

Data-Informed Inversion Model (DIIM): a framework to retrieve marine optical constituents using a three-stream irradiance model

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Abstract. Within the New Copernicus Capability for Trophic Ocean Networks (NECCTON) project, we aim to improve the current data assimilation system by developing a method for accurately estimating marine optical constituents from satellite-derived Remote Sensing Reflectance. We compared two frameworks based on the implicit inversion of a semi-analytical model derived from the classical Radiative Transfer Equation. The first approach employed an iterative Bayesian inversion with a Gaussian approximation, which provides Maximum A Posteriori (MAP) estimates of the optical constituents along with their associated uncertainties. To improve the model performance, we optimized the model parameters using historical in-situ measurements from the BOUSSOLE buoy and a Markov Chain Monte Carlo (MCMC) algorithm, which reduced the Root Mean Square Error (RMSE) between the retrieved and observed values. The second approach employed the Stochastic Gradient Variational Bayes (SGVB) estimator, which is designed to approximate the MAP estimates of the optical constituents while simultaneously optimizing the model parameters through maximum likelihood. This method resulted in faster computations than the iterative Bayesian inversion, while maintaining comparable RMSE values. While the iterative Bayesian inversion provided reliable uncertainty estimates, the SGVB estimator offered faster computations of the optical constituents. Moreover, using a dataset of in-situ sea surface chlorophyll-a concentrations across a broad region of the Northwestern Mediterranean Sea, we compared the inversion techniques with a state-of-the-art algorithm used within the Copernicus Marine Service, finding comparable performances across methods. Notably, the SGVB estimator showed the highest correlation between in-situ measurements and retrievals throughout the analyzed region. We conclude that both inversion methods achieve a performance comparable to existing state-of-the-art algorithms. The Gaussian approximation offers robust uncertainty quantification, while the SGVB estimator provides a reliable and computationally efficient alternative.

1 INTRODUCTION

Operational systems, like Copernicus, use satellite-derived data, combined with data assimilation techniques, to obtain estimates of the marine ecosystem status. Traditionally, the assimilated variable is the chlorophyll retrieved data; nowadays, state of the art biogeochemical models are progressively including refined bio-optical models able to simulate optical variables such as Remote Sensing Reflectance, enabling the direct assimilation of multispectral reflectance measured by satellite sensors.

In this work, we aim to derive a framework to estimate the ocean inherent optical properties (IOPs), such as absorption and scattering coefficients, from measurements of satellite-derived apparent optical properties (AOPs), like irradiance and Remote Sensing Reflectance. The IOPs are of interest in their own right, as they carry key information about ecosystem variables, such as chlorophyll, which can be used as indicators of the trophic condition of large marine areas (Longhurst et al., 1996). Most importantly, the framework is intended to be employed as a module in a data assimilation scheme (Bruggeman et al., 2023), within operational model services, to perform Remote Sensing Reflectance assimilation in a coherent way, providing an aligned forward and inverse procedure.

The retrieval of the IOPs of water bodies from measurements of the AOPs, is referred to as the inverse problem of ocean optics. This is crucially important since directly measuring IOPs with an extended spatial coverage is very difficult (Gordon, 2002).

The first step to compute the IOPs is to establish the forward relationship between the AOPs and the IOPs. In this context, the AOPs are described as a function of the IOPs using the Radiative Transfer Equation (RTE). Due to the complexity of the RTE, this computation is carried out in simple scenarios, resulting in simplified equations that can be solved analytically. Other approaches involve using semi-analytical equations or empirical relations, where the latter are combined with simplified expressions of the RTE. The inverse problem is solved using these forward computations to estimate the IOPs either explicitly, by analytically inverting the forward process (Zaneveld, 1989; Leathers et al., 1999; Tao et al., 1994; McCormick, 1996; Stramska et al., 2000; Salama and Verhoef, 2015; Lazzari et al., 2024), or implicitly, by using an estimate of the IOPs in the forward process and then iteratively adjusting the IOP values to match measurements of the AOPs (Gordon and Boynton, 1997; Boynton and Gordon, 2000; Michalopoulou et al., 2009; Salama and Verhoef, 2015; Erickson et al., 2023; Lazzari et al., 2024).

In this work, we focused on an implicit inverse method following Lazzari et al. (2024), but giving the method a probabilistic interpretation, allowing for the uncertainty estimation of the retrieved quantities. The forward model is the bio-optical model presented in Dutkiewicz et al. (2015) and described in section 2.1, a three-stream semi-analytical irradiance model. The IOPs from the bio-optical model are the absorption, scattering, and backward scattering coefficients of four optical constituents: water, chlorophyll- α (whose increase or decrease is associated with changes in the concentration of phytoplankton), Chromophoric Dissolved Organic Matter, and Non Algal Particles. We focused on finding the sea surface concentration of these optical constituents, since we estimated the former IOPs as linear combinations of the latter. The model also depends on ad hoc parameters, originally computed as part of empirical relations from different studies (Morel, 1974; Aas, 1987; Dutkiewicz et al., 2015; Mason et al., 2016; Álvarez et al., 2023). We also optimized these parameters such that the retrieved quantities are accurate with respect to historical in-situ observations.

We compared two different frameworks. The first one is a Bayesian estimation, where we used a linearization of the forward process for estimating the uncertainties of the optical constituents, and Markov Chain Monte Carlo (MCMC) (Chib and Greenberg, 1995; Andrieu and Thoms, 2008) for the uncertainty of the parameters. This approach is described in section 4.

The second approach is based on Variational Bayes, by using the Stochastic Gradient Variational Bayes (SGVB) estimator, introduced by Kingma and Welling (2013), and described in section 4.4. It allows for the estimation of parameters while also learning an estimate of the posterior distribution of the optical constituents. The idea is to approximate the probability

distribution of the optical constituents given the satellite-derived Remote Sensing Reflectance using a neural network. This is the same framework used to train generative models known as Variational Auto Encoders (VAE), which have also been used to solve inversion problems (Zhong et al., 2019, 2021; Zhao et al., 2023; Shmakov et al., 2024). Originally proposed to solve inversion problems for cases when the posterior distribution is intractable (practically impossible to compute), this framework provides a fast way of estimating optical constituents, which are consistent with the forward model and the in-situ observations.

We employed three data sources covering a period from 2005 to 2012: A dataset of historical satellite-derived Remote Sensing Reflectance, a dataset from the Ocean–Atmosphere Spectral Irradiance Model (OASIM, used as boundary conditions for the bio-optical model (Gregg and Casey, 2009)), and a set of in-situ measurements from the BOUSSOLE buoy, located in the Ligurian basin of the northwestern Mediterranean Sea (coordinates 7.54°E, 43.22°N) (Antoine et al., 2008). The description of the different datasets is presented in section 3.

2 BIO-OPTICAL MODEL

We now describe the Bio-optical model (Aas, 1987; Ackleson et al., 1994; Dutkiewicz et al., 2015; Álvarez et al., 2023), which details the interaction of the radiance with different constituents in the sea, called optical constituents. In section 2.1 we present the model of the water-leaving radiance, based on the classical Radiative Transfer Model (Dutkiewicz et al., 2015). In section 2.2, we use this model to compute the theoretical Remote Sensing Reflectance (R_{rs}^{MODEL}) (Aas and Højerslev, 1999). The inversion problem aims to use this model, named the forward model, and satellite measurements to retrieve optical constituents that are consistent with future observations. For this end, we used historical in-situ observations described in section 2.3.

2.1 Radiative Transfer Model

To simulate the water-leaving radiance, we followed Dutkiewicz et al. (2015), using a one-dimensional, three-stream radiance model, where the vertical component of the radiance over the water column is decomposed into three interacting components (see Fig. 1) following the system of equations,

$$\begin{aligned} \frac{dE_{\text{dir}}(h, \lambda)}{dh} &= -\frac{a(\lambda) + b(\lambda)}{\cos \theta} E_{\text{dir}}(h, \lambda), \\ \frac{dE_{\text{dif}}(h, \lambda)}{dh} &= -\frac{a(\lambda) + r_s b_b(\lambda)}{v_s} E_{\text{dif}}(h, \lambda) + \frac{r_u b_b(\lambda)}{v_u} E_u(h, \lambda) + \frac{b(\lambda) - r_d b_b(\lambda)}{\cos \theta} E_{\text{dir}}(h, \lambda), \\ \frac{dE_u(h, \lambda)}{dh} &= -\frac{r_s b_b(\lambda)}{v_s} E_{\text{dif}}(h, \lambda) + \frac{a(\lambda) + r_u b_b(\lambda)}{v_u} E_u(h, \lambda) - \frac{r_d b_b(\lambda)}{\cos \theta} E_{\text{dir}}(h, \lambda). \end{aligned} \quad (1)$$

These three equations describe how the vertical direct irradiance $E_{\text{dir}}(h, \lambda)$ is attenuated by absorption, with $a(\lambda)$ the total absorption coefficient, and scattered into downward $E_{\text{dif}}(h, \lambda)$, and upward irradiance $E_u(h, \lambda)$, $b(\lambda)$ the total scattering coefficient, $b_b(\lambda)$ the total backward scattering coefficient, r_d , r_s and r_u the effective scattering coefficients normalized with respect to the backward scattering coefficients, $\cos(\theta)$, v_s and v_u the average cosines of the irradiance components, θ the Sun zenith angle, h the depth, and λ the wavelength.

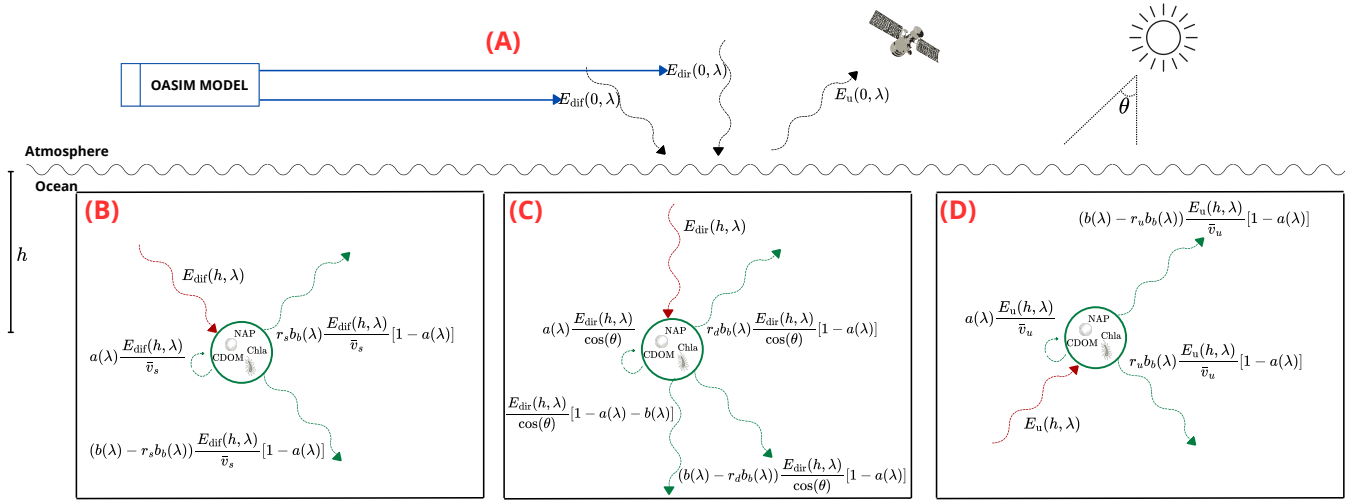


Figure 1. Diagram illustrating the main components of Eq. 1, showing: (A) the incoming irradiance (modeled using the OASIM model; see Sec. 3), and how it interacts with chlorophyll, non-algal particles, and colored dissolved organic matter (CDOM), leading to the attenuation and scattering of: (B) the diffuse, (C) direct, and (D) upward component into upward and downward fluxes.

Following Dutkiewicz et al. (2015), the values for r_d , r_s , r_u , v_s and v_u are approximated as constants (see Tab. 2). See Dutkiewicz et al. (2015), appendix B, for a derivation starting from the classical radiative transfer equation. For previous studies where similar transfer models have been used, see Aas (1987); Ackleson et al. (1994); Salama and Verhoef (2015); Álvarez et al. (2023) and Lazzari et al. (2024).

90 The total absorption and scattering coefficients are modeled as,

$$\begin{aligned}
 a(\lambda) &= a_w(\lambda) + a_{\text{phy}}(\lambda)\text{chla} + a_{\text{CDOM}}(\lambda)\text{CDOM} + a_{\text{NAP}}(\lambda)\text{NAP}, \\
 b(\lambda) &= b_w(\lambda) + b_{\text{phy}}(\lambda)C + b_{\text{NAP}}(\lambda)\text{NAP}, \\
 b_b(\lambda) &= b_{b,w}(\lambda) + b_{b,\text{phy}}(\lambda)C + b_{b,\text{NAP}}(\lambda)\text{NAP},
 \end{aligned} \tag{2}$$

with chla, NAP and CDOM the concentration of the optical constituents Chlorophyll- α , Non Algal Particles and Chromophoric Dissolved Organic Matter respectively; $a_w(\lambda)$ is the water-specific absorption coefficient, $b_w(\lambda)$ and $b_{b,w}(\lambda)$ the water-specific scattering and backward scattering coefficients, $a_{\text{phy}}(\lambda)$ the chlorophyll-specific absorption coefficient of phytoplankton, $b_{\text{phy}}(\lambda)$ and $b_{b,\text{phy}}(\lambda)$ the carbon-specific scattering coefficients of phytoplankton (see Tab. 1), C the carbon concentration, which is derived as a function of chlorophyll and irradiance (Geider et al., 1997), with the chla:C ratio represented as a sigmoid curve dependent on Photosynthetic Available Radiation (PAR), as

$$C = \text{chla} / \left(\Theta_{\text{chla}}^0 \frac{e^{-(\text{PAR}-\beta)/\sigma}}{1 + e^{-(\text{PAR}-\beta)/\sigma}} + \Theta_{\text{chla}}^{\min} \right), \tag{3}$$

Table 1. Parameters dependent of λ used for the Radiative Transfer Model evaluation, with the water-specific absorption coefficient $a_w(\lambda)$ from Mason et al. (2016), the water-specific scattering and backward scattering coefficients $b_w(\lambda)$, $b_{b,w}(\lambda)$ with values interpolated from Morel (1974), the phytoplankton-specific absorption coefficient $a_{phy}(\lambda)$ interpolated from the average values of different phytoplankton functional types from (Álvarez et al., 2023), and the carbon-specific scattering and backward scattering coefficients $b_{phy}(\lambda)$ $b_{b,phy}(\lambda)$ from (Dutkiewicz et al., 2015).

