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Bayesian methodology for inverting satellite ocean-color data

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ABSTRACT

The inverse ocean color problem, i.e., the retrieval of marine reflectance from top-of-atmosphere (TOA) reflectance, is examined in a Bayesian context. The solution is expressed as a probability distribution that measures the likelihood of encountering specific values of the marine reflectance given the observed TOA reflectance. This conditional distribution, the posterior distribution, allows the construction of reliable multi-dimensional confidence domains of the retrieved marine reflectance. The expectation and covariance of the posterior distribution are computed, which gives for each pixel an estimate of the marine reflectance and a measure of its uncertainty. Situations for which forward model and observation are incompatible are also identified. Prior distributions of the forward model parameters that are suitable for use at the global scale, as well as a noise model, are determined. Partition-based models are defined and implemented for SeaWiFS, to approximate numerically the expectation and covariance. The ill-posed nature of the inverse problem is illustrated, indicating that a large set of ocean and atmospheric states, or pre-images, may correspond to very close values of the satellite signal. Theoretical performance is good globally, i.e., on average over all the geometric and geophysical situations considered, with negligible biases and standard deviation decreasing from 0.004 at 412 nm to 0.001 at 670 nm. Errors are smaller for geometries that avoid Sun glint and minimize air mass and aerosol influence, and for small aerosol optical thickness and maritime aerosols. The estimated uncertainty is consistent with the inversion error. The theoretical concepts and inverse models are applied to actual SeaWiFS imagery, and comparisons are made with estimates from the SeaDAS standard atmospheric correction algorithm and in situ measurements. The Bayesian and SeaDAS marine reflectance fields exhibit resemblance in patterns of variability, but the Bayesian imagery is less noisy and characterized by different spatial de-correlation scales. Experimental errors obtained from match-up data are similar to the theoretical errors determined from simulated data. Regionalization of the inverse models is a natural development to improve retrieval accuracy, for example by including explicit knowledge of the space and time variability of atmospheric variables.

1. Introduction

The classic approach to ocean-color remote sensing from space (Antoine & Morel, 1999; Gordon, 1997; Wang, 2010) consists of (i) estimating the aerosol reflectance in the red and near infrared where the ocean can be considered black (i.e., totally absorbing), and (ii) extrapolating the estimated aerosol reflectance to shorter wavelengths. The water reflectance is then retrieved by subtraction. This process is referred to as atmospheric correction. Depending on the application context, the retrieved water reflectance may then be related to chlorophyll-a concentration using a bio-optical model, semi-analytical or empirical (e.g., O'Reilly et al., 1998), or used in inverse schemes of varied complexity to estimate optical properties of suspended particles and dissolved organic matter (see Lee, 2006).

The process of atmospheric correction is inherently difficult to achieve with sufficient accuracy, since only a small fraction (10% or less) of the measured signal may originate from the water body. Furthermore, the surface and atmospheric constituents, especially aerosols, whose optical properties are influential, exhibit high space and time variability. However this two-step approach has been successful, and it is employed in the operational processing of imagery from most satellite ocean-color sensors. Variants and improvements to the classic atmospheric correction scheme have been made over the years, especially to deal with non-null reflectance in the red and near infrared, a general situation in estuaries and the coastal zone. The improvements in these regions consider spatial homogeneity for the spectral ratio of the aerosol and water reflectance in the red and near infrared (Ruddick, Ovidio, & Rijkeboer, 2000) or for the aerosol type, defined in a nearby non-turbid area (Hu, Carder, & Muller-Karger, 2000). They also use iteratively a bio-optical model (Bailey, Franz, & Werdell, 2010; Siegel, Wang, Maritorena, & Robinson, 2000; Stumpf, Arnone, Gould, Martinolich, & Ransibrahmanakul, 2003), exploit differences in the spectral shape of the aerosol and marine reflectance Lavender, Pinkerton, Moore, Aiken,

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and Blondeau-Patissier (2005), or make use of observations in the short-wave infrared, where the ocean is black, even in the most turbid situations (Bo-Cai, M.M.J.A.Z., & D.C.O., 2000; Oo et al., 2008; Wang, Son, & Shi, 2009; Wang, Tang, & Shi, 2007).

Other empirical approaches to atmospheric correction have been proposed in the literature. In Frouin, Deschamps, Gross-Colzy, Murakami, and Nakajima (2006), the TOA reflectance in selected spectral bands is combined linearly, so that the atmosphere/surface effects are reduced substantially or practically eliminated. This algorithm assumes that the perturbing signal, smooth spectrally, can be modeled by a low-order polynomial, and the polynomial is selected so that the linear combination is sufficiently sensitive to chlorophyll-a concentration. In Steinmetz, Deschamps, and Ramon (2011), the atmospheric reflectance is approximated by a polynomial with non-spectral and spectral terms that represent atmospheric scattering and surface reflection, including adjacency effects from clouds and white surfaces. The water reflectance is modeled as a function of chlorophyll concentration and a backscattering coefficient for non-algal particles, and spectral matching is applied to tune the atmospheric and oceanic parameters.

