Chapter 3

Uncertainties in the Products of Ocean-Colour Remote Sensing

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Data products retrieved from the inversion of *in situ* or remotely sensed ocean-colour data are generally distributed or reported without estimates of their uncertainties. The accuracy of inversion products such as chlorophyll-a or IOPs is frequently evaluated by comparison with *in situ* measurements, but these analyses are not always sufficient to determine the level of uncertainty of an ocean-colour product. This is particularly true for remote sensing data where match-up analyses (McClain *et al.*, 2000; http://seabass.gsfc.nasa.gov/matchup_results.html) can only be performed for an infinitesimal fraction of a sensor's records. Although very useful, these analyses cannot provide reliable estimates of how ocean-colour uncertainties vary with time and/or space. Moreover, because the uncertainties of the input data (for example the normalized water-leaving radiance, L_{wN}) vary in space and time, the uncertainties of the output products cannot be reported simply as a single global value unless it is intended to provide general bounds. Some ocean-colour products are also used as input to other models (for example, to calculate primary production or to assimilate phytoplankton carbon into ecosystem models) for which uncertainty budgets cannot be properly established without knowledge of the uncertainties associated with the input data. It is thus important that the variations of the uncertainty in L_{wN} and in the products derived from them are documented in time and space. This section discusses the various types of uncertainties present in ocean-colour data or products and emphasizes recent approaches that allow uncertainties of satellite ocean-colour products to be estimated on a pixel-by-pixel basis.

3.1 Sources of Uncertainty

3.1.1 Uncertainties in *in situ* measurements (L_{wN}, R_{rs}, C, IOP)

In situ data are used for algorithm development and for validation of algorithms and data products. While *in situ* measurements are frequently considered as "the reference" to which other data (*e.g.* satellite data) are compared, they contain significant levels of uncertainties caused by various experimental and environmental factors. Calibration, dark signal, data processing, deployment strategy, sea and sky states all introduce uncertainties in the radiometric measurements (Siegel *et al.*, 1995; Hooker and Maritorena, 2000; Hooker *et al.*, 2001). Close compliancy to establish measurement protocols (*e.g.* Mueller and Austin, 1995 and follow up) along with regular and rigorous calibrations and good characterization of instruments are key to the minimization of uncertainties in the *in situ* measurements. Measurements of biogeochemical variables have their own set of difficulties and resulting uncertainties (Mitchell *et al.*, 2000; Van Heukelem *et al.*, 2002; Claustre *et al.*, 2004). Most of the data sets that are publicly available (*e.g.*, SeaBASS) do not contain information regarding the estimated uncertainties of the various variables they contain (*e.g.*, the differences between the triplicate chlorophyll measurements and the uncertainties in the radiometer reading, based on its variability through the sampling period and its calibration history). It is frequently assumed that the uncertainties of *in situ* data are small and in any case much smaller than the uncertainties arising from the natural spatial/temporal variability of a given variable.

Another uncertainty arises from the fact that the match-up field data usually characterize an area of around 1–10 m while the satellite spatial scale is often 100–1,000 m. This environmental mismatch in scales introduces an uncertainty that is often hard to quantify. Also, satellite measurements represent a water-column weighted average (Gordon and Clark, 1980; Sathyendranath and Platt, 1989; Zaneveld *et al.*, 2005a), while *in situ* measurements usually come from discrete depths. Therefore, for vertically inhomogeneous waters, uncertainties arise when the two are compared with each other. Some sampling platforms such as on-line sampling from steaming vessels, undulating vehicles, gliders, and autonomous underwater vehicles (AUVs) are likely to be fruitful approaches in quantifying these uncertainties.

3.1.2 Uncertainties in satellite measurements (L_{wN})

Various sources of random and systematic error contribute to disagreements between measured normalized water-leaving radiances and their actual values. Uncertainties in L_{wN} are introduced through a variety of factors such as pre-launch characterization of the sensor, atmospheric and bi-directional corrections, and uncertainties in the monitoring of the changes in the sensor's performance. Errors in geo-location, contamination with light emanating from adjacent pixels or other factors like white caps can also add to this uncertainty. The calibration/validation activities of each ocean-colour mission are designed to assess and minimize the magnitude of this uncertainty (and remove any bias). Prelaunch and on-orbit characterization of the sensors (*e.g.*, measurements of reflected Sun and/or Moon light) along with vicarious calibrations (*e.g.*, the MOBY buoy) and match-up analyses are the major procedures used to quantify uncertainties of normalized water-leaving radiances.