λ [nm]	$a_w(\lambda)$ [m^{-1}]	$b_w(\lambda)$ [m^{-1}]	$b_{b,w}(\lambda)$ [m^{-1}]	$a_{phy}(\lambda)$ [$\text{m}^2(\text{mgChla})^{-1}$]	$b_{phy}(\lambda)$ [$\text{m}^2(\text{mgC})^{-1}$]	$b_{b,phy}(\lambda)$ [$\text{m}^2(\text{mgC})^{-1}$]
412.5	0.00271	0.00535	0.002674	0.03713	0.00318	3.25E-06
442.5	0.00574	0.00437	0.002184	0.04019	0.00311	3.30E-06
490.0	0.01460	0.00284	0.001421	0.02741	0.00335	3.41E-06
510.0	0.03300	0.00247	0.001234	0.01981	0.00347	3.42E-06
555.0	0.06098	0.00167	0.000836	0.00917	0.00353	3.39E-06

with Θ_{chla}^0 , β , σ , $\Theta_{\text{chla}}^{\min}$ constant parameters (see Tab. 2), $a_{\text{CDOM}}(\lambda)$, $a_{\text{NAP}}(\lambda)$ and $b_{\text{NAP}}(\lambda)$ the mass-specific absorption and scattering coefficients for CDOM and NAP respectively (Álvarez et al., 2023), with the latter calculated as,

$$\begin{aligned}
 a_{\text{CDOM}}(\lambda) &= d_{\text{CDOM}} e^{-S_{\text{CDOM}}(\lambda-450)}, \\
 a_{\text{NAP}}(\lambda) &= d_{\text{NAP}} e^{-S_{\text{NAP}}(\lambda-440)}, \\
 b_{\text{NAP}}(\lambda) &= e_{\text{NAP}} \left(\frac{550}{\lambda} \right)^{f_{\text{NAP}}},
 \end{aligned} \tag{4}$$

with S_{CDOM} , d_{CDOM} , S_{NAP} , d_{NAP} , e_{NAP} , f_{NAP} constant parameters (see Tab. 2), and $b_{b,\text{NAP}} = b_{r,\text{NAP}} b_{\text{NAP}}$, with $b_{r,\text{NAP}}$ the backscattering-to-scattering ratio of NAP.

PAR was computed following Lazzari et al. (2020), as,

$$\text{PAR} = \frac{10^6}{N_A h c} \int_{400\text{nm}}^{700\text{nm}} (E_{\text{dif}}(0, \lambda) + E_{\text{dir}}(0, \lambda)) \lambda d\lambda \tag{5}$$

with N_A the Avogadro's number, c the speed of light and h the plancks constant.

For the rest of this work, we assumed only one homogeneous layer with constant densities. For deep case 1 waters, like the one studied in the present work, during winter, the chlorophyll concentration in the first layer is approximately constant due to mixing (see Mignot et al. (2011), Fig. 1), while most of the downward irradiance comes from the first 10 to 20 meters (see Simpson and Dickey (1981), Fig. 1 and Fig. 2). During summer, there is no mixing, but still there is a region of around 20 to 50 meters with constant chlorophyll concentrations, making the assumption justified.

2.2 Remote Sensing Reflectance

We used the system of equations in Eq. (1), subject to the boundary conditions

$$E_{\text{dir}}(0, \lambda) = E_{\text{dir}}^{\text{OASIM}}(0, \lambda), E_{\text{dif}}(0, \lambda) = E_{\text{dif}}^{\text{OASIM}}(0, \lambda), E_u(\infty, \lambda) = 0, \tag{6}$$

Table 2. Parameters independent of λ used for the Radiative Transfer Model evaluation, $r_d, r_s, r_u, v_s, v_u, S_{\text{CDOM}}, d_{\text{CDOM}}$ from Dutkiewicz et al. (2015) who took them from Aas (1987), $\Theta_{\text{chla}}^0, \Theta_{\text{chla}}^{\min}, \sigma, \beta$ computed as an empirical model from data in the BOUSSOLE Site (Lazzari et al., 2024), $S_{\text{NAP}}, d_{\text{NAP}}, e_{\text{NAP}}, f_{\text{NAP}}$ and $b_{r,\text{NAP}}$ from Álvarez et al. (2023), Q_a and Q_b from Aas and Højerslev (1999), and, T and γ from Lee et al. (2002).

Parameter name	Symbol	Value from literature	Units
Normalized effective scattering coefficient for direct irradiation	r_d	1.0	-
Normalized effective scattering coefficient for downward radiation,	r_s	1.5	-
Normalized effective scattering coefficient for backward radiation,	r_u	3.0	-
Average cosine for downward scattered radiation	v_s	0.83	-
Average cosine for upward scattered radiation	v_u	0.4	-
-	Θ_{chla}^0	0.03	$\text{mgChla}(\text{mgC})^{-1}$
-	$\Theta_{\text{chla}}^{\min}$	0.005	$\text{mgChla}(\text{mgC})^{-1}$
-	σ	20	$(\text{mmol})\text{m}^{-2}\text{s}^{-1}$
-	β	500	$(\text{mmol})\text{m}^{-2}\text{s}^{-1}$
CDOM mass-specific absorption at 450 nm	d_{CDOM}	0.015	$\text{m}^2(\text{mgCDOM})^{-1}$
CDOM mass-specific absorption spectral slope between 350 and 500 nm	S_{CDOM}	0.017	nm
NAP mass-specific absorption at 440 nm	d_{NAP}	0.0013	$\text{m}^2(\text{mgNAP})^{-1}$
NAP mass-specific absorption spectral slope between 350 and 500 nm	S_{NAP}	0.013	nm
NAP mass-specific scattering at 550 nm	e_{NAP}	0.02875	$\text{m}^2(\text{mgNAP})^{-1}$
-	f_{NAP}	0.5	-
Backscattering-to-scattering ratio of NAP	$b_{r,\text{NAP}}$	0.005	-
-	Q_a	5.33	-
-	Q_b	0.45	-
-	T	0.52	-
-	γ	1.7	-

115 with $E_{\text{dir}}^{\text{OASIM}}(0, \lambda)$, $E_{\text{dif}}^{\text{OASIM}}(0, \lambda)$, the direct and diffuse downward irradiance on the surface of the ocean. For this work, we used the values from the OASIM model (Gregg and Casey, 2009). By assuming an infinitely deep and homogeneous column of water (Ronald and Zaneveld, 1982), the system of equations can be solved analytically, with the final expression presented in Appendix A.

The Remote Sensing Reflectance $R_{rs}^{\text{MODEL}}(\lambda)$ can be computed from the solution $E_u(0, \lambda)$ (Aas and Højerslev, 1999) as

$$120 \quad R_{rs}^{\text{MODEL}}(\lambda) = \frac{E_{u,\lambda}(0)}{Q(\theta) (E_{\text{dir},\lambda}(0) + E_{\text{dif},\lambda}(0))} \quad (7)$$

with

$$Q(\theta) = Q_a e^{-Q_b \sin(\pi/180(90-\theta))}, \quad (8)$$

Q_a and Q_b constant parameters (see Tab. 2).

Due to the interaction in the interface between the sea surface and the atmosphere, a correction has to be added to the R_{rs}^{MODEL} (Lee et al., 2002), with the relation,

$$R_{rs,down}(\lambda) = \frac{R_{rs,up}(\lambda)}{T + \gamma R_{rs,up}(\lambda)} \quad (9)$$

where T and γ are constant parameters (see Tab. 2), $R_{rs,down}(\lambda)$ is the Remote Sensing Reflectance just under the sea surface, and $R_{rs,up}(\lambda)$ is the Remote Sensing Reflectance just up the sea surface.

Thus, the final expression for R_{rs}^{MODEL} is a model that depends on the optical constituents and the boundary conditions.

Since the Satellite Remote Sensing Reflectance measures are a merged product of many satellite samples (see Sec 3) during the day, the direct and diffuse downward irradiance on the surface of the ocean were computed as daily averages, only during hours with sun. For this reason, the densities involved in the computation of Eq. 7 are also daily averages.

2.3 Model of the in-situ observations

We aim to model the chlorophyll- α as the retrieved quantity from the inversion problem. The particulate backward scattering coefficient ($b_{b,p}(\lambda)$) is modeled as the contribution to backward scattering from the phytoplankton and NAP,

$$b_{b,p}(\lambda) = b_{b,phy}(\lambda)C + b_{b,NAP}(\lambda)NAP \quad (10)$$

where the carbon C is calculated as Eq. (3). The downward light attenuation coefficient (k_d) is computed by the relation,

$$E_{\text{dir}}(h, \lambda) + E_{\text{dif}}(h, \lambda) = (E_{\text{dir}}^{\text{OASIM}}(0, \lambda) + E_{\text{dif}}^{\text{OASIM}}(0, \lambda))e^{-k_d h}. \quad (11)$$

3 DATA ACQUISITION

3.1 Ocean–Atmosphere Spectral Irradiance Model (OASIM)

The OASIM model (Gregg and Casey, 2009) uses as input the cloud, aerosol, and atmospheric conditions to simulate the propagation of light in the atmosphere, and return the irradiance at the surface of the ocean. We used the validated outputs for the BUOSSOLE site (Antoine et al., 2008) computed in Lazzari et al. (2020) as the boundary conditions in Eq. 6. The outputs are the surface downward direct irradiance E_{dir} and the surface downward scattered irradiance E_{dif} , from which the Photosynthetic Available Radiation PAR can be computed (Lazzari et al., 2020). The output from the model is in 33 wavelengths from 200 nm to 4 μm . As described in Lazzari et al. (2020), these values are further interpolated at wavelengths 412.5 nm, 442.5 nm, 490 nm, 510 nm and 555 nm.

3.2 Satellite-derived Remote Sensing Reflectance

We used a Level 3 product provided by the E.U. Copernicus Marine Service Information (CMEMS). This is a merge of Level 2 Remote Sensing Reflectance from different satellite sources, as explained in Colella et al. (2023). This product provides pre-processed Remote Sensing Reflectance with daily resolution, spatial resolution of one kilometer, at six different wavelengths:

412 nm, 443 nm, 490 nm, 510 nm, 555 nm and 670 nm. Due to the fact that for oligotrophic and mesotrophic water, the absorption of water for wavelengths higher than 555 nm is dominant over the other constituents (Lee et al., 2002), we focus our attention on the data with wavelengths less than or equal to 555 nm. The values at the wavelengths 412 nm and 443 nm were assumed to be the same as the values with wavelengths at 412.5 nm and 442.5 nm in order to match the values computed with the OASIM model.

3.3 In-situ observations

We used three in-situ observations: chlorophyll- α , particulate backward scattering coefficient, and downward light attenuation coefficient, with data from the BOUSSOLE buoy (Antoine et al., 2008) retrieved as explained in Lazzari et al. (2024).

The three sets of measurements had 15 15-minute resolution. We used only measurements between 10:00 and 14:00 GMT as representative. First, we removed the data coming from the buoy if it reported an absolute tilt higher or lower than 10 degrees. We also removed the ones reported at a depth more than 2 m below the nominal values (4 m and 9 m, depending on the instrument of measurement). Next, the downward light attenuation coefficient data were filtered with a Butterworth high-pass filter, using the package SciPy (Virtanen et al., 2020) from the programming language Python (Van Rossum and Drake, 2009), filtering the noise with a frequency less than 4 hours. Finally, we proceeded to average the daily values.

Due to low vertical variability, the measurements of chlorophyll- α and particulate backward scattering coefficient were considered as the values just below the water-air interface, even if the instruments were at 9 m deep. The former one had measurements at wavelengths equal to 442 nm, 488 nm, 550 nm, and 620 nm.

On the contrary, due to the high vertical variability of the downward light attenuation coefficient, the measurements were considered to be at a depth of 9 m, with values at the wavelengths 412 nm, 442 nm, 490 nm, 510 nm, 555 nm, 560 nm, 665 nm, 670 nm, 681 nm.

For the same reasoning described in section 3.2, we only used the values less than or equal to 555 nm. The values at the wavelengths 412 nm, 442 nm, 488 nm and 550 nm were assumed to be the same as the values with wavelengths at 412.5 nm, 442.5 nm, 490 nm and 555 nm in order to match the values computed with the OASIM model.

In other words, taking into account the previously said assumptions and data availability, the in-situ observations considered are sea surface chlorophyll, 9 meters deep downward light attenuation coefficient in 5 wavelengths, (412.5,442.5,490,510,555) nm, and sea surface particulate backward scattering coefficient at 3 wavelengths (442,490,510)nm.

4 BAYESIAN INVERSE PROBLEM

The model for the Remote Sensing Reflectance (R_{rs}^{MODEL}) depends on the concentration of the optical constituents chl a , NAP and CDOM. The inverse problem consists of retrieving these constituents from the forward model and the satellite observations (R_{rs}^{OBS}). In Sec. 4.1 we formalize the problem and introduce the nomenclature that is going to be used in the next sections, then in Sec. 4.2 and 4.3 we introduce the Bayesian approach to solve the problem (Rodgers, 2000), as well as the approach used to optimize the model.

4.1 Formal statement of the problem

185 We proceed to call $y \in \mathcal{Y}$ the set of wavelength-dependent satellite measurements, modeled with a forward model plus noise,

$$y(\lambda) = R_{rs}^{MODEL}(z, x(\lambda), \lambda; \Lambda) + \epsilon(\lambda), \quad (12)$$

where

$$x(\lambda) = (E_{\text{dif}}^{\text{OASIM}}(0, \lambda), E_{\text{dir}}^{\text{OASIM}}(0, \lambda), \theta, \text{PAR})$$

are available simulated quantities, $x \in \mathcal{X}$, gathered from the OASIM model,

$$\Lambda = (r_s, r_u, r_d, v_s, v_u, a_w(\lambda), a_{\text{phy}}(\lambda), b_w(\lambda), b_{\text{phy}}(\lambda), b_{b,w}(\lambda), b_{b,\text{phy}}(\lambda), \\ 190 \quad d_{\text{CDOM}}, S_{\text{CDOM}}, d_{\text{NAP}}, S_{\text{NAP}}, e_{\text{NAP}}, f_{\text{NAP}}, b_{r,\text{NAP}}, \Theta_{\text{chla}}^0, \Theta_{\text{chla}}^{\min}, \beta, \sigma, Q_a, Q_b, T, \gamma),$$

is the set of parameters listed together with their literature values in Tab. 1 and Tab. 2, and

$$z = (\text{chla}, \text{NAP}, \text{CDOM}) \quad (13)$$

is the set of unknown or latent quantities $z \in \mathcal{Z}$, which are the optical constituents.

By performing the inversion, we compute an estimate of the unknown daily quantity z^d , which only depends on the mea-
 195 surements and OASIM data from the same day. Each day, minimization is independent of the others, like screenshots of the state of the ocean, from which we aim to estimate the average concentrations of the active optical constituents.

Since we have measurements for a discrete set of wavelengths (at a depth $h = 0$ m, except k_d , at a depth $h = 9$ m), the input of the forward model is discretized as a five-dimensional vector, with each component representing values at different wave-
 lengths. To distinguish between continuous functions and their respective discretization, λ is used as a subscript, e.g. $E_{\text{dir},\lambda}$ rep-
 200 represents a component of the five dimensional vector $\mathbf{E}_{\text{dir}}$, with magnitudes $E_{\text{dir}}(0, \lambda)$, where $\lambda = (412.5, 442.5, 490, 510, 555)$ nm. In similar fashion, $x_\lambda = (E_{\text{dif},\lambda}, E_{\text{dir},\lambda}, \theta, \text{PAR})$ is a component of the 4×5 tensor $\mathbf{x}$. Using this notation, the measurements and OASIM-data of the day d are written as $(\mathbf{y}^d, \mathbf{x}^d)$.

The noise ϵ is added to the model to account for the different sources of uncertainty. In this work, we assumed that ϵ is a random Gaussian variable with mean zero, and covariance Σ_ϵ .

205 As a consequence, the model of the measurement is a random variable with a Gaussian probability distribution

$$y \sim p_\Lambda(\mathbf{y}|z, \mathbf{x}) = \mathcal{N}(\mathbf{R}_{rs}^{MODEL}(z, \mathbf{x}; \Lambda), \Sigma_\epsilon). \quad (14)$$

4.2 Bayesian approach to retrieve the latent variable

Under the Bayesian framework (Rodgers, 2000), the probability of the unknown quantity z , $p(z|\mathbf{y}, \mathbf{x})$, given the true probability distribution of the measurement $p(\mathbf{y}|z, \mathbf{x})$, can be retrieved using the Bayes theorem,

$$210 \quad p(z|\mathbf{y}, \mathbf{x}) = \frac{p(\mathbf{y}|z, \mathbf{x})p(z|\mathbf{x})}{p(\mathbf{y}|\mathbf{x})}. \quad (15)$$

Table 3. Root Mean Square Difference (RMSD) between in-situ measurements and the satellite measurements of R_{rs} in the Mediterranean Sea, obtained from a validation of the Copernicus Dataset (Colella et al., 2023).

