Chlorophyll Concentration Profiles from \textit{in situ} Radiances by Ant Colony optimization

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Abstract. A methodology for the reconstruction of vertical profiles of the absorption ($a$) and scattering ($b$) coefficients in natural waters is presented. Reconstruction is performed using single-wavelength \textit{in situ} radiance measurements at several depths. The depth is discretized by a multi-region approach assuming that absorption and scattering coefficients are constant in each region. The inverse problem is iteratively computed employing the radiative transfer equation as direct model, and bio-optical models to correlate the chlorophyll concentration to these coefficients. At every iteration, the inverse solver generates a candidate solution that is a set of discrete chlorophyll concentration values. For each region, the concentration is mapped to the values of absorption and scattering coefficients. The radiative transfer equation is then solved by a parallel version of the Laplace transform discrete ordinate (LTS$N$) method considering polar and azimuthal scattering angles. An objective function is given by the square difference between reconstructed and experimental radiances. In order to compensate the nearly exponential radiance decay with depth, that unbalances the influence of the radiance at different depths, a depth correction factor is applied to weight radiance values at each level. This objective function is minimized by an Ant Colony System (ACS) implementation. A new regularization scheme pre-selects candidate solutions based on their smoothness quantified by the Tikhonov’s norm. A new chlorophyll candidate profile is then generated and iterations proceed. Synthetic and real data show the suitability of the proposed method.

1. Introduction

In the last decades, the development of inversion methodologies for radiative transfer problems has been an important research topic in many branches of science and engineering \cite{17,14}. The direct or forward radiative transfer problem in hydrologic optics, in the steady state, involves the determination of the radiance distribution in a body of water, given the boundary conditions, source term, inherent optical properties (IOPs), as the absorption $a$ and scattering $b$ coefficients, and the scattering phase function. The corresponding inverse radiative transfer problem arises when physical properties, internal light sources and/or boundary conditions must be estimated from radiometric measurements of the underwater light field. In previous works, we tried to establish a general methodology to separately tackle the reconstruction of internal sources \cite{30}, IOP estimation \cite{29,8,10,9}, the identification of boundary conditions \cite{5,7,22}, or even a joint
inversion scheme [29]. In these works, the inverse model is an implicit technique for parameter and/or function estimation from in situ synthetic radiometric measurements.

The algorithm is formulated as a constrained nonlinear optimization problem, in which the direct problem is iteratively solved for successive approximations of the unknown parameters. Iteration proceeds until an objective function, representing the least-square fit of model results and experimental data added to a regularization term, converges to a specified small value. An overview of this technique, as well as a survey of the results, can be found in [6] or in [4].

This work presents a methodology to reconstruct vertical profiles of the absorption and scattering coefficients in natural waters from in situ radiance measurements in several depths and single wavelength. The inverse problem is iteratively solved using the radiative transfer equation (RTE) as direct model. A former work [29] employed a step-by-step reconstruction methodology, estimating \(a\) and \(b\) in an alternate manner. A deterministic optimizer was employed to solve the associated inverse problem. In the current work, bio-optical models [18] are employed to correlate the chlorophyll concentration to \(a\) and \(b\). At every iteration, the inverse solver generates a candidate solution that is a set of discrete chlorophyll concentration values. The spatial domain (geometrical depth) is discretized in 10 regions \((R = 10)\). These coefficients and thus the chlorophyll concentration are assumed as being constant in each region. The discrete chlorophyll profile is then defined by 10 points.

The inverse problem is formulated as an optimization problem and iteratively solved using the radiative transfer equation as direct model. An objective function is given by the square difference between computed and experimental radiances at every iteration. However, the radiance values near the surface are much higher than those in deeper water, since radiance value decays nearly exponentially with depth.

A depth correction factor for the radiances was first proposed by [31]. This work employs a new correction factor based on the mean radiance at each depth level/region. Preliminary version of the methodology was presented in [27]. Here, the methodology is fully described and applied for a high level noise data, and employed to the real problem, where the radiances were measured in the Brazilian sea experimental campaign with the Chl-a concentration obtained from a PNF instrument.