The calibration/validation activities and the reduction of the uncertainties in the derived L_{wN} should be one of the primary tasks of space agencies providing the ocean-colour data and much effort must be invested in minimizing it for various missions. In the remainder of this chapter we will therefore assume the uncertainty in the L_{wN} is known and documented, although at present uncertainties in atmosphere correction still dominates errors in L_{wN} of coastal waters.

3.1.3 Uncertainties and assumptions in the functional relationship that links L_{wN} and IOP and in the inversion procedure used to derive the products

Uncertainties in the products derived from the inversion of L_{wN}, however, do not benefit from the same level of effort. In what follows we will address these uncertainties with reference to the type of algorithm designed to produce them, distinguishing between empirical and semi-analytical inversion algorithms. The approaches used in some recent works to provide ocean-colour product uncertainties are also described.

3.1.3.1 Obtaining uncertainties in products based on empirical algorithms

Empirical algorithms are developed from data sets where *in situ* radiometry and a to-be-derived product (*e.g.*, chlorophyll-a, POC) have been collected at the same spot of the ocean and within a narrow period of time. A regression is most often performed to obtain the 'best-fit' function between the two variables and to define the formulation that relates the two quantities. The type of regression used to relate two variables is relevant to the uncertainty discussion because regression methods work under different assumptions about uncertainties in the data involved. Type-I regressions (Laws, 1997) are the most frequently used and are based on the assumption that only the dependent variable (*i.e.* y, the product) has an uncertainty, while the independent variable (*i.e.* x, the input data) is error free. In Type-I regressions, the individual uncertainties in the input data are not taken into account and it is generally assumed that the relative error in the variable is constant. Conversely, Type-II regressions (Press *et al.*, 1992; Laws, 1997) assume that both variables have uncertainties and are thus better adapted for ocean colour where substantial uncertainties frequently exist in the variables involved (*e.g.*, reflectance ratio, chlorophyll).

An empirical algorithm is as good as the data it is based on, and on how representative the data are of the environment or bio-optical provinces where the algorithm is to be applied. *In situ* data sets are often geographically and seasonally biased due to constraints in the timing and location of oceanic cruises (Claustre and Maritorena, 2003).

In general, it is crucial that data sets used in the development (or validation) of an ocean-colour algorithm have complete information about the location and time at which the data were collected and about their quality (*i.e.* associated uncertainties). The geographical and temporal extent of a data set determines the water types where the algorithm can be applied, whereas uncertainties in products require information on uncertainties in the input data.

For empirical algorithms, the dispersion of the y-axis data (*i.e.* the product) around the “mean” relationship of the resulting algorithm provides, to some degree, information about the uncertainties that can be expected at any given x-axis value (*i.e.* the input data). However, this only represents the uncertainties associated with the data set used in the regression and cannot be generalized unless the data set fully encompasses all the natural variability that exists for the water types included. Ideally, to evaluate the uncertainties of an empirical algorithm one needs a different data set than that with which the algorithm was developed; the statistics of the differences between the inverted products and the measured products in this independent data set can then be used to evaluate the uncertainties in the product. Additionally, an uncertainty propagation analysis to evaluate the effect of the uncertainties in the L_{wN} on the output has to be carried out to establish whether or not this uncertainty is a significant source for uncertainty in the product (*e.g.*, to what extent a 5% relative uncertainty in L_{wN} at 440 and 555 nm affects the IOPs retrieved).

In the case of neural network (NN) based algorithms, uncertainties should be determined from a rigorous statistical approach. Aires *et al.* (2004) provided an example of such an approach to products derived from remote sensing (other than ocean colour). They use a Bayesian technique to evaluate the uncertainties in the NN parameters which are then used to compute the uncertainties in the outputs.

Another way to determine whether the measured reflectance spectrum is within the domain of the bio-optical models used to simulate reflectance spectra, which in turn were used to train a neural network, has been developed for the Medium Resolution Imaging Spectrometer (MERIS) (Doerffer and Schiller, 2000; Krasnopolsky and Schiller, 2003). For this purpose one network is trained to determine concentrations from the eight MERIS bands together with the solar and viewing zenith angles and the azimuth difference between viewing and sun direction (see Chapter 6). A second, forward, network is trained with the same data set, which takes the derived concentrations as input and produces reflectances. The deviation, calculated as the Chi^2 (Sokal and Rohlf, 1981), over all eight bands between the measured and the computed spectrum, is then used as an indicator to see if the measured spectrum is within the training range, and thus within the scope of the algorithm. In the case of the MERIS ground segment, a flag is raised whenever the Chi^2 deviation exceeds a certain threshold. However, the Chi^2 value can also be used as an uncertainty measure. Furthermore, a technique has been developed (Schiller and Doerffer, 2005), which combines the neural networks with an optimization procedure, to estimate the uncertainty of a product on a pixel-by-pixel basis.