$R_{rs,\lambda}$	RMSD($R_{rs,\lambda}$)
$R_{rs,412.5}$	1.5×10^{-3} sr
$R_{rs,442.5}$	1.2×10^{-3} sr
$R_{rs,490}$	1×10^{-3} sr
$R_{rs,510}$	8.6×10^{-4} sr
$R_{rs,555}$	5.7×10^{-4} sr

The probability distribution $p(z|\mathbf{y}, \mathbf{x})$ is called the posterior probability distribution, or just the posterior, $p(\mathbf{y}|z, \mathbf{x})$ the likelihood, and $p(z|\mathbf{x})$ the prior probability distribution, or just the prior.

Since we are dealing with random variables, computing the posterior is equivalent to retrieving z . In the case when this computation is not possible, common approaches attempt to estimate the value of z that maximizes the posterior, named
215 Maximum A Posteriori (MAP) estimate.

In the case of little knowledge of the value of z , it is common practice to use an improper prior, $p(z|\mathbf{x})$, as an uninformative prior, where each value of z is equally probable. With this choice of prior, the MAP is equivalent to finding the Maximum Likelihood Estimate (MLE).

In this work, we used a log-normal distribution prior (Campbell, 1995) for the latent variable z , with parameters μ_z, Σ_z . This
220 is equivalent to making the change of variable $\tilde{z} = \log(z)$ with a Gaussian prior with mean μ_z and covariance Σ_z . With this prior, and the Gaussian likelihood which can be derived from the forward model $\mathbf{R}_{rs}^{MODEL}$, we can define the loss function

$$\begin{aligned} \mathcal{L}^{z,d}(\mathbf{y}^d, \mathbf{x}^d, \tilde{z}^d; \Lambda) &= -2 \log(p_\Lambda(\tilde{z}^d | \mathbf{y}^d, \mathbf{x}^d)) \\ &= (\mathbf{y}^d - \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}^d; \Lambda))^T \Sigma_\epsilon^{-1} (\mathbf{y}^d - \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}^d; \Lambda)) + (\tilde{z}^d - \mu_z)^T \Sigma_z^{-1} (\tilde{z}^d - \mu_z) + c_0 \end{aligned} \quad (16)$$

with c_0 a constant. It can be shown that minimizing the loss function in Eq. (16), is the same as maximizing the posterior (Rodgers, 2000). In other words, We are interested in finding the $\tilde{z}^d$ that minimizes this loss function, as an estimate of the true
225 value for the optical constituents (under the log-normal assumptions).

As an estimate of Σ_ϵ , we used a diagonal matrix, with elements equal to the square of the Root Mean Square Difference (RMSD) between in-situ measurements and the satellite measurements of R_{rs} in the Mediterranean Sea, shown in Tab. 3, obtained from a validation of the Copernicus Dataset (Colella et al., 2023). This choice for Σ_ϵ is equivalent to assuming independence between measurements y_λ^d with different wavelengths.

230 For the prior parameters, we used $\mu_z = 0$ and $\Sigma_z = \mathbb{1}\alpha$, with $\mathbb{1}$ a diagonal matrix of dimension 3×3 , and α a hyperparameter to be determined. This choice of Σ_z is equivalent to a ℓ_2 regularization. In Appendix B we explain the criteria used to tune α .

To retrieve $\tilde{Z}^* = \{\tilde{z}^{d*}\}_{d=1}^D$, the MAP estimate of the latent variable $\tilde{z}$ for each day d , we want to minimize $\mathcal{L}^{z,d}$ with respect of $\tilde{z}^d$ for every day d . We can perform this retrieval for all the historical data by minimizing the loss function, i.e., we aim to

find:

$$\begin{aligned} \tilde{Z}^* &= \operatorname{argmin}_{\tilde{Z}} \mathcal{L}^z \\ &= \operatorname{argmin}_{\tilde{Z}} \sum_{d=0}^D \mathcal{L}^{z,d}(\mathbf{y}^d, \mathbf{x}^d, \tilde{z}^d; \Lambda). \end{aligned} \quad (17)$$

4.2.1 Estimation of the latent variable posterior

We performed the minimization of $\mathcal{L}^z$ using the Adam algorithm, with a learning rate $\gamma = 0.03$, and $\beta_1 = 0.9$, $\beta_2 = 0.999$, which are the default momentum parameters from the library PyTorch (Paszke et al., 2019) version 2.4.1. We used 90% of all the historical data per iteration, selected randomly across the entire period. The remaining 10% was used as the test set. A copy of the code availability for every algorithm described in this work is in Soto (2025).

After $\tilde{Z}^*$, the set of latent variables for the entire training set, has been retrieved, in order to estimate the uncertainty, we linearized $\mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}; \Lambda)$ around $\tilde{z}^{d*}$, as

$$\begin{aligned} &\mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}; \Lambda) \\ &\approx \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^{d*}}, \mathbf{x}; \Lambda) + \nabla_{\tilde{z}^d} \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}; \Lambda)|_{(\tilde{z}^d = \tilde{z}^{d*})} (\tilde{z}^d - \tilde{z}^{d*}) \\ &= \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^{d*}}, \mathbf{x}; \Lambda) + \mathbf{K}(\tilde{z}^d - \tilde{z}^{d*}). \end{aligned} \quad (18)$$

Where $\mathbf{K}$ is the Jacobian of $\mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^{d*}}, \mathbf{x}; \Lambda)$ with respect of $\tilde{z}^d$. Then, as shown in (Rodgers, 2000), the covariance matrix of the approximate posterior can be written as

$$\Sigma_{\tilde{z}^{d*}} = (\mathbf{K}^T \Sigma_{\epsilon}^{-1} \mathbf{K} + \Sigma_z^{-1})^{-1}. \quad (19)$$

In this way, the standard deviation is computed as the root square of the diagonal elements $\sigma_{\tilde{z}}$ of $\Sigma_{\tilde{z}^{d*}}$.

Then, since the resulting retrieved values $\tilde{Z}^*$ are normally distributed, $Z^* = \exp(\tilde{Z}^*)$ has a log-normal distribution and thus, the uncertainty can be computed with the 68% confidence interval (here we match the convention of using the standard deviation as uncertainty for variables with normal distribution).

The uncertainty for derived variables like kd and $b_{b,p}$ is computed with standard error propagation (Arras, 1998), i.e. $\Delta F(\mathbf{x})^2 = \nabla_x F(\mathbf{x}) \Sigma^x \nabla_x F(\mathbf{x})^T$, where $\Delta F(\mathbf{x})$ is the error of a function $F(\mathbf{x})$, $\nabla_x F(\mathbf{x})$ is the Jacobian, and Σ^x is the covariance matrix of x , in our case, $\Sigma^x = \Sigma_{\tilde{z}^{d*}}$. These equations assume that each component of $\mathbf{x}$ is not correlated with the others, and is only an approximation for nonlinear functions.

The previous procedure is equivalent to estimating the latent variable posterior with a log-normal distribution. A comparison of the true posterior and the estimated posterior can be appreciated in Figure 7, where the true posterior was computed by sampling using the Metropolis-Hasting Algorithm (see Algorithm 2). The discrepancy between the mean and standard deviation is due to the linearization step in Eq. 18. Algorithm 1 summarizes the steps used for the posterior estimate.

Algorithm 1 Algorithm for estimating the daily posterior estimate of the unknown latent variable z^d , and the derived quantities kd^d and b_{bp}^d :

Input: x^d, y^d .

1. Find $\tilde{z}^{d*} = \text{argmin}_{z^d} \mathcal{L}^{z,d}(y^d, x^d, z^d; \Lambda)$ using a minimization algorithm (For example, Adam).
2. Compute $\mathbf{K}$, the Jacobian of $\mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^{d*}}, x; \Lambda)$ with respect of $\tilde{z}^d$.
3. Compute the covariance matrix of the approximate posterior as $\Sigma_{\tilde{z}^{d*}} = (\mathbf{K}^T \Sigma_\epsilon^{-1} \mathbf{K} + \Sigma_z^{-1})^{-1}$.
4. The MAP estimate of the latent variable is equal to $z^{d*} = e^{\tilde{z}^{d*}}$. The uncertainty can be found by computing the 68% confidence interval of the log normal distribution. For this work, only the diagonal elements of $\Sigma_{\tilde{z}^{d*}}$ were used, assuming independence between the latent variables.
5. Use Eq. 10 and Eq. 11 to compute b_{bp}^d and kd^d respectively, and use standard error propagation for their uncertainties.

4.3 Model optimisation scheme

We retrieved the latent variable posterior in order to accurately estimate the daily average of chlorophyll, Non-Algal particles, and Colored Dissolved Organic Matter concentrations. To asses the accuracy of the inversion, we used the in-situ observations $H^{OBS} = \{(kd^{d,obs}, b_{bp}^{d,obs}, chla^{d,obs})\}_{d=1}^D$ where D is the number of days with observations available, $kd^{d,obs}$ is a vector of dimension five containing daily in-situ observations of the downward light attenuation coefficient, $b_{bp}^{d,obs}$ is a vector of dimension three with observations of particulate backward scattering coefficient, only for the wavelengths $\lambda = (442.5, 490, 555)\text{nm}$, and $chla^{d,obs}$ is a scalar observation of sea surface chlorophyll concentration.

By comparing the modeled observation operator $H^{MODEL} = (kd(z^d; x^d, \Lambda), b_{bp}(z^d; x^d, \Lambda), chla)$ with the daily observations, we aimed to optimize the forward model $\mathbf{R}_{rs}^{MODEL}(\tilde{z}, x^d; \Lambda)$ by adjusting the parameters Λ . We looked for Λ^* such that $\sum_{d=1}^D \|H^{MODEL}(z^{d*}; x^d, \Lambda^*) - H^{OBS}\|$ is minimized, for some suitable choice of distance. Since not every day has observations available, and also occur that the observations corresponding to some of the wavelengths are missing, we worked with daily vectors with dimension equal to the total number observations available, e.g. days with all observations available correspond with vectors of dimension nine (five for kd^d , three for b_{bp} and one for $chla$), while days with less observations correspond to lower dimensional vectors.

Since we also want to estimate the uncertainty of the retrieved parameters, we used the standard deviation over all the training data as a measure of the spread of each observation, and defined the loss function,

$$\mathcal{L}^H = \sum_{d=0}^D \frac{(\mathbf{H}^{MODEL,d}(Z^*; \mathbf{X}, \Lambda) - H^{OBS,d})^2}{\sigma_{OBS}^2} \quad (20)$$

where σ_{OBS} is the standard deviation of the observations computed only with the train data. We want to minimize this loss function and get an estimate for the uncertainty of the retrieved parameters. For this aim, we proceed to use a Markov Chain Monte Carlo algorithm, described in the next section.

4.3.1 Markov Chain Monte Carlo algorithm for optimizing the model parameters

280 In order to estimate the posterior distribution of the parameters, $p(\Lambda|H^{\text{OBS}}, \hat{Z}, \mathbf{X})$, we used the Metropolis-Hasting Algorithm (Chib and Greenberg, 1995; Andrieu and Thoms, 2008).

The algorithm returns samples from a probability density function $\pi(x)$ by defining a Markov process with transition probability $p(x, y)$ of moving from state x to state y . It can be shown that by a suitable definition of this transition probability, the Markov Chain process can converge asymptotically to the target distribution $\pi(x)$. The Metropolis-Hasting Algorithm uses the
285 transition probability

$$p(x, y) = q(x, y)\alpha(x, y), \quad \alpha(x, y) = \min \left[\frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}, 1 \right] \quad (21)$$

where $q(x, y)$ is the proposal transition probability, and $\alpha(x, y)$ is the acceptance probability. With this definition, samples from $\pi(x)$ can be drawn by following Algorithm 2.

Algorithm 2 Metropolis-Hasting Algorithm (Chib and Greenberg, 1995; Andrieu and Thoms, 2008). It consists in defining a Markov process. It is useful to sample from a target distribution $\pi(x)$ without knowing the normalization constant.

Define: Proposal transition probability $q(x, y)$.

Input: Length L_{chain} .

Initialize: x_0 .

1. x = array of length L_{chain} .
 2. $x[0] = x_0$.
 3. For $i=0$ to $i = L_m - 1$ do
 1. Sample a proposed new point $y \sim q(x[i], y)$.
 2. Compute $\alpha(x[i], y)$ as stated in Eq. 21.
 3. Sample a random number from a uniform distribution between 0 and 1. If the output is smaller than $\alpha(x[i], y)$ $x[i+1] = y$ else $x[i+1] = x[i]$.
 4. Discard the first samples (reaching the asymptotical behaviour) and the correlated ones.
-

Some drawbacks are known, for example, the iterations have to be performed multiple times before the algorithm converges
290 to its asymptotical behaviour, or that successive iterations tend to be strongly correlated, so many iterations have to be performed in order to obtain uncorrelated samples. These difficulties increase as the dimensionality of the sampling space gets higher. In our case, to mitigate some of these effects, we didn't perturb all the parameters, leaving those that are more precisely measured in the literature unperturbed, like the water-specific absorption and scattering coefficients.

A further complication is that the probability density that we want to sample depends on Z^* , the latent variable. This means
295 that, each time we want to do an iteration of the Metropolis-Hasting Algorithm, we would need to find the MAP estimate of Z , increasing the computational time. To mitigate this problem, we use an estimate $\hat{Z}$, consisting of a few iterations towards the MAP estimate.

Our model for the negative log-likelihood is the loss function $\mathcal{L}^H$ described in 4.3, which give us the expression for the Likelihood

$$p(H^{OBS}|\Lambda, \hat{Z}, \mathbf{X}) \propto e^{-\frac{1}{2}\mathcal{L}^H(H^{OBS}, \hat{Z}, \mathbf{X}, \Lambda)}. \quad (22)$$

The density function, $\pi(x)$, that we want to sample from is the posterior probability for the parameters. By using a uniform prior, and $q(\Lambda_i, \Lambda_j) = \mathcal{N}(\Lambda_i, \alpha_q \mathbf{1})$, where α_q is a hyperparameter equal to the standard deviation of the distance between steps. We compute the acceptance probability as

$$\alpha(\Lambda_i, \Lambda_j) = \min \left[e^{-\frac{1}{2}(\mathcal{L}^H(H^{OBS}, \hat{Z}, \mathbf{X}, \Lambda_j) - \mathcal{L}^H(H^{OBS}, \hat{Z}, \mathbf{X}, \Lambda_i))}, 1 \right]. \quad (23)$$

Regarding the perturbed parameters, we consider the literature values Λ^0 as close estimates of the optimal ones. For this reason, we perturbed them as $\Lambda^* = \delta_\Lambda^T \Lambda^0$, where δ_Λ is a vector of small perturbations from unity, referred to as perturbation factors.

The values of the λ dependent vector of dimension five representing the phytoplacton-specific absorption coefficients $\mathbf{a}_{\text{phy}}$ were perturbed as: $\mathbf{a}_{\text{phy}}^* = \delta_{a_{\text{phy}}} \mathbf{a}_{\text{phy}}^0$ with $\delta_{a_{\text{phy}}}$ a learnable scalar, and $\mathbf{a}_{\text{phy}}^0$ the literature values. We chose it like this to maintain the shape of the function $a_{\text{phy}}(\lambda)$ unperturbed.

For the carbon-specific scattering and backscattering coefficients $b_{\text{phy}}(\lambda)$ and $b_{b,\text{phy}}(\lambda)$, we first linearly interpolated them with the literature values, and perturbed the tangent and the intercept of the linear interpolations, $b_{\text{phy}}(\lambda)^* = \delta_{b_{\text{phy},\text{int}}} b_{\text{phy},\text{int}}^0 + \delta_{b_{\text{phy},\text{T}}} b_{\text{phy},\text{T}}^0 \lambda$.