At each iteration, the RTE is solved using the candidate set of \(a\) and \(b\) values by the Laplace transform discrete ordinate (LTS\(_N\)) method [1, 23, 24]. The associated optimization problem is solved by an Ant Colony System (ACS) [12] implementation. A recent intrinsic regularization scheme that pre-selects candidate solutions based on their smoothness is applied, quantified by a Tikhonov norm. This scheme was proposed in a crystal growth inverse problem to reconstruct the diffusion coefficient [21].

A subsequent chlorophyll candidate profile is generated and iterations proceed. As hundreds of iterations are typically demanded and the direct model demands most of the processing time, a parallel implementation of the ACS is used and executed in a distributed memory machine. The code was parallelized using the Message Passing Interface (MPI) communication library [13]. The parallelization scheme distributes the pre-selected candidate solutions of the current iteration among the processors.

Results show the suitability of the proposed method using synthetic data with 5% and 30% noisy data, and also employing radiances collected in the experiment on board of the Brazilian oceanographic scientific ship. Reconstructions were performed using the proposed methodology with no depth correction factor for the radiances and with the new factor. The reconstructed profiles with the new depth correction factor have good agreement to the exact curves.

2. Radiative Transfer Equation in Hydrological Optics

The Radiative Transfer Equation (RTE) models the transport of photons through a medium [25]. Light intensity is given by a directional quantity, the radiance \(I\), that measures the rate
of energy being transported at a given point and in a given direction. Considering a horizontal plane, this direction is defined by a polar angle $\mu$ (relative to the normal of the plane) and a azimuthal angle $\phi$ (a possible direction in that plane). At any point of the medium, light can be absorbed, scattered or transmitted, according to the absorption ($a$) and scattering ($b$) coefficients and to a scattering phase function that models how light is scattered in any direction. An attenuation coefficient $c$ is defined as $c = a + b$ and the geometrical depth is mapped to an optical depth $\tau$ that imbeds $c$. Assuming a plane-parallel geometry, and a single wavelength, the unidimensional integral-differential RTE, can be written as:

$$
\mu \frac{\partial}{\partial \tau} I(\tau, \mu, \phi) + I(\tau, \mu, \phi) = \frac{\tau_0(\tau)}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} \beta(\mu, \phi; \mu', \phi') I(\tau, \mu', \phi') d\phi' d\mu' + S(\tau, \mu, \phi)
$$  \hspace{1cm} (1)

where $\mu \in [-1,1]$ and $\phi \in [0,2\pi]$ are the cosine of the incident polar angle $\theta$ and the incident azimuthal angle, respectively. $\tau_0(\tau) = b(\tau)/c(\tau)$ is the single scattering albedo. The scattering phase function $\beta(\mu, \phi; \mu', \phi')$, gives the scattering beam angular distribution, mapping the incident beam direction $(\mu, \phi)$ to the scattered direction $(\mu', \phi')$, and the source term is $S(\tau, \mu, \phi)$. The heterogeneous medium, in this case offshore ocean water is then modeled as a set of $R$ homogeneous finite layers. Boundary conditions are defined between regions, at the surface (incident light) and the bottom of the water. Each layer is denoted as being a region $r$ of the multiregion domain:

$$
\tau_0(\tau) = \tau_r \hspace{1cm} r = 1,2,\ldots,R .
$$  \hspace{1cm} (2)

There are several resolution methods, most of them adopting the Chandrasekhar’s decomposition on the azimuthal angle [11] that generates $L + 1$ integral-differential equations, each one with no dependence on $\phi$. For the discrete ordinate method, the above equations are approximated by a colocation method, where the $\mu$ integral is computed by the Gauss-Legendre quadrature formula. This yields a set of $N$ differential equations for each azimuthal mode. Each set (discretized RTE) is solved by the LTS$_N$ method [1, 23, 24], that generates a system of equations of order $R \times N$. For the considered test cases, it was assumed $R = 10$, $N = 20$ and $L = 0$ (azimuthal simmetry on $\phi$).

