^{-1}\), and $\sim 18\% (N = 150)$ for $a(443)$ greater than 0.4 m\(^{-1}\).

Applying the curvature algorithm of Barnard et al.,\textsuperscript{10} yields a rmse value of approximately 43\% for the entire $a(443)$ range. The rmse values are $\sim 36\%$ for $a(443)$ less than 0.07 m\(^{-1}\), $\sim 13\%$ for $a(443)$ between 0.07 and 0.4 m\(^{-1}\), and $\sim 103\%$ for $a(443)$ greater than 0.4 m\(^{-1}\). It is clear from Fig. 2 that this curvature algorithm overestimates $a(443)$ for values less than 0.07 m\(^{-1}\), and substantially underestimates $a(443)$ for values greater than 0.4 m\(^{-1}\). However, this curvature algorithm works quite well for the middle range (0.07–0.4 m\(^{-1}\)), which is consistent with the results of Barnard et al.\textsuperscript{10}

It is interesting that both algorithms performed similarly for the middle range, but the two-band-ratio algorithm performed better at both low- and high-absorption values. These results suggest that three or more curvature algorithms with different sets of wavelength bands could be useful for different ranges of total absorption coefficients. If one uses the two-band-ratio algorithm, another empirical algorithm might be required for $a(443)$ values greater than 1.0 m\(^{-1}\), such as the switch method by Gordon et al.\textsuperscript{20} for the Coastal Zone Color Scanner algorithm.

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