The parameters d_{CDOM} , $b_{r,\text{NAP}}$, S_{CDOM} , $\Theta_{\text{chla}}^{\min}$, Θ_{chla}^0 , β , σ , Q_a and Q_b perturbations consisted in per parameter scalar multiplications. All the other parameters were left unperturbed.

In this way, we perturbed 24 parameters, 9 of them by multiplying them for a scalar δ_i , i equal to each of the perturbed parameters, the five components of $\mathbf{a}_{\text{phy}}$ by multiplying them by the same scalar $\delta_{a_{\text{phy}}}$, and finally, $b_{\text{phy}}(\lambda)$ and $b_{b,\text{phy}}(\lambda)$ by linearly interpolating them, and perturbing the tangent and the intercept of each of them, making a total of 14 perturbation factors.

In this manner, the perturbations δ_Λ were initialized with ones, then using alternate minimization (AM), alternating between finding the MAP estimate of Z^* and the MLE of the parameters. Finally, we used the Metropolis-Hasting Algorithm to estimate the posterior, as described in Algorithm 3.

4.4 Data Informed Inversion Method (DIIM): A Variational Bayes approach

As the dimension of the posterior increases, MCMC methods become increasingly more challenging, and even point-wise estimates, like the one obtained with Alternate Minimization, could not converge, due to the nonconvexity of our models. As an alternative approach, we present a framework based on the Stochastic Gradient Variational Bayes (SGVB) estimator (Kingma and Welling, 2013).

The SGVB based framework considers a random latent variable $z \in \mathcal{Z}$ sampled from an unknown distribution $p_{\Lambda^*}(z)$, and a random variable $\mathbf{y} \in \mathcal{Y}$ sampled from a distribution $p_{\Lambda^*}(\mathbf{y}|z)$ conditional on the latent variable z . For example, $\mathbf{y}$ could be measurements from a known physical process, conditional on unknown physical hidden processes.

Algorithm 3 Metropolis-Hasting Algorithm with alternate minimization. Here we expand the Metropolis-Hasting Algorithm in combination with the alternate minimization to sample from the posterior probability of the parameter space

Define: Transition probability $q(\Lambda_i, \Lambda_j) = \mathcal{N}(\Lambda_i, \alpha_q \mathbf{1})$.

Input: L_{chain} (Length of MCMC chains), N_{steps} (Number of AM steps), N_{z_steps} (steps towards the min of z^*).

Initialize: Λ_0 as the literature values.

1. Alternate minimization to estimate the MLE of the parameters.

1. For $i=0$ to $i=N_{\text{steps}}$ do

- Find an estimate of all the latent variables $\hat{Z}^* \approx \text{argmin}_{\tilde{z}} \mathcal{L}^z(\mathbf{y}, \mathbf{x}, \tilde{z}; \Lambda_0)$ by performing N_{z_steps} iterations towards the minimum of the loss function.
- Perform one step towards the minimization of $\mathcal{L}^H(\mathbf{y}, \mathbf{x}, \hat{Z}^*; \Lambda_0)$, and set Λ_0 to the new value.

2. Define an empty array Λ of length L_{chain} .

3. $\Lambda[0] = \Lambda_0$.

4. For $i=0$ to $i = L_{\text{chain}} - 1$ do

1. Sample a proposed new point $\Lambda_j \sim \mathcal{N}(\Lambda[i], \alpha_q \mathbf{1})$.

2. Find an estimate of all the latent variables $\hat{Z}^* \approx \text{argmin}_{\tilde{z}} \mathcal{L}^z(\mathbf{y}, \mathbf{x}, \tilde{z}; \Lambda_j)$ by performing a finite amount of iterations towards the minimum of the loss function.

2. Compute $\alpha(\Lambda_i, \Lambda_j)$ as stated in Eq. 23 using the estimate $\hat{Z}^*$ instead of the true minimum Z^* .

3. Sample a random number from a uniform distribution between 0 and 1. If the output is smaller than $\alpha(\Lambda_i, \Lambda_j)$, make $\Lambda[i+1] = \Lambda_j$ else $\Lambda[i+1] = \Lambda[i]$.

5. Discard the first samples (reaching the asymptotical behaviour) and the correlated ones.

The aim is to efficiently approximate the Maximum Marginal Likelihood estimate of the parameters Λ ,

$$\Lambda^* = \text{argmax}_{\Lambda} (p_{\Lambda}(y)). \quad (24)$$

For this end, the posterior probability distribution $p_{\Lambda}(z|\mathbf{y})$ is estimated as a parameterized function $q_{\phi}(z|\mathbf{y})$. It can be shown that finding Λ^* and ϕ^* such that

$$\Lambda^*, \phi^* = \text{argmax}_{\Lambda, \phi} \mathcal{L}_{ELBO},$$

$$335 \quad \mathcal{L}_{ELBO} = -D_{KL}(q_{\phi}(z|\mathbf{y})||p_{\Lambda}(z)) + \mathbb{E}_{q_{\phi}(z|\mathbf{y})}[\log(p_{\Lambda}(\mathbf{y}|z))] \quad (25)$$

where $D_{KL}(\cdot||\cdot)$ is the Kullback-Leibler divergence (DKL divergence), an asymmetric, positively defined measure of the proximity between two probability distributions (Shlens, 2014), $p_{\Lambda}(z)$ is the prior distribution of the latent variable z , and $\mathbb{E}_{q_{\phi}(z|\mathbf{y})}[\cdot]$ stands for the expected value over the probability distribution $q_{\phi}(z|\mathbf{y})$, is approximately equal to finding the Maximum Likelihood estimate.

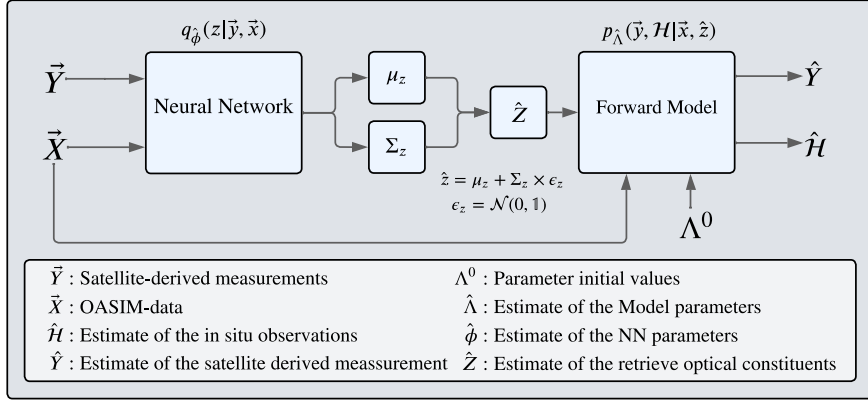


Figure 2. Diagram of the Variational Bayes framework, adapted for the inversion problem, where the estimated $\hat{Z}$ is retrieved using a parameterized probabilistic function $q_\phi(z|\mathbf{y}, \mathbf{x})$, which for our case, is a feed forward neural network (diagram in Fig. 3) and whose parameters ϕ are learned simultaneously as the parameters Λ , the parameters from the Forward model.

340 This is because $\mathcal{L}_{ELBO}$, where ELBO stands for “Evidence Lower Bound”, is a lower bound of the data log-likelihood $\log p_\Lambda(\mathbf{y})$ (see appendix C).

Kingma and Welling (2013) presented the SGVB estimator for the expected value (in the case where the D_{KL} can not be computed analytically, it can also be estimated) as,

$$\hat{\mathcal{L}}_{ELBO} \approx -D_{KL}(q_\phi(z|\mathbf{y})||p_\Lambda(z)) + \frac{1}{L} \sum_{l=1}^L \log(p_\Lambda(\mathbf{y}|z_l)), \quad z_l \sim q_\phi(z|\mathbf{y}, \mathbf{x}). \quad (26)$$

345 If the SGVB is used with a neural network as the approximate probability distributions $q_\phi(z|\mathbf{y})$, then the neural network architecture and minimization scheme is known as Variational Auto-Encoders (Kingma and Welling, 2013), where the model $q_\phi(z|\mathbf{y})$ is usually called the “Encoder”, and $p_\Lambda(\mathbf{y}|z)$ the “Decoder”.

Sohn et al. (2015) generalized this framework for what they called, Conditional Variational Auto-Encoders (CVAE), where the likelihood and posterior probabilities are allowed to be conditional distributions on a third set of random variables $x \in \mathcal{X}$, $y \sim p_\Lambda(y|\mathbf{z}, x)$, and $\mathbf{z} \sim q_\phi(\mathbf{z}|y, x)$. This is the final configuration we used, but instead of training a generative model as CVAE are usually used to, we used it to solve the inversion problem while simultaneously finding approximate values for the parameters Λ^* , as explained in Sec. 4.4.1.

4.4.1 Variational Bayes approach to solve the Inversion Problem with the SGVB estimator

CVAEs are commonly used to train a generative model $p_\Lambda(\mathbf{y}|\mathbf{z}, \mathbf{x})$ from a probability distribution $p(\mathbf{z}|\mathbf{x})$ that is easy to sample, in order to generate samples that well approximate the target probability distribution (Doersch, 2021). They have been used to solve inverse problems, like image recovery (Zhong et al., 2019, 2021; Zhao et al., 2023), unfolding in high energy physics

(Shmakov et al., 2024), among other applications. In contrast to previous applications of VAEs and CVAEs to inverse methods, in this work, instead of first training a CVAE with latent variables that lack a physical interpretation, we directly used the SGVB estimator for the inverse method. Here, $p_\Lambda(\mathbf{y}|z, \mathbf{x})$ is the likelihood described in Eq. (14), where Λ represents the parameters of the forward function that we aim to optimize, and the latent variable $\mathbf{z}$ is the vector that we want to retrieve.

To do so, we used a neural network $q_\phi(z|\mathbf{y}, \mathbf{x})$ (diagram shown in Fig. 3) as an approximation of the posterior $p(z|\mathbf{y}, \mathbf{x})$.

Our model for the Likelihood was,

$$-\frac{1}{L} \sum_{l=1}^L \log(p_\Lambda(\mathbf{y}|z_l)) = \frac{1}{2L} \sum_{l=0}^L (\mathbf{y}^d - \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}^d; \Lambda))^T \Sigma_\epsilon^{-1} (\mathbf{y}^d - \mathbf{R}_{rs}^{MODEL}(e^{\tilde{z}^d}, \mathbf{x}^d; \Lambda)) + (\mathcal{H}^d(e^{\tilde{z}^d}, \mathbf{X}; \Lambda) - H^{OBS,d})^T \Sigma_H^{-1} (\hat{\mathcal{H}}^d(e^{\tilde{z}^d}, \mathbf{X}; \Lambda) - H^{OBS,d}) \quad (27)$$

where Σ_ϵ^{-1} was the equivalent to the covariance matrix introduced in Sec. 4.2, Σ_H^{-1} was chosen in order to have the equivalent to $\mathcal{L}^H$ from Eq. (20) and L is the number of samples used per iteration to approximate the expected value. We performed experiments with $L = 1$, $L = 10$, and $L = 100$. The performance of using higher values for L was not significantly higher, for which we decided to use $L = 10$.

We used a neural network composed of two parts, one having as output the mean μ_{q_z} , and the other one the covariance matrix Σ_{q_z} , of a Gaussian probability distribution. Since the prior for z is a multivariate Gaussian, the D_{KL} divergence in Eq. 26 is,

$$D_{KL}(q_\phi(z|\mathbf{y})||p_\Lambda(z)) = \frac{1}{2} \left[\frac{|\Sigma_z|}{|\Sigma_{q_z}|} + \text{Tr}(\Sigma_{q_z}^{-1} \Sigma_z) + (\mu_{q_z} - \mu_z)^T \Sigma_{q_z}^{-1} (\mu_{q_z} - \mu_z) - \dim_z \right] \quad (28)$$

where $|\Sigma_z|$ stands for the determinant of the scaled covariance matrix used for the prior introduced in 4.2, $\text{Tr}(\mathbf{A})$ stands for the trace of a matrix $\mathbf{A}$, and $\dim_z = 3$, the dimension of z .

Finally, we added a ℓ_2 regularization for the parameters Λ , since it helped for the convergence of the Neural Network. With all the components at hand, the inversion task plus the inference on the parameters is equivalent to approximate the posterior with a parametrized function $q_\phi(z|\mathbf{x}, \mathbf{y})$, and find the parameters $\{\phi, \Lambda\}^*$ that minimize the loss function,

$$L_{NN} = D_{KL}(q_\phi(z|\mathbf{y})||p_\Lambda(z)) - \frac{1}{L} \sum_{l=1}^L \log(p_\Lambda(\mathbf{y}|z_l)) - \alpha_\Lambda \|\Lambda - 1\|_2 \quad (29)$$

where $\alpha_\Lambda(\Lambda - 1)^2$ is the regularization term, with α_Λ a hyperparameter tuned as explained in the next section, together with all the other hyperparameters of the method.

4.5 Architecture and Training of the Neural Network

As illustrated in Fig. 3, the Neural Network (NN) is composed of three sections. The first part has two hidden layers, whose function is to reduce the dimensionality of the input layer by projecting it into the space of the in-situ observations. To achieve it, this part was trained separately from the rest of the NN with in situ observations corresponding to the training data. This preprocessing was done to facilitate the convergence of the final output to physically plausible values. The second and third

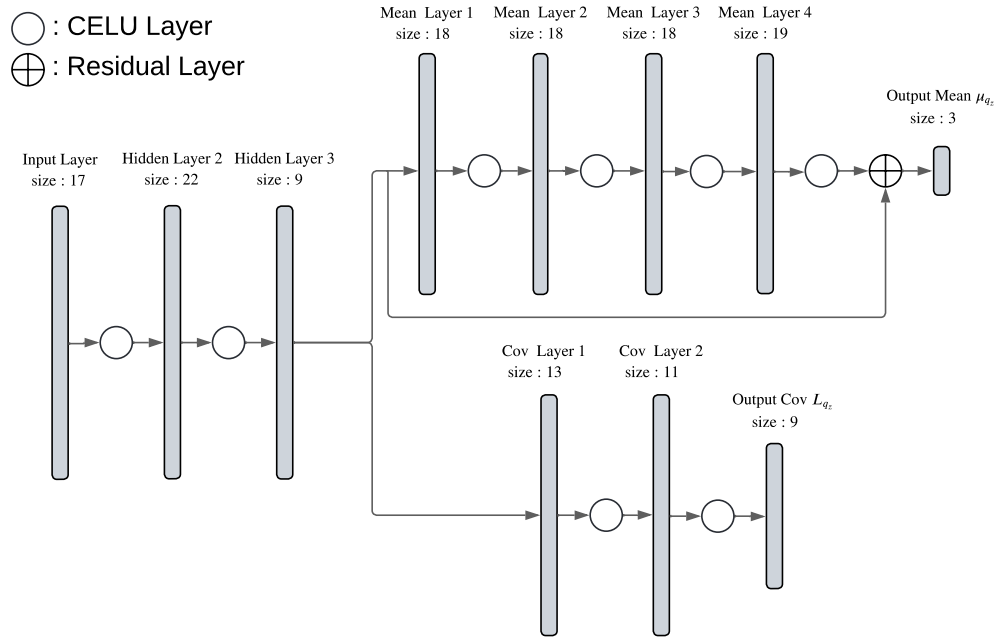


Figure 3. Diagram of the Neural Network (Soto, 2025) used as the parameterized probabilistic function $q_\phi(z|\mathbf{x}, \mathbf{y})$. It is composed of three sections, the first two hidden layers reduce the dimensionality of the input layer by projecting it into the space of the in-situ observations. The output of the second layer is the input of the layers that learn the mean value of the latent variable μ_{q_z} , and those that learn the components of the square root of the covariance matrix $\Sigma_{q_z} = L_{q_z}^T L_{q_z}$. The dimension of the hidden layers and the number of hidden layers are tuned using Ray Tune (Liaw et al., 2018).