This work employs a bio-optical models to correlate the absorption and scattering coefficients of each region to the chlorophyll concentration. These coefficients are assumed to be constant in each region. Therefore discrete values $a_r$ and $b_r$ can be estimated for each region from the discrete values $C_r$.

Usually, chlorophyll profiles can be represented according Gaussian distributions [18]. A particular profile, corresponding to the Celtic Sea was considered:

$$
C(z) = 0.2 + \frac{144}{9\sqrt{2} \pi} \exp \left[-\frac{1}{2} \left(\frac{z-17}{9}\right)^2\right]
$$  \hspace{1cm} (3)

where $z$ is the depth in meters and $C$ is given in $mg/m^3$. This profile can be shown in section 5 of this work, termed exact profile. A bio-optical model was formulated by [19] for the absorption coefficient,

$$
a_r = \left[a^w + 0.06 \ a^c C_r^{0.65}\right] \left[1 + 0.2 \ e^{-0.014(\lambda-440)}\right]
$$  \hspace{1cm} (4)

where $a^w$ is the pure water absorption and $a^c$ is a nondimensional, statistically derived chlorophyll-specific absorption coefficient, and $\lambda$ is the considered wavelength, while another was $a^c_y$ formulated by [15] for the scattering coefficient,

$$
b_r = \left(\frac{550}{\lambda}\right) 0.30 C_r^{0.62}
$$  \hspace{1cm} (5)
The considered Celtic Sea profile refers to a type of water that present a high concentration of phytoplankton in comparison to organic particles [20]. The values of \( a^w \) and \( a^c \) depend on the wavelength and can be found in tables [18].

3. Inversion Scheme

This work formulates the inverse problem according to an implicit approach, leading to an optimization problem [16]. The set of parameters to be estimated, is given by \( p \), in this case, the \( R \) discrete values of the chlorophyll concentration \( C \) at optical depths \( \tau \) taken at the interface of the regions. Thus \( p_r = C(\tau_r) \) for \( r = 0, 1, ..., R - 1 \).

Experimental data are the discrete radiances \( I(\tau_r, \mu_i) \) for \( r = 0, 1, ..., R \) and \( i = 1, 2, ..., N \). The objective function \( J(p) \) is given by the square difference between experimental and model radiances plus a regularization term:

\[
J(p) = \sum_{r=0}^{R} \sum_{i=1}^{N} [I_{\text{exp}}(\tau_r, \mu_i) - I_p(\tau_r, \mu_i)]^2 + \gamma \Omega(p)
\]

The \( R \) discrete values of the concentration are estimated from \((R+1) \times N\) radiance values. \( \Omega(p) \) is the regularization function, that is weighted by a regularization parameter \( \gamma \). For instance, the 2nd order Tikhonov regularization [32] is defined by

\[
\Omega[p] = \sum_{i=2}^{R-1} (p_{i+1} - 2p_i + p_{i-1})^2 .
\]

The regularization term is required for noisy data due to the ill-posedness nature of inverse problems. Then, small changes in radiance data cause big changes in the concentration profile. There are some criteria for the choice of \( \gamma \), but an optimal value can be difficult to adjust, as it requires a choice criteria (Morozov discrepancy principle, L-curve, etc. [5]) that may demand many executions of the inverse solver. A value too small may yield a profile with fluctuations, while the opposite makes the profile flat.

The influence of radiance data of higher depths can be underestimated since radiances decrease is nearly exponential with depth. Therefore, a depth correction factor may be used in the objective function.

