Matching reflectances for the estimation of inherent optical properties

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Abstract

A novel approach based on an analytical bio-optical model is developed for the retrieval of Inherent Optical Properties, from which the water quality constituent concentrations can be obtained. The proposed method generates synthetic (sub)surface irradiance reflectances ($R(0)$) for different values of the unknown parameters and matches them to the measured reflectances; the values of the parameters that generate the best match are taken to be the parameter estimates. Through Monte Carlo simulations the method is shown to be superior to linear matrix inversion, consistently producing estimates very close to the true values of absorption and backscattering.

I Introduction

Analytical inversion of bio-optical models leads to retrieval of optical water quality parameters and estimation of their concentrations from remotely sensed data. Such parameters include total suspended matter, phytoplankton pigments, and colored dissolved organic matter. Inversion methods [1, 2, 3, 4] developed to date have strengths and weaknesses; no single method can accurately derive concentrations of all optically active water quality parameters in oceanic and coastal waters from remotely sensed data. Accurate estimation of these parameters (chlorophyll-a being the main concern) forms the basis for determining primary productivity and estimation of organic carbon produced by phytoplankton, which is critical in global change studies.

For the estimation of inherent optical properties (IOPs) of oceanic (case 1) water, a linear model has been established [1] relating reflectance to absorption of phytoplankton, CDOM absorption and backscattering. The radiance models describe the generation of upwelled water-leaving spectral radiance caused by backscatter and absorption of incident downwelling solar irradiance. This extends work in [5] for IOPS, from which constituent concentrations can be obtained. The model describes the generation of upwelled water-leaving spectral radiance caused by backscatter and absorption of incident downwelling solar irradiance and relies on expressing reflectance R as:

$$\frac{R}{Q} = l_1 X + l_2 X^2, \tag{1}$$

where $l_1 = 0.0949$, $l_2 = 0.0794$, Q is the ratio of upwelling radiance to upwelling irradiance towards zenith, and

$$X = \frac{b_b}{b_b + a}, \tag{2}$$

a and b_b being total absorption and backscattering, respectively. Equation 2 can be rewritten as

$$a + b_b(1 - 1/X) = a + b_b v = 0. \tag{3}$$

Total absorption a includes phytoplankton, CDOM, and detritus components. For case 1 waters, CDOM and detritus absorptions can be combined into a single component a_d; one can then write $a_{ph} + a_d + a_w = a_t + a_w = a$, where a_{ph} is the phytoplankton absorption, a_w is the known natural absorption of water, and a_t is the combined absorption of phytoplankton, CDOM, and detritus. Separating absorption of water constituents, natural water absorption, and backscattering components, Eq. 3 leads to:

$$a_t + b_{bt} v = -a_w - b_{bw} v, \tag{4}$$

where $b_b = b_{bt} + b_{bw}$, where b_{bw} is the seawater backscatter and b_{bt} is the total constituent backscatter.

Assuming reflectance measurements at three wavelengths λ_i, $i = 1, 2, 3$, one can then write three equations of the type:

$$a_{ph}(\lambda_i) + a_d(\lambda_i) + b_{bt}(\lambda_i) v(\lambda_i) = h(\lambda_i), \tag{5}$$

where $h(\lambda_i)$ is the righthand side of Eq. 4.

As explained in [1], an effort is then made to express $a_{ph}(\lambda_i)$, $a_d(\lambda_i)$, and $b_{bt}(\lambda_i)$ in terms of a single a_{ph}, a_d and b_{bt} at a single wavelength, so that we can use Eq. 5 to write three equations with three unknowns. We write

$$b_{bt}(\lambda_i) = b_{bt}(\lambda_b)(\lambda_b/\lambda_i)^n, \tag{6}$$

$$a_d(\lambda_i) = a_d(\lambda_d)exp(-S(\lambda_i - \lambda_d)), \tag{7}$$

and

$$a_{ph}(\lambda_i) = a_{ph}(\lambda_g)exp(-(\lambda_i - \lambda_g)^2/(2g^2)). \tag{8}$$

Wavelengths λ_b, λ_d, and λ_g are reference wavelengths. Constant n typically takes values between 0 and 4.1. Quantity S is the CDOM-detritus slope [1], and g is the width of the Gaussian model for phytoplankton absorption. Quantities n, S, and g are typically selected based on empirical knowledge.