385 parts are the predicted mean of the latent variable μ_{q_z} and the square root of the covariance matrix $\Sigma_{q_z} = L_{q_z}^T L_{q_z}$. In addition, experiments showed that a residual layer at the end of the second part of the NN (adding the first component of the output of the first part) improved the generalization error.

To decide the best hyperparameters of the neural network, we used the library Ray Tune (Liaw et al., 2018), a Python library designed for parameter tuning, together with the Bayesian Optimization HyperBand algorithm (Falkner et al., 2018) to search
 390 in the hyperparameter space. These include the number of hidden layers, the size of the hidden layers, the learning rate, the different moments for the Adam Algorithm used to train the neural network, and the size of the mini-batches.

In the same manner as with the MCMC algorithm, we used the same 90% of the data for training, from which we select randomly five percent of it as validation for each iteration of the hyperparameter search.

Also, we did an exploration within the activation functions, finding the CELU activation function as the one that returned the
 395 best results. The CELU function is similar to the Rectified Linear Unit (ReLU) function, where instead of being the identity for positive inputs and truncating to zero for negative inputs, it truncates to minus one for negative values and makes a smooth

transition between the identity part and the truncation part (Barron, 2017),

$$CELU(x) = \max(0, x) + \min(0, \alpha_c e^{x/\alpha_c} - 1). \quad (30)$$

With α_c , a hyperparameter also tuned with Ray Tune.

400 A diagram of the neural network $q_\phi(z|\mathbf{y}, \mathbf{x})$ is presented in Fig. 3, which is part of the framework described in Fig. 2. To train the neural network, first the measurements and OASIM-data $(\mathbf{X}, \mathbf{Y})$ are passed to it, returning an estimate for the mean and the covariance matrix of the latent variable Z . From these estimates, a random sample is computed, $\hat{Z} = \mu_z + \Sigma_z \epsilon_z$, $\epsilon_z \sim \mathcal{N}(0, \mathcal{I})$, and subsequently used as an estimate in the forward model $\mathbf{R}_{rs}^{MODEL}(e^{\hat{z}^d}, \mathbf{x}^d; \Lambda)$, and with the observation function $\mathcal{H}(\hat{Z}, \mathbf{X}; \Lambda)$.

405 5 RESULTS

The results are divided into four parts: the first one focuses on the Bayesian retrieval of the optically active constituents on the surface of the sea and the uncertainty estimation, the second on the parameter optimization, the third part talks about the comparison between the Bayesian outputs and the Variational Bayes approach, and the last one talks about a comparison with a state of the art algorithm for satellite sea surface chlorophyll a estimation.

410 5.1 Bayesian Inversion

We performed the Bayesian inversion from 2005 to 2013. As shown in Fig. 4, the retrieved sea surface chlorophyll manages to reproduce the interannual variability, including the spring algal blooms. The reported uncertainty serves as an estimate of the average expected discrepancy between retrieved data and in-situ measurements, not restricted to chlorophyll observations, but also to the downward light attenuation coefficient and particulate backward scattering coefficient observations. We tested the
415 performance of the inversion with a random sample consisting of 10% of the days with observations. The Root Mean Square Error between the observations and the inverted data was computed (see Tab. D1), as well as the Spearman rank correlation coefficient ρ (Tab. D2), and the relative Median Absolute Deviation rMAD (Tab. D3).

Figure 7 shows a comparison between the true posterior distribution, sampled using the Metropolis-Hasting Algorithm, and the estimated one using the linear approximation, for the inversion of the Remote Sensing Reflectance of February 18, 2005.
420 The true posterior means and standard deviations are closely approximated by the linearization, even if the Forward function is highly nonlinear. This result is closely related to the choice of the prior $\alpha \mathbf{1} = 1.3 \mathbf{1}$ computed as explained in Sec. C, since it is a strongly informative prior. We can study the effect of the prior by computing the inverse of the Fisher information matrix, since the Cramér–Rao bound states that the variance of the MLE is always higher than or equal to this quantity:

$$\text{Var}[\hat{\psi}] \geq \frac{1}{\mathbf{I}(\psi)} \quad (31)$$

425 where $\hat{\psi}$ is an unbiased estimator of a random parameter ψ , and $\mathbf{I}(\psi)$ is the Fisher information matrix, defined as

$$\mathbf{I}(\psi) = -\mathbb{E} \left[\frac{d^2 \mathcal{L}(X; \psi)}{d\psi^2} \right] \quad (32)$$

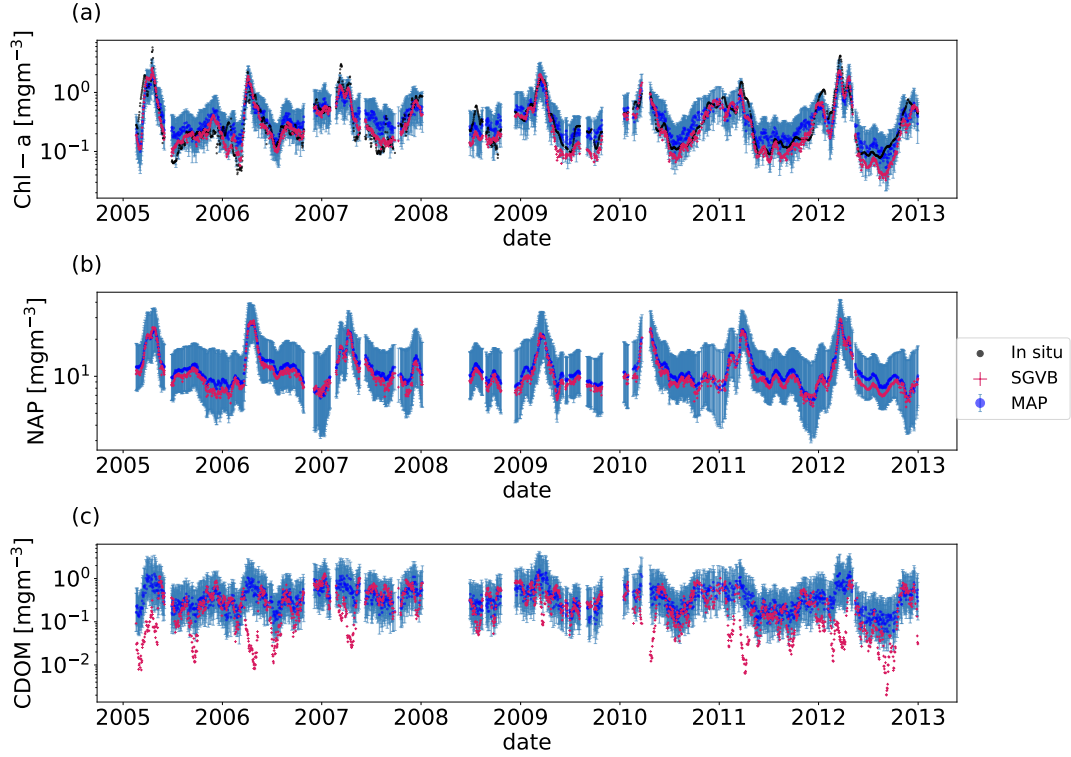


Figure 4. Time series for the chlorophyll- α (a), Non-Algal Particles (b), and Chromophoric Dissolved Organic Matter (c). For all the timelines, the black points are the in-situ observations from the BOUSSOLE buoy, the blue points are the MAP output with uncertainty (blue shadow), using the optimal parameters from the SGVB based framework algorithm, and the red points are the output of the SGVB based framework.

where $\mathcal{L}(X; \psi)$ is the likelihood of a random variable X with parameters ψ (Cramér, 1999). For our case, the Fisher information matrix is equal to

$$I(\Lambda) = \mathbf{K}^T \Sigma_{\epsilon}^{-1} \mathbf{K} \quad (33)$$

430 which is equal to the inverse of Eq. 19 without the effect of the prior. To quantify the effect of the prior, we divided the average Frobenius norm of the inverse of the Fisher information matrix $\|1/I(\Lambda)\|_{2,2}$ and the retrieved covariance matrix $\|\Sigma_{\tilde{z}^d}\|_{2,2}$, obtaining the value of 42.9, which means that the prior is reducing the uncertainty of the MLE by a factor of 42. On the other hand, this highly informative prior is a reasonable prior, since it states that most of the chlorophyll concentration should be within values lower than $\exp(\mu_z + 2\sigma_{\tilde{z}}) = \exp(2.6) = 13.46 \text{mgm}^{-3}$ and higher than $\exp(\mu_z - 2\sigma_{\tilde{z}}) = \exp(-2.6) =$
 435 0.07mgm^{-3} .

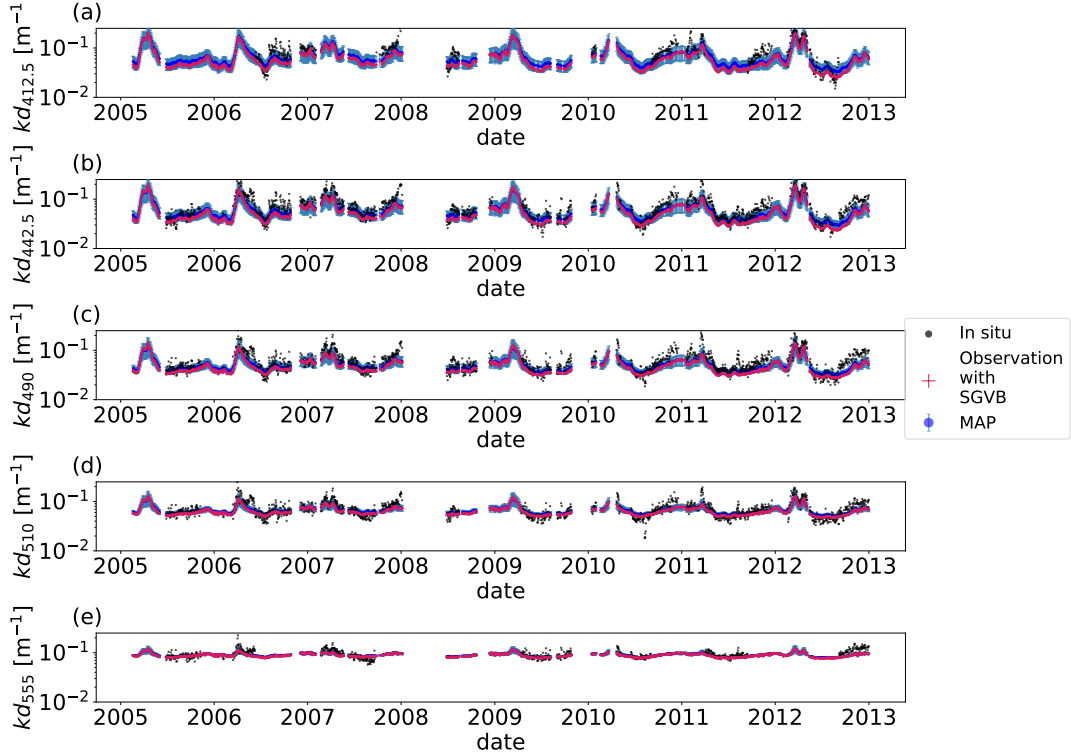


Figure 5. Time series for downward light attenuation coefficient ($k_d(\lambda)$), wavelengths $\lambda = 412.5$ (a), $\lambda = 442.5$ (b), $\lambda = 490$ (c), $\lambda = 510$ (d) and $\lambda = 555$ (e). For all the timelines, the black points are the in-situ observations from the BOUSSOLE buoy, the blue points are the MAP output with uncertainty (blue shadow), using the optimal parameters from the SGVB based framework algorithm, and the red points are the observation operator computed using the output of the SGVB based framework.

5.2 Optimization of the forward model parameters

As described in Sec. 4.3.1, we tuned twenty-four parameters, multiplying them by fourteen perturbation factors, to minimize the distance between retrieved quantities and observation data. We are interested in the optimized parameter values, as well as the uncertainties. If any of our final parameterizations are going to be used in future works, it is important to note that we are finding optimal parameters that are representative of data from different seasons. For this reason, we present a sensitivity analysis, where we can appreciate the annual variability of the sensitivity. Parameters with high variability may need special considerations for models that use different parameterizations for different seasons.

Following Carmichael et al. (1997), the sensitivity of the Remote Sensing Reflectances, downward light attenuation coefficient and backward scattering coefficient can be computed by calculating the partial derivative with respect of the different parameters ($\partial R_{RS}/\partial \delta_i$, $\partial kd/\partial \delta_i$, $\partial b_{b,p}/\partial \delta_i$), named the local sensitivity coefficients, and normalized with respect to the sensitivity coefficient (R_{RS}/δ_i , kd/δ_i , $b_{b,p}/\delta_i$) to obtained adimensional quantities. The results can be observed in Fig. 8.

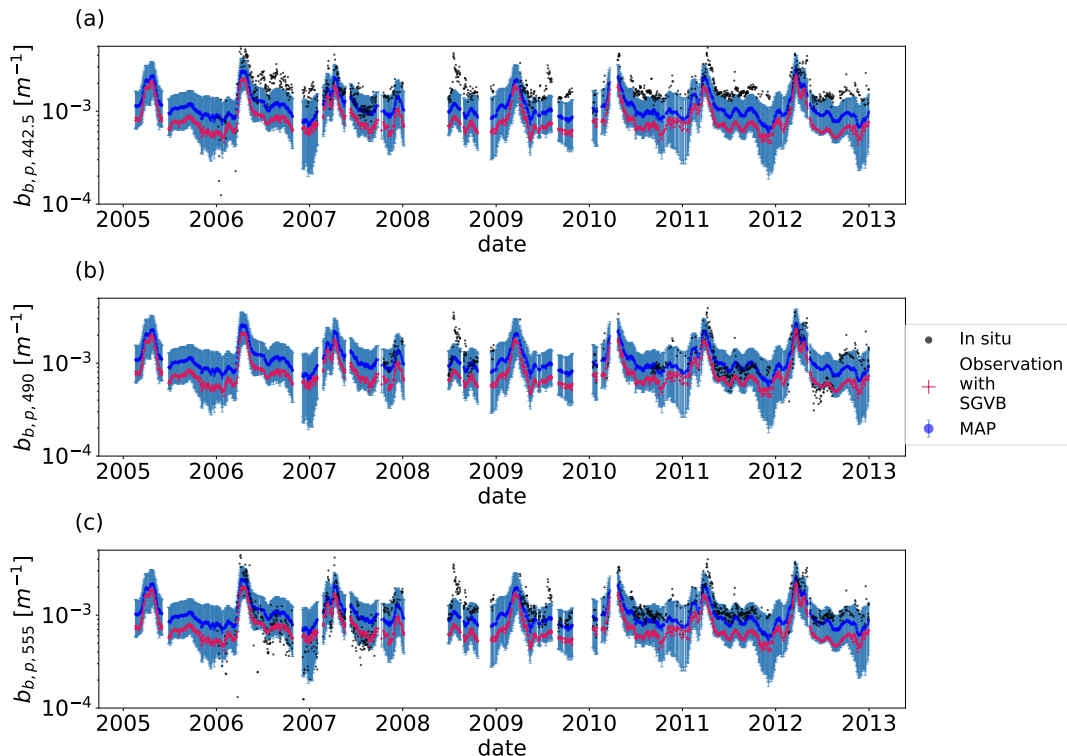


Figure 6. Time series for particulate backward scattering coefficient for the wavelengths $\lambda = 442.5$ (a), $\lambda = 490$ (b) and $\lambda = 555$ (c). For all the timelines, the black points are the in-situ observations from the BOUSSOLE buoy, the blue points are the MAP output with uncertainty (blue shadow), using the optimal parameters from the SGVB based framework algorithm, and the red points are the observation operator computed using the output of the SGVB based framework.