It is proposed a new depth correction factor \( (CF_r) \), given by the ratio between the mean radiance \( \overline{I}_r \) related to the polar angle \( \mu \) at each level \( r \) and the mean radiance at the surface \( \overline{I}_1 \). This is done separately for negative/upward \( (u) \) and positive/downward \( (d) \) polar directions. The depth correction factor for the regions \( r = 0, 2, ..., R - 1 \) is given by:

\[
\overline{I}_r = \sum_{i=1}^{N/2} I_{\text{exp}}(\tau_r, \mu_i)/(N/2)
\]

\[
CF^u_{r+1} = \left( \frac{\overline{I}_1}{\overline{I}_r} \right)^2 .
\]

For regions \( r = 1, 2, ..., R \) the depth correction factor is given:

\[
\overline{I}_r = \sum_{i=N/2+1}^{N} I_{\text{exp}}(\tau_r, \mu_i)/(N/2)
\]

\[
CF^d_r = \left( \frac{\overline{I}_1}{\overline{I}_r} \right)^2 .
\]
Thus, the objective function can be written as:

$$J(p) = \frac{N}{2} \sum_{i=1}^{R-1} CF_{r+1} \left[I^{exp}(\tau_r, \mu_i) - Ip(\tau_r, \mu_i)\right]^2 +$$

$$\sum_{i=N/2+1}^{N} \sum_{r=1}^{R} CF_{r} \left[I^{exp}(\tau_r, \mu_i) - Ip(\tau_r, \mu_i)\right]^2 + \gamma \Omega(p) \quad (12)$$

A previous correction factor was proposed by [31], where the radiance values at each level are corrected by \(\sqrt{e^{Z_r}}\). In this expression, \(Z_r = z_r/L\) (r=0,1,...,R), where \(z_r\) is the depth in meters and \(L\) is a scaling factor (in this work, \(L = 1.5\) m). Considering the adopted plane-parallel geometry, Fig. 1 compares the values of the upward depth-corrected radiances, while Fig. 2 compares the values of the downward depth-corrected radiances. In these figures, the radiance decay is shown in function of depth \(z\) and of the polar angle \(\mu\), for two cases: (a) no depth correction factor, and (b) using the proposed factor. Section 5 presents the reconstructed profiles for these two alternatives in a particular test case.

![Figure 1. Upward radiance I(z,\(\mu\)) decay: (a) no depth correction factor, and (b) with the proposed factor.](image)

4. Ant Colony System
The Ant Colony System (ACS) is a method that employs a meta-heuristic based on the collective behaviour of ants choosing a path between the nest and the food source [12]. Each ant marks its path with an amount of pheromone and the marked path is further employed by other ants as a reference. As an example of this, the sequence in Fig. 3 shows how ants, trying to go from point N to point F (a), behave when an obstacle is put in the middle of the original path, blocking the flow of the ants between points B and obstacle (b). Two new paths are then possible, either going to the left of the obstacle. The shortest path causes a greater amount of pheromone to be deposited by the preceding ants and thus more and more ants choose this path (c).

In the ACS optimization method, several generations of ants are produced. For each generation, a fixed amount of ants (\(na\)) is evaluated. Each ant is associated to a feasible path and this path represents a candidate solution, being composed of a particular set of edges of the graph that contains all possible solutions. Each ant is generated by choosing these edges on a probabilistic basis. This approach was succesfully used for the Traveling Salesman Problem...
Figure 2. Downward radiance $I(z, \mu)$ decay: (a) no depth correction factor, and (b) with the proposed factor.

(TSP) and other graph-like problems [2]. The best ant of each generation is then chosen and it is allowed to mark with pheromone its path. This will influence the creation of ants in the further generations. The pheromone put by the ants decays due to an evaporation rate. Finally, at the end of all generations, the best solution is assumed to be achieved.

Figure 3. Ants overcoming an obstacle in the trail – adapted from [12].