3.1.3.2 Obtaining uncertainties in products based on semi-analytical models

Semi-analytical models or algorithms are based on the premise of a known relationship (derived from the radiative-transfer theory) between L_{wN} (or a function of it) and IOPs (generally the absorption, a, and the backscattering, b_b, coefficients). These models contain some level of empiricism in the way IOPs are parameterized (*i.e.* how their variations and spectral shapes are formulated) and they also use simplified assumptions for some of their components (see Chapter 1). The inversion of semi-analytical models generally allows the simultaneous retrieval of several variables contained in the IOP terms. Like empirical algorithms, semi-analytical models are affected by uncertainties in L_{wN} but they are also influenced by uncertainties associated with the chosen relationship between L_{wN} and IOPs, and uncertainties resulting from the assumptions used in their formulation.

Sensitivity analyses are frequently used to assess how assumptions used to describe the component terms of a model affect retrievals (Roesler and Perry, 1995; Hoge and Lyon, 1996; Garver and Siegel, 1997). Although very useful, this approach does not allow the determination of a product's uncertainty on a case-by-case (or pixel-by-pixel) basis, but rather provides a general uncertainty estimate. To our knowledge, only two methods have recently been used with ocean-colour data that can estimate the uncertainties of products retrieved by the inversion of a semi-analytical model on a case-by-case basis. The first one (Maritorena and Siegel, 2005) is a non-linear adaptation of the calculation of confidence intervals in linear regressions. Essentially, this method is based on the projection of the residuals between the observed and reconstructed (from the inverted variables) L_{wN} in the solution (*i.e.* retrieved variables) (Bates and Watts, 1988).

A recent study (Wang *et al.*, 2005) suggests another approach to compute uncertainties of the retrieved variables. In this approach, each of the variables to be retrieved has a predefined set of spectral shapes and the model is inverted for each of the possible combinations of these spectral shapes resulting in an extensive set of possible solutions. These results are then filtered to keep only the "realistic" (e.g., positive) solutions that can closely reproduce the input L_{wN} spectrum (within a pre-described difference from the L_{wN} based on the uncertainties in L_{wN} and the uncertainties in the theoretical relationship between L_{wN} and IOP). The final value for each inversion product and its associated uncertainty is then obtained from the statistics (median and percentiles) on the acceptable solution subset. The key steps in this approach are the choice of the acceptance criteria for the solutions (*e.g.*, what is the acceptable difference between observed L_{wN} and that reconstructed from retrieved IOP) and the choice of range in possible shapes for the spectrum of each individual IOP. The two methods described above do not produce the same kind of uncertainties, and thus they are not directly comparable. Both approaches have benefits and limitations. For example, the Maritorena and Siegel (2005) approach always returns a value for the confidence interval of the retrieved product because the calculations do not depend on spectral criteria but on the sum of the residuals (weighted by the spectral uncertainties of the input data, if they are known). On the other end, this approach does not take into account the uncertainties caused by the model assumptions. In the Wang *et al.* (2005) approach, uncertainties in the model and data are included in the spectral agreement criteria but the inversion may fail to find any solution that satisfies this criteria. Although it uses an efficient linear matrix inversion technique (Hoge and Lyon, 1996), the Wang *et al.* (2005) method is also more computationally demanding (computational demands increase with numbers of possible combinations of different shapes of IOPs).

3.2 Summary

While some preliminary uncertainty estimates for ocean-colour products are available through match-up analyses, uncertainties are generally not provided on a per data point basis. This has caused many users to use ocean-colour products as a qualitative descriptor of patterns rather than a quantitative variable. Others use these products in biogeochemical models (*e.g.*, computing primary productivity) without being able to propagate uncertainties.

For some ocean-colour missions, such as for MERIS, a sophisticated flagging system has been developed. It computes, on a pixel-by-pixel basis, indicators for the reliability of a product by regarding different possible error sources including sun glint, failure in the atmospheric correction, high turbidity in the water, *etc.* A flag for each possible problem is raised if the uncertainty value exceeds a certain threshold. By this method, the user gets a warning and has to decide if he can accept this pixel for further computations.

We have reviewed briefly some of the uncertainties present in ocean-colour data, and have presented different approaches to establish uncertainties in products of ocean-colour remote sensing for either empirical or semi-analytical algorithms. The procedures described above are not complicated and their full application benefits from the knowledge of uncertainties in the input data. Use of such approaches will help the ocean-colour community establish quantitative confidence in the remote-sensing products.