We noticed that R_{RS} and $b_{b,p}$ share a strong variability in the sensitivity with respect to the backward scattering coefficient of phytoplankton $b_{b,phy}$ and backscattering-to-scattering ratio of NAP, $b_{r,NAP}$, as well as the parameters $\Theta_{chla}^{\min}$, Θ_{chla}^0 , β , σ , which form part of the $chl a:C$ ratio relation described in Eq. (3). This agrees with the seasonal variability in the abundance of the different phytoplankton functional types (Lazzari et al., 2012), as well as the variability in concentrations of pollution (Bodin et al., 2004). With this observation, we expect that using only one set of parameters for the full year would result in suboptimal predictions. Nevertheless, we proceed to find the optimal parameters that describe the full historical data set.

To do so, we performed an MCMC algorithm as described in Sec. 4.3.1. An example of the distribution obtained for each parameter can be observed in Fig. 9. The original values as well as the mean and standard deviation for the λ -dependent parameters can be appreciated in Fig. 10. Finally, the original values as well as the statistics obtained using the MCMC algorithm for the λ -independent parameters can be appreciated in Tab. 4.

For completeness, we also computed the covariance matrix between the perturbation factors δ_i , which can be appreciated in Tab. 5.

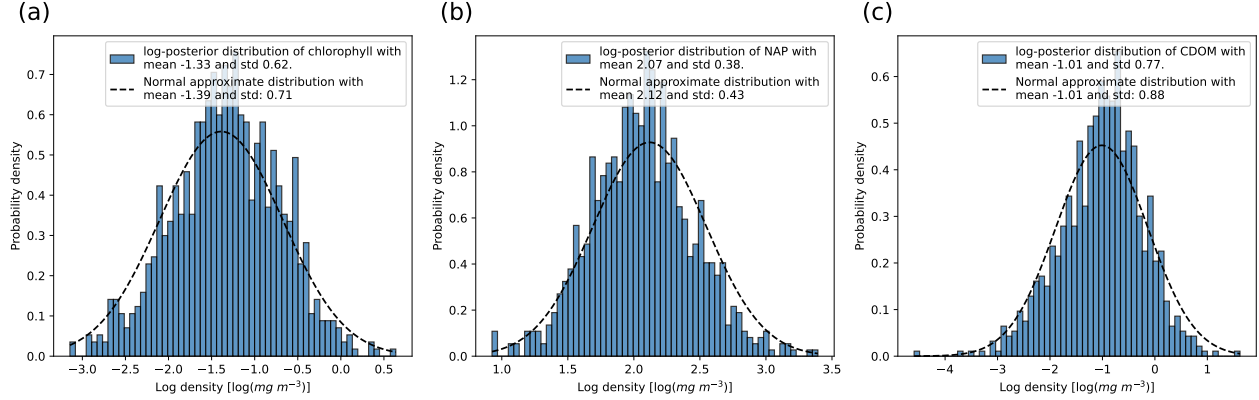


Figure 7. Comparison between the true posterior distribution (Eq. 16) and the approximate posterior by following the algorithm in Algorithm 1 for the log-posterior distribution of (a) chlorophyll- α , (b) Non Algal particles and (c) Colored Dissolved Organic Matter, for the first day of the train data (February 18, 2005). The true posterior (in blue) was sampled using the Metropolis-Hasting Algorithm (see Algorithm 2), while the normal approximation (dashed line) was derived by linearization of the forward model around the MAP estimate.

Table 4. Original values, final values obtained using the SGVB estimator, as well as the mean, standard deviation, and Kolmogorov-Smirnov test coefficient for the sampling with the Metropolis-Hasting Algorithm for the λ -independent parameters.

	Original value	SGVB result	MCMC result	KS test for normality	KS p-value for normality
d_{CDOM} [m ² (mgCDOM) ⁻¹]	0.0150	0.0156	0.0101 $\pm$ 0.0028	0.0536	7.259E-01
S_{CDOM} [nm]	0.0170	0.0111	0.0099 $\pm$ 0.0005	0.0553	6.907E-01
Q_a	5.3300	4.4960	5.3861 $\pm$ 0.2899	0.0495	8.087E-01
Q_b	0.4500	0.4283	0.4441 $\pm$ 0.0463	0.0742	3.250E-01
$\Theta_{\text{chla}}^{\text{min}}$ [mgChla(mgC) ⁻¹]	0.0050	0.0049	0.0048 $\pm$ 0.0006	0.0708	3.810E-01
Θ_{chla}^0 [mgChla(mgC) ⁻¹]	0.0300	0.0251	0.0296 $\pm$ 0.0027	0.0637	5.135E-01
β [mmolm ⁻² s ⁻¹]	500.0000	589.2924	558.5273 $\pm$ 33.5500	0.1090	4.129E-02
σ [mmolm ⁻² s ⁻¹]	20.0000	20.3714	18.8886 $\pm$ 2.2417	0.0732	3.420E-01
$b_{r,\text{NAP}}$	0.0050	0.0024	0.0041 $\pm$ 0.0008	0.0545	7.077E-01

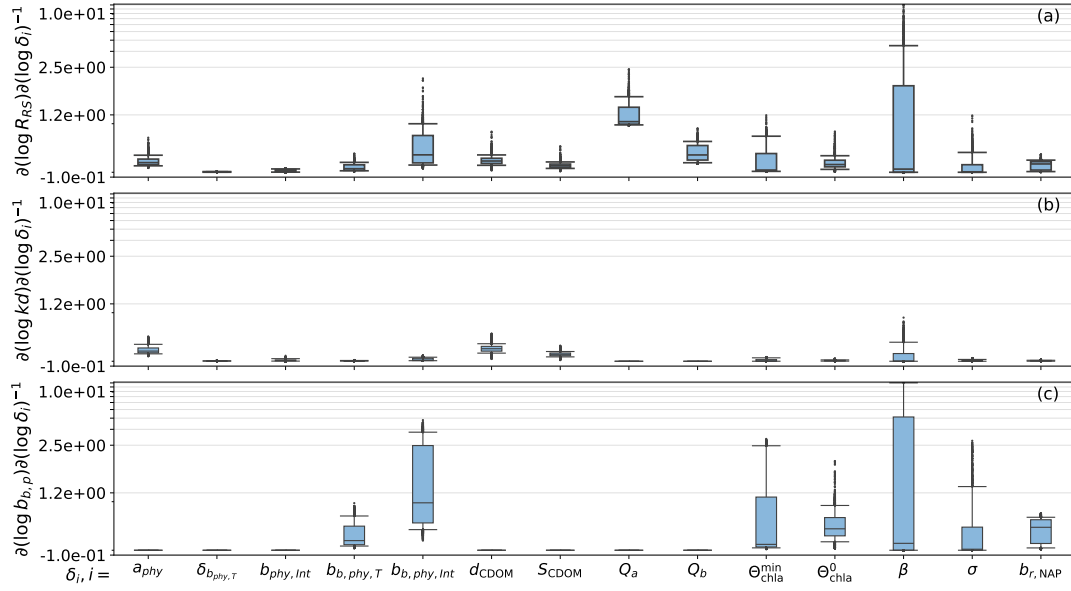


Figure 8. Sensitivity of (a) R_{rs} , (b) kd and (c) $b_{b,p}$ with respect to the perturbation factors δ_i evaluated at $\delta_i = 1$, the box plots represent the quartiles of the sensitivity for each day.

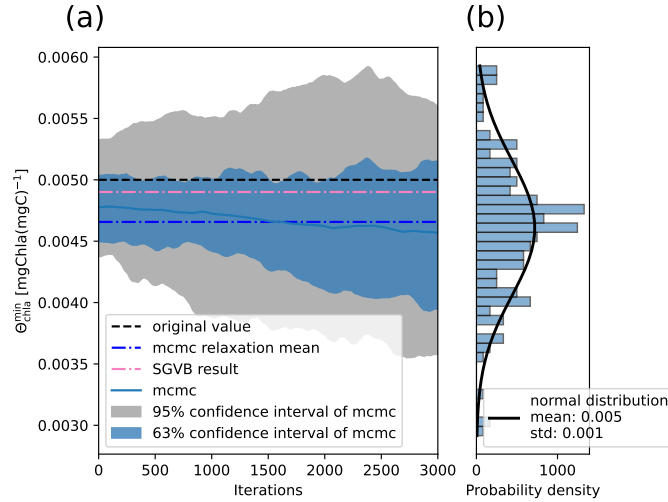


Figure 9. Result of the Metropolis-Hasting Algorithm for the parameter $\Theta_{\text{chla}}^{\text{min}}$ [$\text{mgChla}(\text{mgC})^{-1}$], using the transition probability shown in Eq. (23), with initial conditions close to the value obtained after performing Alternate Minimization. (a) Evolution of the parameter after each iteration of the algorithm, (b) final probability density estimated as a Gaussian distribution.

The main result of the new parametrization is a decrease in the Root Mean Square Error RMSE between the test data of sea surface chlorophyll observations and inverted values. A key aspect to note is that the MLE computed using the train data can

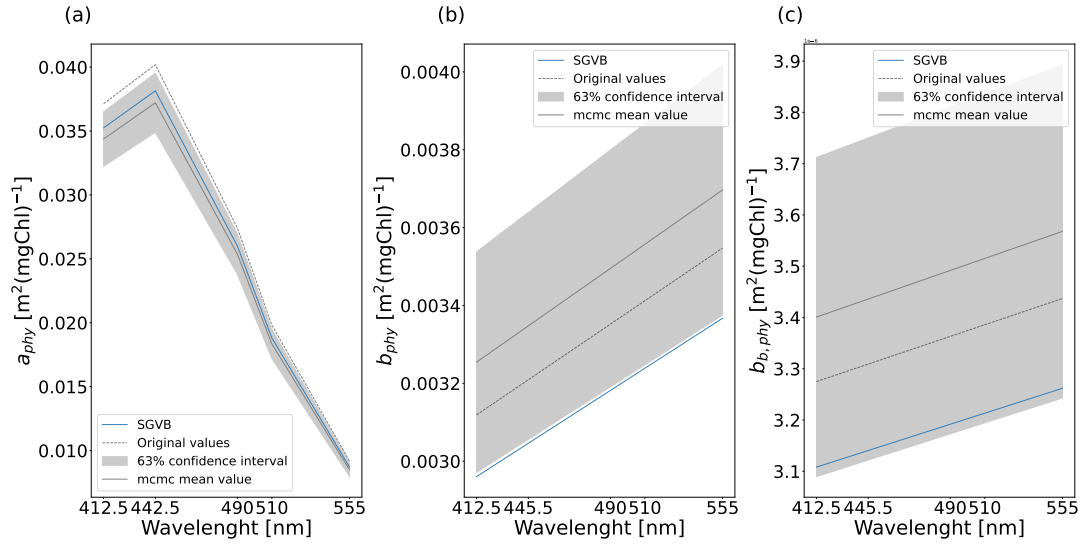


Figure 10. Original values (dashed line), final values using the SGVB based framework (blue) as well as the mean and standard deviation (gray) for the λ -dependent parameters (a) absorption coefficient of phytoplankton $a_{phy}(\lambda)$, (b) scattering coefficient of phytoplankton $b_{phy}(\lambda)$ and (c) backward scattering coefficient of phytoplankton $b_{b,phy}(\lambda)$.

Table 5. Correlation matrix between the perturbation factors δ_i , computed using the samples from the Metropolis-Hasting Algorithm.

$\delta_i, i =$	a_{PH}	$b_{phy,T}$	$b_{phy,Int}$	$b_{b,phy,T}$	$b_{b,phy,Int}$	d_{CDOM}	S_{CDOM}	Q_a	Q_b	$\Theta_{chl a}^{\min}$	$\Theta_{chl a}^0$	β	σ
a_{PH}	1.00												
$b_{phy,T}$	-0.04	1.00											
$b_{phy,Int}$	0.17	0.12	1.00										
$b_{b,phy,T}$	0.05	-0.01	-0.01	1.00									
$b_{b,phy,Int}$	0.06	-0.08	-0.07	0.09	1.00								
d_{CDOM}	0.47	-0.05	0.02	-0.04	0.03	1.00							
S_{CDOM}	0.19	0.09	0.08	-0.04	-0.05	0.61	1.00						
Q_a	-0.52	0.10	-0.04	-0.02	-0.03	-0.05	0.38	1.00					
Q_b	0.28	-0.10	-0.08	-0.01	0.08	0.06	-0.16	-0.28	1.00				
$\Theta_{chl a}^{\min}$	0.02	-0.02	0.07	-0.11	0.13	0.11	-0.04	0.01	0.19	1.00			
$\Theta_{chl a}^0$	-0.07	-0.25	0.08	0.10	-0.07	0.05	0.08	0.11	-0.00	-0.01	1.00		
β	-0.44	-0.23	-0.23	0.28	0.16	-0.30	-0.32	0.34	-0.18	0.02	0.12	1.00	
σ	-0.02	0.07	0.23	-0.16	-0.05	0.02	0.20	0.19	-0.13	-0.19	-0.02	-0.07	1.00
$b_{r,NAP}$	0.24	-0.13	-0.00	-0.19	-0.04	0.42	0.41	-0.01	0.11	0.08	0.28	-0.44	0.15

present overfitting; for this reason, we had to use early stopping during the Alternate Minimization step, and then we proceeded

to use the mean value of the estimated posterior estimated with the MCMC samples. Since for the test data, we observed a decrease in the RMSE (see Tab. D1), we can say that the posterior mean is good for generalization.

5.3 Comparison between Bayesian retrievals and the Variational Bayes approach

465 As described in Sec. 4.4, we used the SGVB estimator to find an optimal parametrization. The results can be appreciated in Tab. 4 and Fig. 10. Taking into account the uncertainty of the MCMC results, and using the 95% confidence interval, 22 of the 24 parameters perturbed with the SGVB estimator agree with the MCMC estimation, in the sense that the SGVB output is within the uncertainty of the MCMC estimate. The two parameters with high discrepancy between the two frameworks are: Q_a , in average, the most sensitive parameter concerning Remote Sensing Reflectance, and $b_{r,NAP}$, one of the most sensitive
470 parameters concerning particulate backward scattering.

To assess the performance of each set of parameters, we evaluated the MAP estimates of the optical constituents z given each set of parameters (MAP estimate obtained with the MCMC algorithm and the MLE obtained with the SGVB estimator) for the test dataset. I recall that this data set was not used for any parameter tuning before, so these results serve as a confirmation of the robustness of the methods.

475 The main indicator will be the sea surface chlorophyll observations, as it is the least noisy and scattered observation data. Based on the Root Mean Square Error (RMSE) and relative Median Absolute Deviation (rMAD) between measurements and retrieved estimates (Tab. D1 and Tab. D3), both parameter sets improved the inversion results. However, the parameter set optimized using the SGVB estimator yielded the best performance.

The observations of the downward light attenuation coefficient and the particulate backward scattering coefficient are much
480 more scattered and noisy than the chlorophyll, yet the SGVB parameters optimized all the model output matching observations, while the MCMC favors better outputs only for the k_d values. We speculate that this is due to overfitting, as the measurements of particulate backward scattering are highly scattered, and as particulate backward scattering is sensitive to $b_{r,NAP}$, the estimated value from the MCMC could be affected by the noise. In the case of NN training, we used minibatch minimization, which may have helped to find a parameter value that is better for generalization.