Expanding Eq. 5, we can write

$$Ax = b, \tag{9}$$

where

$$A = \begin{pmatrix} exp(-(\lambda_1 - \lambda_g)^2/(2g^2)) & exp(-S(\lambda_1 - \lambda_d)) & (\lambda_b/\lambda_1)^n v(\lambda_1) \\ exp(-(\lambda_2 - \lambda_g)^2/(2g^2)) & exp(-S(\lambda_2 - \lambda_d)) & (\lambda_b/\lambda_2)^n v(\lambda_2) \\ exp(-(\lambda_3 - \lambda_g)^2/(2g^2)) & exp(-S(\lambda_3 - \lambda_d)) & (\lambda_b/\lambda_3)^n v(\lambda_3) \end{pmatrix},$$

$$x = \begin{pmatrix} a_{ph}(\lambda_g) \\ a_d(\lambda_d) \\ b_{bt}(\lambda_b) \end{pmatrix},$$

and

$$b = \begin{pmatrix} h(\lambda_1) \\ h(\lambda_2) \\ h(\lambda_3) \end{pmatrix}.$$

In [1], the system of Eq. 9 is solved for calculation of the vector of unknowns x containing a_{ph}, a_d, and b_{bt} at reference wavelengths. Using Equations 6, 7, and 8, we can then calculate

a_{ph}, a_d and b_{bt} at desired wavelengths. Because the system can be readily solved by inverting matrix A, this estimation method is often referred to as the linear matrix inversion method. Matrix A has been shown to rarely exhibit ill-conditioning or singularities [1]. In the absence of such problems, the system can be solved in a straightforward manner using standard techniques such as elimination or Cramer's rule. When matrix A is ill-conditioned, Singular Value Decomposition or other regularization methods can be applied for the solution of the system.

II A least-squares method for inherent optical property estimation

In this work we propose an alternate method for extracting a_{ph}, a_d, and b_{bt} from reflectance data. We assume that the mathematical model of Equation 1 is still valid. The difference is that now, instead of solving the system of Eq. 9 for retrieving a_{ph}, a_d and b_{bt}, we generate synthetic reflectances using Equations 1 and 2 for the wavelengths at which data points are available and values of the three parameters on a three dimensional grid. Each parameter takes values in the interval [0.1 2] with a spacing of 0.1. We then compute the squared error between measured and synthetic reflectances. The values for a_{ph}, a_d, and b_{bt} for which the error is minimized are taken to be the parameter estimates.

III Performance evaluation

To evaluate the proposed method, we selected values for a_{ph}, a_d, and b_{bt} and we generated reflectance R for a set of wavelengths between 413 and 750 nm. The selected values for reflectance data generation were $a_{ph} = 1.0$, $a_d = 0.8$ and $b_{bt} = 0.2$. Also $\lambda_g = \lambda_b = \lambda_s =$ 430 nm, $S = 0.025$, $g = 40$, $n = 1.4$, $\lambda_1 = 404$, $\lambda_2 = 443$, and $\lambda_3 = 555$ nm.

Even when the mathematical model relating reflectance with absorption and backscattering is exactly correct, the measured reflectance will be a noisy version of the true reflectance. To generate realistic data, we perturbed the generated reflectance to obtain 100 noisy realizations. Noisy data generation was performed by adding Gaussian noise to the "true" reflectance. To test the estimation methods, matrix inversion and least squares, under mild noise conditions, we selected a high Signal to Noise Ratio (43 dB). One noisy realization along with the true reflectance is shown is Figure 1.

Linear matrix inversion and least-squares were then applied to the generated data realizations. Figure 2 shows the histograms obtained for the three parameters: the first column shows the matrix inversion results and the second column presents the least-squares results. There is a larger spread (error) in the matrix inversion estimates around the true parameter values than in the least-squares estimates, as seen from the histograms. Moreover, for certain realizations, the amount of noise in the data (although numerically tiny as can be seen from Figure 1) produces non- physical, negative estimates for the unknowns. Medians of the estimates are presented in Table 1, showing clearly that the estimates obtained through least-squares are much closer to the true values of the parameters than the estimates obtained through matrix inversion. The suboptimal performance of matrix inversion is attributed to the fact that the relationship between the measured R and the parameters is not truly linear, because the measured R contains a noise component. This deviation from linearity introduces errors in the results. The least-squares method, matching real to synthetic reflectances, appears much more promising in the estimation of water constituents' absorption and backscattering.