Another approach to satellite ocean-color inversion is to determine simultaneously the key properties of aerosols and water constituents by minimizing an error criterion between the measured reflectance and the output of a radiative transfer model (e.g., Chomko & Gordon, 1988; Kuchinke, Gordon, Harding, & Voss, 2009; Land & Haigh, 1996; Stamnes et al., 2007). This belongs to the family of deterministic solutions to inverse problems; for a mathematical treatment of the subject, we refer the interested reader to Engl, Hanke, and Neubauer (1996). Through systematic variation of candidate aerosol models, aerosol optical thickness, hydrosol backscattering coefficient, yellow substance absorption, and chlorophyll-a concentration, or a subset of those parameters, a best fit to the spectral top-of-atmosphere reflectance (visible and near infrared) is obtained in an iterative manner. The advantage of this approach, compared with the standard, two-step approach, resides in its ability to handle both Case 1 and Case 2 waters. It also can handle both weakly and strongly absorbing aerosols, even if the vertical distribution of aerosols, an important variable in the presence of absorbing aerosols, is not varied in the optimization procedure. A main drawback is that convergence of the minimizing sequence may be slow in some cases, making it difficult to process large amounts of satellite data. To cope with this issue, a variant proposed in Brajard, Jamet, Moulin, and Thiria (2006) and Jamet, Thiria, Moulin, and Crépon (2005) consists of approximating the operator associated to the radiative transfer (RT) model by a function which is faster in execution than the RT code, e.g., by neural networks. Still, convergence speed of the minimization algorithm remains an issue. It may also not be easy to differentiate absorption by aerosols and water constituents like yellow substances, processes that tend to decrease the TOA signal in a similar way. As a result, the retrievals may not be robust to small perturbations on the TOA reflectance. This reflects the fact that atmospheric correction is an ill-posed inverse problem; in particular, different values of the atmospheric and oceanic parameter can correspond to close values of the TOA reflectance. In the context of deterministic inverse problem, stability of the solution can be obtained by regularization (see Engl et al., 1996), but to the best of our knowledge, regularization strategies are not implemented in the approaches described above.

Another route is to cast atmospheric correction as a statistical inverse problem and to define a solution in a Bayesian context. In this setting, one group of approaches consists of estimating, based on simulations, a function performing a mapping from the TOA reflectance to the marine reflectance. In Shroeder, Behnert, Schaale, Fischer, and Doerffer (2007), a neural network model is fitted to simulated data. A similar approach is studied in Gross, Colzy, Frouin, and Henry (2007a,b), where the (finite-dimensional) TOA signal, corrected for gaseous absorption and molecular scattering, is first represented in a basis such that the correlation between the ocean contribution and atmosphere contribution is, to some extent, minimized. This representation of the TOA reflectance makes the function approximation problem potentially easier to solve. In these studies, data are simulated for all the observation geometries. In Frouin and Pelletier (2007) and Pelletier and Frouin (2004, 2005), the angular information is decoupled from the spectral reflectance, and atmospheric correction is considered as a collection of similar inverse problems indexed by the observation geometry. These methods can all be formalized in a Bayesian context; see Kaipio and Somersalo (2004) and Tarantola (2005) for an introduction on the subject.

The Bayesian approach to inverse problem consists of first specifying a probability distribution, called the prior distribution, on the input parameters (atmospheric and oceanic) of the RT model. As the name implies, the prior distribution reflects prior knowledge that may be available before the measurement of the TOA reflectance. A probabilistic modeling of any perturbation of the TOA reflectance is also typically considered, in the form of an additive random noise. The solution to the inverse problem is then expressed as a probability distribution which, in the present context of atmospheric correction, measures the likelihood of encountering values of water reflectance given the TOA reflectance (i.e., after it has been observed). The posterior distribution is a very rich object, and its complete reconstruction and exploration can rapidly become prohibitive from the computational side. Instead, one may reduce the ambition to extracting useful quantities, like its expectation and covariance. In the present setting of atmospheric correction, the expectation provides an estimate of the water reflectance, while the covariance allows a quantification of uncertainty in the water reflectance estimate.

In this paper, we address ocean-color remote sensing in a Bayesian context. We make the following contributions. First of all, we formulate the atmospheric correction problem at a certain depth of physical modeling, and we use the angular decoupling as in Frouin and Pelletier (2007) and Pelletier and Frouin (2004, 2005). Prior distributions suitable for use at a global scale, as well as a noise model, are determined. Second, we define and implement numerical approximations of the expectation and covariance of the posterior distribution (i.e., the complete Bayesian solution). The procedure is developed for the marine reflectance as well as for the atmospheric parameters, hence these quantities are retrieved simultaneously from the TOA reflectance, and measures of uncertainties are provided along with the retrievals. The modeling choices in this work have been governed by keeping the execution time of the models small, and by having theoretical guarantees on the performance. Let us point out that it is a forward model which is inverted and that, as precise as the physical modeling can be, it is important to detect cases where the model is limited in view of the measured TOA reflectance. So as a final contribution, we define and implement a model, based on level sets, to detect these situations where the retrievals become meaningless.

The paper is organized as follows. In Section 2, the inverse problem of atmospheric correction is defined, and the Bayesian solution is formulated. In Section 3, the inverse applications that will be implemented in practice are specified. In Sections 4 and 5, the modeling of the satellite signal and the approximation of the forward operator are described. In Section 6, the practical implementation of the inverse applications is detailed. Some technical details are gathered in Appendices A and B at the end of the paper. In Section 7, performance is evaluated on simulated data, and the ill posed-ness of the inverse problem is illustrated and discussed. In Section 8, the theoretical concepts and inverse models are applied to Sea-viewing Wide Field-of view Sensor (SeaWiFS) imagery, and comparisons are made with estimates from the standard atmospheric correction algorithm and in-situ measurements. In Section 9, conclusions are given about the Bayesian methodology in terms of performance, robustness, and generalization, as well as a perspective on future work.

2. Bayesian approach to atmospheric correction

2.1. Problem position

Let L_{toa} be the radiance measured by the satellite ocean-color sensor in a given spectral band. Express L_{toa} in terms of bidirectional reflectance