485 The SGVB estimator also provides an efficient way of computing estimates of the optical constituents z , which, by construction, are also consistent with the forward model, with optimal RMSE between measurements and estimates. Since they are computed with a neural network, the computational time outperforms the standard implicit inversion methods, required in cases where the expression of the RTE is too complicated to invert it analytically. For comparison, the estimated optical constituents $\hat{z}$ using the SGVB estimator are shown in Fig. 4, Fig. 5 and Fig. 6, and the statistics for the observation operator
490 using these estimates are shown in Tab. D1, Tab. D3 and Tab. D2.

We observe that the standard Bayesian estimate and those using the SGVB estimator are close to each other (Fig. 4), since the SGVB estimator outputs are within the uncertainty of the Bayesian estimate. Differences between both could be due to model errors, since the SGVB estimator requires approximating the posterior with a parameterized probability distribution, in our case, a Neural Network, or differences between the training algorithms. The Variational Bayes method also estimates the

495 covariance matrix between the latent variables Z , nevertheless, since the uncertainty was underestimated, we only plotted the mean values.

5.4 Comparison with satellite products

To asses the validity of the results with respect of state of the art algorithms, we compared the capability of the DIIM system in a wider region in the North West Mediterranean Sea characterized by high dynamics regimes of vertical mixing during the spring period and stratification during summer. The comparison is carried out using additional in-situ data (not used in the calibration of DIIM) based on High-Performance Liquid Chromatography (HPLC, Di Biagio et al., 2025) and a standard Ocean Color retrieval approach used with Copernicus Marine Service, the MedOC4.2020 (Colella et al., 2025). The latter approach is based on a calibrated nonlinear regression of the maximum Rrs in the wavelengths at 443, 490, and 510 nm, normalized over Rrs at 555 nm:

$$\text{chlorophyll}_{\text{satellite}} = 10^{(a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4)}, \quad X = \log_{10} \left(\frac{\max(R_{rs,443}, R_{rs,490}, R_{rs,510})}{R_{rs,555}} \right)$$

505 $a_0 = 0.327, a_1 = -2.994, a_2 = 2.722, a_3 = -1.226, a_4 = -0.568.$ (34)

To do so, we computed the surface downward direct and scattered irradiance as described in Lazzari et al. (2020) for the days and places where in-situ measurements were taken (see Fig. 11, (A)). We chose a square of $4^\circ \times 4^\circ$ close to the BOUSSOLE buoy for the samples, and selected those with a bathymetry lower than 200 m, and samples performed at less than 10 meters deep. For the Remote Sensing Reflectance (CMEMS), we used an average of 5 days, ~ 5 km window around the points. Finally, we used the SGVB estimator to invert the Remote Sensing Reflectance and estimate the Chlorophyll concentration. The outputs can be observed in Fig. 11.

Results are consistent between in-situ data and inversion models, suggesting that the present approach is applicable over spatially heterogeneous conditions.

6 Discussion

515 In the last years, there has been an increasing number of applications of neural networks in earth sciences, like forecasts of the El Niño-Southern Oscillation (ENSO) by using historical simulations and a convolutional neural network (Ham et al., 2019), fusion of satellite data (Chapman and Charantonis, 2017; Denvil-Sommer et al., 2019; Bocquet et al., 2020), classification of regions on the ocean (Richardson et al., 2003; Saraceno et al., 2006), finding drivers of net primary productivity using self organizing maps (Lachkar and Gruber, 2012), reconstruction of oceanographic variables (Martinez et al., 2020; Pietropolli et al., 2022), classification of the anomalies of water leaving radiance (Mustapha et al., 2014), data reconstruction (Manucharyan et al., 2021; George et al., 2021), inversion of oceanographic variables (Brajard et al., 2006; Irrgang et al., 2019; Dessailly, 2012), pattern recognition (Maze et al., 2017; Jones et al., 2019; Jones and Ito, 2019; Boehme and Rosso, 2021; Desbruyères et al., 2021), forecast imposing physical constrains (De Bézenac et al., 2019; Erichson et al., 2019), increase of the resolution of modeling (Barthélémy et al., 2022), among others.

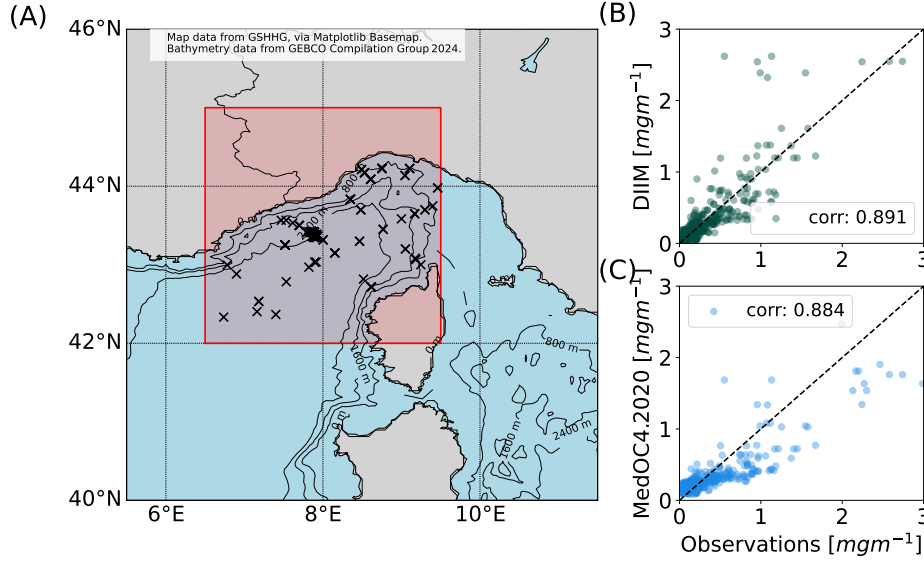


Figure 11. (A) Region in red and place with in-situ measurements (x) for the comparison between (B) the inverted values of chlorophyll a using the SGVB estimator, and (C) a standard Ocean Color retrieval approach used with Copernicus Marine Service (Colella et al., 2025).

Our work makes use of a neural network to approximate the posterior probability distribution of optical constituents in the sea by employing the SGVB estimator. As described in Sec. 4.4.1, we maximise the ELBO loss function, which simultaneously optimizes the forward model by finding the MLE of the parameters, deriving in situ biogeochemical parameters for reflectance observations, linking the neural network procedure to an interpretable model. As stated by Kingma and Welling (2013), this approach is especially useful to do inference of intractable posteriors and to find the MLE of the forward model parameters, a situation commonly encountered in data assimilation problems, where the number of parameters to optimize makes the problem intractable. This work serves as a test bed, comparing the more traditional Bayesian Inference approach with the results obtained with the SGVB estimator, as well as presenting a pointwise observation operator for the active optical constituents chlorophyll, NAP and CDOM.

Our results with the SGVB estimator under-estimated the uncertainty of the optical constituents, computation that is of crucial importance for multiple applications, like objective comparison of simulations against observations, efficient assimilation of data with methods like the Kalman Filters, among others (Brankart et al., 2012). A further analysis of the effect that each term of the loss function has on the NN covariance matrix would be needed, as well as whether the inclusion of a regularization term is affecting the uncertainty estimation. For the moment, the requirement of reliable uncertainty estimations leads us to use only the point-wise estimate of the neural network. Furthermore, we explored the Bayesian approach, approximating the final posterior distribution of the optical constituents, $p_{\Lambda}(z|y, \mathbf{x})$, with a Gaussian probability distribution. This method returns estimates with reliable uncertainty estimations that can be used in real operational systems.

In particular, in addition to the optical constituents, we aimed to find the optimal model with respect to all the in-situ observations for the entire period. This ambitious goal made the final results suboptimal for some individual measurements. For example, Salama and Verhoef (2015) used a similar forward model to estimate the downward light attenuation coefficient at a wavelength of 490 nm, $kd(490)$, at different depths, obtaining a rMAD of 11.84%, while our result using the MCMC parameters presented a rMAD value of 21%. We noticed that by optimizing only one in-situ measurement, we could find a set of parameters that made that measurement more precise. Nevertheless, we decided to use the parameters presented to balance the global accuracy. For example, in terms of the rMAD of the Remote Sensing Reflectance at a wavelength of 490 nm, $R_{rs}(490)$, we obtained a value of rMAD of 1.8%, outperforming previous works.

Our approach also differs from other works on Bayesian estimation of optical constituents (Gordon and Boynton, 1997; Boynton and Gordon, 2000; Michalopoulou et al., 2009; Erickson et al., 2023), since we are employing a three stream model, derived from the Radiative Transfer Model (Dutkiewicz et al., 2015), and using it to derived the in-situ observations for all the wave-lengths available. This feature allows scientists to understand the automatic learning process in terms of meaningful physical parameters.

The approach can be extended in different directions, in particular, the addition of more optical constituents, which will be facilitated once the information of the new satellite missions PRISMA (Hyperspectral Precursor of the Application Mission), with 12 nm spectra resolution ranging from 400 to 2500 nm, and PACE (Plankton, Aerosol, Cloud, Ocean Ecosystem) with a 5 nm resolution ranging from 350 to 890 nm, is used as input of the system, or the addition in the Forward model of terms that take into account the interaction with the sea floor, crucial for the analysis of shallow waters.

7 CONCLUSIONS

By utilizing the Bayes theorem and linearizing the forward function, we achieved the inversion of the optical constituents, with an estimate of the uncertainty. The latter is fundamental for the assimilation of Remote Sensing Reflectance.

By using an MCMC algorithm, we computed a set of parameters that optimized the forward model and showed that the method was robust by obtaining coherent values with the SGVB estimator. Moreover, the Variational Bayes framework can be used as an alternative to find point-wise estimates of optimal parameters, and also as an efficient way of computing point-wise estimates of the optical constituents.

Regarding the computational advantages of the SGVB estimator, as long as the uncertainty is not required, it is the best option to estimate the optical constituents in operational systems, since, after training, the evaluation of the neural network is much faster than the iterative minimization (effect known as amortization). Nevertheless, the posterior probability learned by the neural network underestimates the uncertainty of the result, which makes the MAP algorithm preferred when the uncertainty is a requirement. Since the computational time for the MAP estimate depends on the initial conditions, we proposed to use the SGVB estimates as initial conditions for the MAP algorithm, which, by making experiments with our current implementation, we found to be capable of reducing the number of steps by more than 50%.

For future work, it would be important to apply and verify the accuracy of the approach with more optical constituents and
 575 to test Remote Sensing Reflectance assimilation in a biogeochemical model.

Code and data availability. The version used to produce the results is archived on Zenodo, as are the input data and scripts to run the model and produce the plots for all the simulations presented in this paper, under the DOI 10.5281/zenodo.14609747 (Soto, 2025).

We used the MedBGCins data set for in-situ data based on High-Performance Liquid Chromatography. Data set available in Zenodo under the DOI <https://doi.org/10.5281/zenodo.15489967> (Di Biagio et al., 2025).

580 Appendix A

In this section, we expand the solution of Eq. (1) subject to the boundary conditions (6), under the homogeneity assumption. First, for simplicity, we re-write Eq. (1) as,

$$\begin{aligned}\frac{dE_{\text{dir}}(h, \lambda)}{dh} &= -c_d(\lambda)E_{\text{dir}}(h, \lambda), \\ \frac{dE_{\text{dif}}(h, \lambda)}{dh} &= -C_s(\lambda)E_{\text{dif}}(h, \lambda) + B_u(\lambda)E_u(h, \lambda) + F_d(\lambda)E_{\text{dir}}(h, \lambda), \\ \frac{dE_u(h, \lambda)}{dh} &= -B_s(\lambda)E_{\text{dif}}(h, \lambda) + C_u(\lambda)E_u(h, \lambda) - B_d(\lambda)E_{\text{dir}}(h, \lambda),\end{aligned}$$

subject to,

$$E_{\text{dir}}(0, \lambda) = E_{\text{dir}}^{\text{OASIM}}(0, \lambda), E_{\text{dif}}(0, \lambda) = E_{\text{dif}}^{\text{OASIM}}(0, \lambda), E_u(\infty, \lambda) = 0, \quad (\text{A1})$$

were,

$$\begin{aligned}c_d(\lambda) &= \frac{a(\lambda) + b(\lambda)}{\cos \theta}, \\ C_s(\lambda) &= \frac{a(\lambda) + r_s b_b(\lambda)}{v_s}, \\ B_u(\lambda) &= \frac{r_u b_b(\lambda)}{v_u}, \\ F_d(\lambda) &= \frac{b(\lambda) - r_d b_b(\lambda)}{\cos \theta}, \\ B_s(\lambda) &= \frac{r_s b_b(\lambda)}{v_s}, \\ C_u(\lambda) &= \frac{a(\lambda) + r_u b_b(\lambda)}{v_u}, \\ 585 \quad B_d(\lambda) &= \frac{r_d b_b(\lambda)}{\cos \theta}.\end{aligned} \quad (\text{A2})$$

Equation (A1) is a linear system of Ordinary Differential Equations, which can be solved by, first solving the equation for $E_{\text{dir}}(h, \lambda)$, followed by solving the system of equations for $E_{\text{dif}}(h, \lambda)$ and $E_u(h, \lambda)$, taking the solution of $E_{\text{dir}}(h, \lambda)$ as the

in-homogeneous part of the system of equations. The final expression is,

$$\begin{aligned}
E_{\text{dir}}(h, \lambda) &= E_{\text{dir}}^{\text{OASIM}}(0, \lambda) e^{-hc_d}, \\
E_{\text{dif}}(h, \lambda) &= c^+ e^{-k^+ h} + x_{\text{dif}} E_{\text{dir}}(h, \lambda), \\
E_u(h, \lambda) &= c^+ r^+ e^{-k^+ h} + y_u E_{\text{dir}}(h, \lambda),
\end{aligned} \tag{A3}$$

590 where,

$$\begin{aligned}
c^+ &= E_{\text{dif}}^{\text{OASIM}}(0, \lambda) - x E_{\text{dir}}^{\text{OASIM}}(0, \lambda), \\
k^+ &= D - C_u, \\
r^+ &= \frac{B_s}{D}, \\
D &= \frac{1}{2} \left(C_s + C_u + \sqrt{(C_s + C_u)^2 - 4B_s B_u} \right), \\
x &= \frac{-(C_u + c_d)F_d - B_u B_d}{(c_d - C_s)(c_d + C_u) + B_s B_u}, \\
y &= \frac{(-B_s F_d + (-C_s + c_d)B_d)}{(c_d - C_s)(c_d + C_u) + B_s B_u}.
\end{aligned} \tag{A4}$$

In the case when the expression $(c_d - C_s)(c_d + C_u) + B_s B_u = 0$, then the expression for c^+ has to be exchange to $c^+ = E_{\text{dif}}^{\text{OASIM}}(0, \lambda)$.

Appendix B: Tuning of the hyperparameter α

595 As seen in Sec. 4, the final covariance matrix for the retrieve $\tilde{Z}^*$ depends on the hyperparameter α by the equation $\Sigma_z = \alpha \mathbb{I}$. We selected the value of α to fulfill two criteria: The retrieved $\tilde{Z}^*$ should be robust on α , meaning, small changes on α should not change the retrieved quantity, and the estimated uncertainty has to be close to the discrepancy between retrieved data and in-situ observations.

600 For this end, we defined the error of the forward model $\epsilon_{R_{rs}}(\alpha)$ as the Root Mean Square Difference between the satellite Remote Sensing Reflectance and that predicted by the model. The aim is to make this quantity robust on α .

We also defined the error between the predicted uncertainty and the actual discrepancy between model and data $\epsilon_{\delta_{\text{chla}}}(\alpha)$, where the predicted uncertainty is estimated as the mean value of the standard deviation of the predicted $\text{chla}^{\text{MODEL}}$, and the discrepancy between model and data is estimated as the Root Mean Square Difference between chla^{OBS} and $\text{chla}^{\text{MODEL}}$.