A solution is composed of linking $ns$ nodes and in order to connect each pair of nodes, $np$ discrete values can be chosen. This approach was used to deal with a continuous domain. Therefore, there are $ns \times np$ possible paths $[i,j]$ available. Denoting by $\rho$ the pheromone decay rate and $\tau_0$ the initial amount of pheromone, the amount of pheromone $\tau_{ij}$ at generation $t$ is given by:

$$\tau_{ij}(t + 1) = (1 - \rho)\tau_{ij}(t) + \tau_0 . \quad (13)$$

In this work, $\tau_0$ is calculated as suggested by [3] using an evaluation $Q$ of the function to be optimized obtained with a greedy heuristics:

$$\tau_0 = 1/(ns \times Q), \quad (14)$$
The probability of a given path \([i, j]\) be choosed is then

\[
P_{ij}(t) = \frac{[\tau_{ij}(t)]^\alpha [\eta_{ij}]^\beta}{\sum_l ([\tau_{il}(t)]^\alpha [\eta_{il}]^\beta)}
\]

where \(l \in [1, np]\) and \(\eta_{ij}\) is the visibility/cost of each path, a concept that arises from the TSP, where the cost is the inverse of the distance of a particular path. The above equation assumes that all paths are possible for any ant, but the TSP does not allow this assumption. The parameters \(\alpha\) and \(\beta\) are weights that establish the trade-off between the influence of the pheromone and the visibility in the probability of each path.

However, there is a further scheme for the choice of a path for a new ant. According to a roulette, a random number in the range \([0, 1]\) is generated for the new ant and it is compared with a parameter \(q_0\) chosen for the problem. If the random number is greater than this parameter, the path is taken according to \(P_{ij}\). If not, the most marked path is assigned.

In this work, the set of parameters (nodes) to be estimated is \(ns = R + 1\) discrete values of the Chl-a concentration \(C_r\), for \(r = 0, 1, ..., R\) at optical depths \(\tau\) taken at the upper interface of the regions. In Figure 4 is illustrated a hypothetical case where only three ants are used in the ACS method, in order to find the best Chl-a concentration profile, given by discrete values of \(C_r\).

![Figure 4](image)

**Figure 4.** Example of estimated Chlorophyll concentration profile obtained by three ants in the ACS algorithm. Bolded profile is the one with lowest objective function cost, in each ant generation/iteration.

In the current work, a ACS based inverse solver with a recent implicit regularization scheme [21] is proposed and employed without the explicit regularization \((\gamma = 0)\). Since here is an a priori information about the smoothness of the solution profile, such knowledge is included in the generation of the candidate solutions, by means of pre-selecting the smoother ants.

This information can be used as an alternative for the visibility \(\eta_{ij}\) of each path. First, an overpopulation of ants is generated, making \(\alpha = 1\) and \(\beta = 0\) in Equation (15) and after, a
certain fraction containing the smoother ants/paths is selected. Thus the visibility is assumed to be associated to the smoothness of the path. The criteria chosen to select the paths according to their smoothness was precisely the 2nd order Tikhonov norm - Equation (7), that is normally used as a regularization function. Such procedure is a kind of pre-regularization, and the usual regularization term is not required.

It was difficult to find an ACS visibility/cost criteria in this problem since it does not belong to the TSP class and this issue lead to choice of the smoothness for the path of each ant. It can be shown that the ACS has poor performance compared to other stochastic optimization algorithms when no visibility information can be defined. In addition, the proposed strategy leads to a reduction of the number of evaluations of the objective function and therefore improves the performance since the direct model demands a significant amount of processing time.

5. Numerical Results
The inverse solver, based on a ACS implementation, was tested for a multi-region \((R = 10)\) offshore ocean water radiative transfer problem considering \(N = 20\) polar angles and \(L = 0\) (azimuthal symmetry). Two sets of radiance data were used, corrupted with 5% and 30% gaussian noise.

In the test cases, as mentioned in section 2, synthetic data was used to simulate the experimental values of the Celtic sea. In the case of noisy data, no classical regularization was used \((\gamma = 0)\). Instead, the smoothness-based pre-selection was employed in the generation of the ants. The 2nd order Tikhonov norm was used as smoothness criteria.