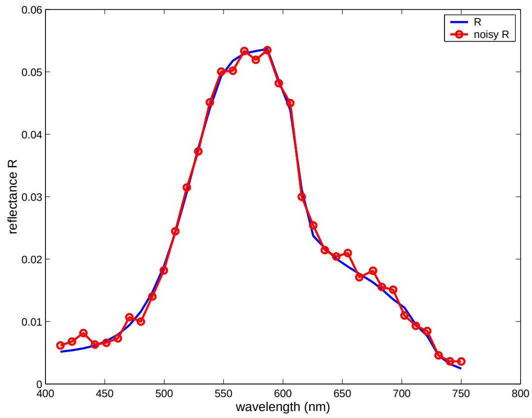

Figure 1: True (synthetic) reflectance R and one noisy realization of R.

Table 1: Medians of estimates from 100 realizations for matrix inversion and least-squares.

parameter	true value	matrix inversion	least-squares
a_{ph}	1.0	0.6003	1.0
a_d	0.8	-0.0025	0.9
b_{bt}	0.2	0.0685	0.2

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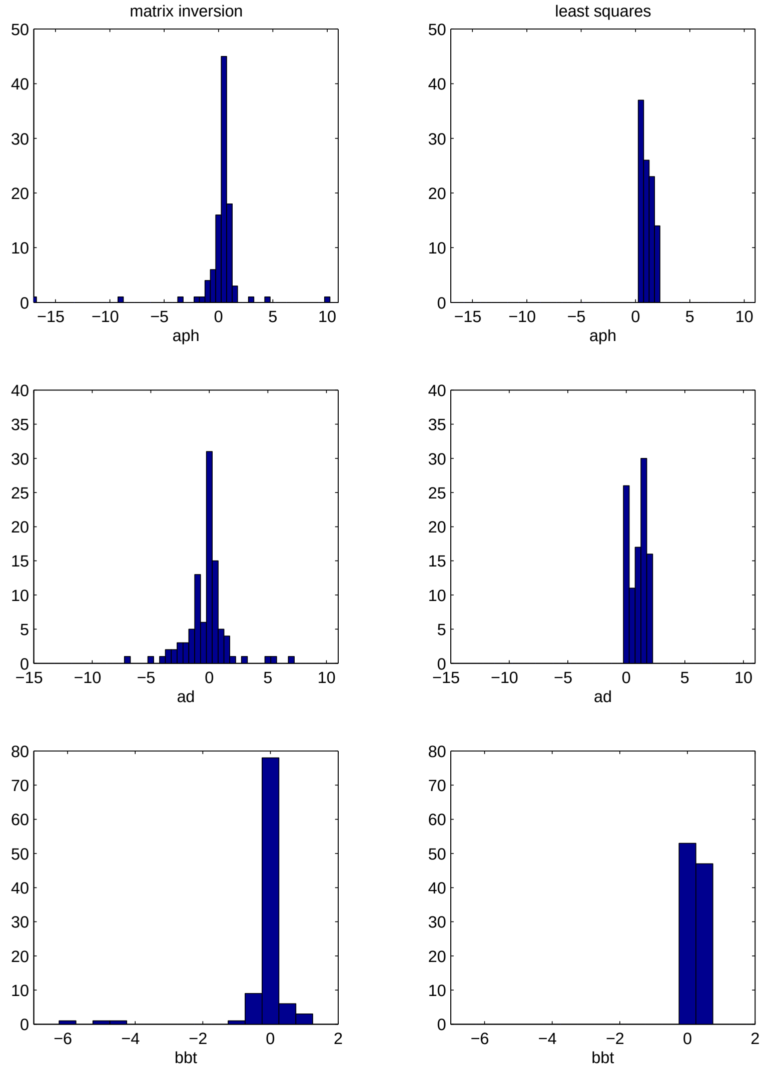

Figure 2: Histograms of estimates for matrix inversion (left column) and least-squares (right column).

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