605 We computed $\epsilon_{R_{rs}}(\alpha)$ and $\epsilon_{\delta_{\text{chla}}}(\alpha)$ for different values of α until the curve $\epsilon_{R_{rs}}(\alpha)$ flattens. With the errors computed, we re-scaled the error functions $\epsilon_{R_{rs}}(\alpha)$ and $\epsilon_{\delta_{\text{chla}}}(\alpha)$ between zero and one in order to minimize both functions simultaneously by minimizing the loss function

$$\mathcal{L}^\alpha = \overline{\epsilon_{R_{rs}}(\alpha)} + \overline{\epsilon_{\delta_{\text{chla}}}(\alpha)}, \tag{B1}$$

where the line over the errors stands for the rescaling. Figure B1 shows the final value of α selected, as a function of $\epsilon_{R_{rs}}(\alpha)$, $\epsilon_{\delta_{\text{chla}}}(\alpha)$ and $\mathcal{L}^\alpha$.

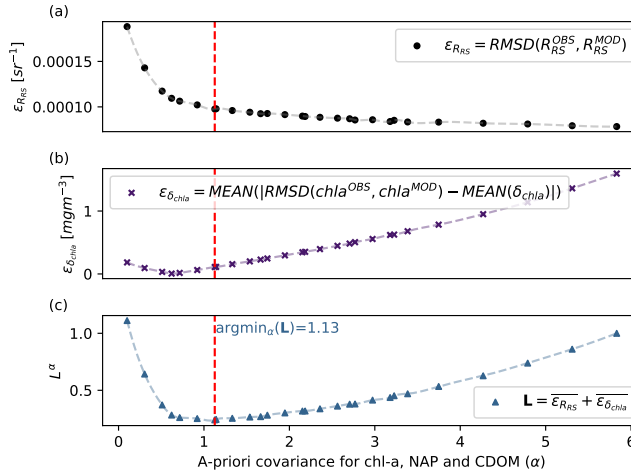


Figure B1. Illustration of how the hyper-parameter α was chosen. Using a higher α decreases the Root Mean Square Difference between the Remote Sensing Reflectance observed by satellite, and the one obtained with the model (a), but increases the error between the predicted uncertainty and the actual discrepancy between model and data (b). The value chosen was the one that minimized the $\mathcal{L}^\alpha$ loss function (c).

610 Appendix C

This section shows that $\mathcal{L}_{ELBO}$ is a lower bound of the data log-likelihood. First, we write the expression for the log-likelihood by marginalizing over all possible values of the latent variable z

$$\log(p_\Lambda(\mathbf{y})) = \log\left(\int_{\mathcal{Z}} p_\Lambda(\mathbf{y}|z)p(z)dz\right), \quad (C1)$$

next we introduce the parameterized probability distribution $q_\phi(z|\mathbf{y})$

$$615 \quad = \log\left(\int_{\mathcal{Z}} p_\Lambda(\mathbf{y}|z)\frac{q_\phi(z|\mathbf{y})}{q_\phi(z|\mathbf{y})}p(z)dz\right), \quad (C2)$$

Finally, we use Jensen's inequality to find a lower bound for the log-likelihood,

$$\begin{aligned} &\geq \int_{\mathcal{Z}} \log\left(\frac{p_\Lambda(\mathbf{y}|z)p(z)}{q_\phi(z|\mathbf{y})}\right)q_\phi(z|\mathbf{y})dz \\ &= \int_{\mathcal{Z}} \log\left(\frac{p(z)}{q_\phi(z|\mathbf{y})}\right)q_\phi(z|\mathbf{y}) + \int_{\mathcal{Z}} \log(p_\Lambda(\mathbf{y}|z))q_\phi(z|\mathbf{y})dz \\ &= -D_{KL}(q_\phi(z|\mathbf{y})||p(z)) + \mathbb{E}_{q_\phi(z|\mathbf{y})}[\log(p_\Lambda(\mathbf{y}|z))] \\ &= \mathcal{L}_{ELBO}. \end{aligned} \quad (C3)$$

The inequality is an equality for the case $q_\phi(z|\mathbf{y}) = p(z|\mathbf{y})$, the true posterior distribution, in which case $\mathcal{L}_{ELBO} = \log(p_\Lambda(\mathbf{y}))$. In other words, maximising the $\mathcal{L}_{ELBO}$ equals maximising the marginal log-likelihood.

620 **Appendix D**

In this section, we include the Root Mean Square Error (RMSE), Pearson correlation coefficients (ρ), and relative Median Absolute Deviation (rMAD) for all the measurements and observations, using the MAP estimates with unperturbed parameters, MAP estimate with parameters from the MCMC algorithm, MAP estimate with parameters from the SGVB estimator, and outputs from the SGVB estimator. All the quantities are computed using only the test data, which is 10% of the data, not used
625 in the MCMC algorithm or in the training of the neural network. Finally, we include tables with the symbols used across this work.

Table D1. Root Mean Square Error between satellite and in-situ observations, and the modeled data using the Maximum A-posterior (MAP) estimate with unperturbed parameters, optimized parameters with the MCMC algorithm, optimized parameters with the SGVB based framework, and modeled data purely with the SGVB based framework. Notice that a log transform was performed before the computations.

	Root Mean Square Error, $\text{RMSE}(\text{OBS}, \text{MOD}) = \sqrt{\text{MEAN}((\text{OBS} - \text{MOD})^2)}$			
	MAP with unperturbed parameters	MAP with MCMC parameters	MAP with SGVB parameters	SGVB output
$R_{RS,412.5}$	0.039998	0.040920	0.042113	0.128636
$R_{RS,442.5}$	0.019901	0.022441	0.019984	0.117474
$R_{RS,490}$	0.033773	0.023230	0.029305	0.071944
$R_{RS,510}$	0.033258	0.038340	0.039021	0.059382
$R_{RS,555}$	0.019328	0.031546	0.033822	0.091312
$k_{d,412.5}$	0.395717	0.419141	0.378790	0.429363
$k_{d,442.5}$	0.327759	0.322888	0.303636	0.365043
$k_{d,490}$	0.324604	0.300414	0.299151	0.339610
$k_{d,510}$	0.221749	0.210633	0.213028	0.214196
$k_{d,555}$	0.135205	0.130366	0.133158	0.137648
$b_{b,p,442.5}$	0.457789	0.334198	0.512618	0.787984
$b_{b,p,490}$	0.446384	0.506215	0.405386	0.549156
$b_{b,p,555}$	0.439231	0.521719	0.423929	0.550503
chl _a	0.603652	0.587130	0.502672	0.447947
Total	3.49835	3.48918	3.33661	4.29020

Table D2. Pearson correlation coefficient r between satellite and in-situ observations, and the modeled data using the Maximum A-posterior (MAP) estimate with unperturbed parameters, optimized parameters with the MCMC algorithm, optimized parameters with the SGVB framework, and modeled data purely with the SGVB framework.

	Spearman rank-order correlation coefficient ρ			
	MAP with unperturbed parameters	MAP with MCMC parameters	MAP with SGVB parameters	SGVB output
$R_{RS,412.5}$	0.99304	0.98841	0.99041	0.98306
$R_{RS,442.5}$	0.99851	0.99747	0.99801	0.99192
$R_{RS,490}$	0.99715	0.99622	0.99479	0.98670
$R_{RS,510}$	0.99201	0.99105	0.97962	0.94380
$R_{RS,555}$	0.99378	0.99142	0.97987	0.92020
$k_{d,412.5}$	0.80801	0.81693	0.81097	0.81300
$k_{d,442.5}$	0.88324	0.88525	0.88408	0.87611
$k_{d,490}$	0.84371	0.85139	0.85001	0.84049
$k_{d,510}$	0.85792	0.86398	0.86020	0.85466
$k_{d,555}$	0.71051	0.69352	0.68246	0.68541
$b_{b,p,442.5}$	0.65502	0.67547	0.68759	0.68896
$b_{b,p,490}$	0.52632	0.57810	0.61910	0.61431
$b_{b,p,555}$	0.65197	0.67520	0.68754	0.68674
chla	0.85199	0.86955	0.87259	0.87400
Total	11.76319	11.87396	11.89723	11.75935

Table D3. relative Median Absolute Deviation (rMAD) between satellite and in-situ observations, and the modeled data using the Maximum A-posterior (MAP) estimate with unperturbed parameters, optimized parameters with the MCMC algorithm, optimized parameters with the SGVB framework, and modeled data purely with the SGVB framework.

	rMAD = $\text{MEAN}(\text{OBS} - \text{MOD} /\text{OBS})$			
	MAP with unperturbed parameters	MAP with MCMC parameters	MAP with SGVB parameters	SGVB output
$R_{RS,412.5}$	0.029481	0.031956	0.032869	0.122038
$R_{RS,442.5}$	0.014825	0.016953	0.014725	0.110805
$R_{RS,490}$	0.028941	0.018827	0.024378	0.066319
$R_{RS,510}$	0.029412	0.034112	0.031342	0.046536
$R_{RS,555}$	0.015851	0.025844	0.022127	0.071504
$k_{d,412.5}$	0.267226	0.284409	0.262888	0.270284
$k_{d,442.5}$	0.226699	0.224069	0.219680	0.245279
$k_{d,490}$	0.222441	0.212747	0.214475	0.228192
$k_{d,510}$	0.168964	0.167468	0.169385	0.159414
$k_{d,555}$	0.101646	0.100650	0.101680	0.101663
$b_{b,p,442.5}$	0.316195	0.256815	0.350178	0.509545
$b_{b,p,490}$	0.376320	0.556826	0.311682	0.317715
$b_{b,p,555}$	0.384337	0.568183	0.365311	0.379714
chl _a	0.725247	0.694534	0.488889	0.305717
Total	2.90758	3.19339	2.60961	2.93472

Table D4. Table of Symbols used for the Radiative Transfer Model.

Symbol	Meaning
E_{dir}	Vertical Direct irradiance
E_{dif}	Vertical scattered downward irradiance
E_{u}	Vertical scattered upward irradiance
θ	Sun zenith angle
h	depth at which a measurement is assumed to be taken.
λ	Wavelength at which a measurement is assumed to be taken.
$a(\lambda)$	Total absorption coefficient
$b(\lambda)$	Total scattering coefficient
$b_b(\lambda)$	Total backward scattering coefficient
w	Water
phy	Phytoplankton
chla	Chlorophyll- α
CDOM	Chromophoric Dissolved Organic Matter
NAP	Non Algal Particles
$a_w(\lambda)$	Water-specific absorption coefficient
$a_{\text{phy}}(\lambda)$	Chlorophyll-specific absorption coefficient of phytoplankton
$a_{\text{CDOM}}(\lambda)$	Mass-specific absorption coefficient of CDOM
$a_{\text{NAP}}(\lambda)$	Mass-specific absorption coefficient of NAP
$b_w(\lambda)$	Water-specific scattering coefficient
$b_{\text{phy}}(\lambda)$	Carbon-specific scattering coefficient of phytoplankton
$b_{\text{NAP}}(\lambda)$	Mass-specific scattering coefficient of NAP
$b_{b,w}(\lambda)$	Water-specific backward scattering coefficient
$b_{b,\text{phy}}(\lambda)$	Carbon-specific backward scattering coefficient of phytoplankton
$b_{b,\text{NAP}}(\lambda)$	Mass-specific backward scattering coefficient of NAP
PAR	Photosynthetic Available Radiation
$E_{\text{dir}}^{\text{OASIM}}(0, \lambda)$	Direct downward irradiance on the surface of the ocean, from the OASIM model
$E_{\text{dif}}^{\text{OASIM}}(0, \lambda)$	Scattered downward irradiance on the surface of the ocean, from the OASIM model
$E_{\text{u}}(\infty, \lambda)$	Scattered upward irradiance on the floor of the ocean
R_{rs}	Remote Sensing Reflectance
$b_{b,p}$	Particulate backward scattering coefficient
k_d	Downward light attenuation coefficient

Table D5. Table of symbols and notation used for the Bayes formalism.

Symbol	Meaning
$\mathbf{y}$	Vector, discretization of a continuous function in discrete values of λ
y_λ	Component of a vector with magnitude $y(\lambda)$
z^*	Optimal value of a retrieved quantity z , solution of a minimization problem
$\hat{z}$	Estimation of the optimal value of a quantity z
$\operatorname{argmin}_z \mathcal{L}(z)$	Quantity z that minimized the loss function $\mathcal{L}$
$\operatorname{argmax}_z p(y z)$	Quantity z that maximises the likelihood $p(y z)$
$\mathbf{y}^d$	Remote Sensing Reflectance data from day d
$\mathbf{x}^d$	OASIM data from day d
$\mathbf{z}^d$	Optical constituents from day d
Λ	Set of parameters from the forward model
$\mathbf{Y}$	Set of many days with Remote Sensing Reflectance data, which represents the train set when it is used for training, and the test set when it is used for testing
$\mathbf{X}$	Set of many days with OASIM data, which represents the train set when it is used for training, and the test set when it is used for testing
$\mathbf{Z}$	Set of many days with retrieved optical constituents, which represents the train set when it is used for training, and the test set when it is used for testing
$p_\Lambda(\mathbf{y} z, \mathbf{x})$	Probability distribution of the variable $\mathbf{y}$ conditional on z , and $\mathbf{x}$, as a function of Λ
$\mathcal{N}(\mu, \Sigma)$	Gaussian probability distribution with mean μ and covariance matrix Σ
H^{OBS}	in-situ observations
H^{MODEL}	Model of the in-situ observations
$\mathcal{H}$	Observation operator, equal to H^{OBS} when there were observations, and zero otherwise
I^d	Presence-absence nine dimension indicator function
$\mathcal{L}^H$	Loss function used to minimize the distance between in-situ observations and predicted observations
$\mathcal{L}^z$	Loss function used to maximize the posterior probability $p_\Lambda(\tilde{z}^d \mathbf{y}^d, \mathbf{x}^d)$ for every day d
$\tilde{z}$	optical constituents with the change of variable $\tilde{z} = \log(z)$
Σ_ϵ	Covariance matrix of the Remote Sensing Reflectance
ϵ	Noise of the Remote Sensing Reflectance
δ_Λ	Perturbations on the parameters
$\nabla_{\tilde{z}^d}$	Gradient over every component of $\tilde{z}^d$
Σ_z	Covariance of the prior term associated to the optical constituents $\Sigma_z = \alpha \mathbf{1}$, $\mathbf{1}$ the identity matrix

Table D6. Table of Symbols and notations used for the Variational Bayes formalism.

Symbol	Meaning
z	Latent variable sampled from an unknown distribution $p_{\Lambda^*}(z)$
$\mathbf{y}$	Random variable sampled from a known conditional distribution $p_{\Lambda^*}(\mathbf{y} z)$
$p_{\Lambda}(\mathbf{y})$	data-Likelihood of the parameter Λ
$p_{\Lambda}(z \mathbf{y})$	Posterior probability of the latent variable z
$q_{\phi}(z \mathbf{y})$	Estimate of the posterior probability of the latent variable z
$\mathcal{L}_{ELBO}$	ELBO loss function, where ELBO stands for ‘‘Evidence Lower Bound’’
$D_{KL}(q_{\phi}(z \mathbf{y}) p_{\Lambda}(z))$	Kullback-Leibler divergence between the two probability distributions $q_{\phi}(z \mathbf{y})$ and $p_{\Lambda}(z)$
$\mathbb{E}_{q_{\phi}(z \mathbf{y})}[\log(p_{\Lambda}(\mathbf{y} z))]$	Expected value of $\log(p_{\Lambda}(\mathbf{y} z))$ with respect to the probability distribution $q_{\phi}(z \mathbf{y})$

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