Since radiance decay is nearly exponential with depth, the use of a depth correction factor may be required: radiances near the surface have a greater influence in the objective function than those at higher depths. A new depth correction factor, shown in Section 3, is proposed to balance the radiance values.

Similarly to other stochastic optimization algorithms, the tuning of parameters in the ACS has a big influence in the results. This implementation required adjustment of parameters like \(\rho\), the pheromone decay rate and \(q_0\), used in the roulette scheme. Other parameters may influence the quality of the solution, like the the number of \(np\) possible paths between each pair of the \(ns\) nodes, the number of ants \(na\), or the maximum number of iterations \(mit\). The adopted values for these parameters are shown in Table 1. In each generation, of the 90 \((na)\) ants, 1/6 were pre-selected according to their smoothness.

| seed | ns  | np  | na  | mit | \(\rho\) | \(q_0\) |
|------|-----|-----|-----|-----|--------|--------|
| 33   | 10  | 3000| 90  | 500 | 0.03   | 0.0    |

Figs. 5 and 6 shows the reconstructed profile of the chlorophyll concentration, using 5% and 30% noisy data, respectively. The exact solution is compared to the estimations performed using the ACS-based solver employing no depth correction factor, and the proposed factor for the reconstruction using 5% noisy data. It can be seen that the use of the proposed depth correction factor was decisive for the quality of the solution.

In an oceanographic campaing at the fall 2003 [28], Chl-a concentration was measured in several depths, using a sensor for natural fluorescence (PNF, Biospherical instruments). Experimental data was collected from some stations, numerated as 7448, 7452, 7456, 7457. Three of these stations (7448, 7456, 7457) were described in reference [28]. Station 7456 presented a Chl-a concentration profile similar to the previous profiles used to test the present inverse scheme.
Figure 5. Chlorophyll profile reconstruction using 5% gaussian noisy radiance data with no depth correction factor and with the proposed correction factor.

Figure 6. Chlorophyll profile reconstruction using 30% gaussian noisy radiance data with the proposed depth correction factor.
The PNF instrument is able to measure Chl-a concentration for every depth. For our purpose, it was convenient to choose the 10 depths that correspond to the forward problem in each station, in order to reconstruct the discrete concentration profile using the ACS algorithm.

The Chl-a concentration profile estimated by PNF instrument for stations 7448 and 7452 (solid line in Figures 7 and 8, respectively) showed bi-modal and unimodal profiles. These profiles could be considered real ones, and they are used to produce synthetic noiseless experimental radiances.

The depicted inverse solutions obtained from an average after 10 realizations of the ACS, regarding to 10 different seeds for this stochastic algorithm, is also showed in Figures 7 and 8, for both station profiles. For Figure 7, an unimodal Gaussian is a good representation. Figure 8 presents a two-peaked concentration profile. The numerical inverse solution was not able to identify these two peaks. However, the retrieved concentration profile can be considered satisfactory, since it is close to the exact solution.

![Graph showing Chl-a concentration profiles and inverse solutions.](image)

**Figure 7.** Average Chl-a unimodal profile reconstruction from 10 realizations of ACS, using noiseless synthetic radiances.

### 6. Conclusions

This work presented a methodology for the estimation of the chlorophyll concentration vertical profiles in natural waters from radiance data in several depths. Vertical profiles of the absorption and scattering coefficients that are required by the forward model can be obtained using the chlorophyll profile by means of bio-optical models.

It is proposed here a depth correction factor for the radiances and a recent pre-regularization scheme that filters candidate solutions according to their smoothness. The inverse solver is an implementation of the Ant Colony System meta-heuristics.

The ACS-based inverse solver yielded a good estimation of chlorophyll vertical profiles using the new depth correction factor using noiseless radiance data and also 5% and 30% noisy data. No standard regularization was used in the objective function, since the pre-regularization...
scheme yielded good solutions. The quality of the identified profiles and the performance results were discussed for reconstructions using synthetic experimental data.

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