Probabilistic constraints for nonlinear inverse problems
An ocean color remote sensing example

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Abstract The probabilistic continuous constraint framework complements the representation of uncertainty by means of intervals with a probabilistic distribution of values within such intervals. This paper describes how nonlinear inverse problems can be cast into this framework, highlighting its ability to deal with all the uncertainty aspects of such problems. In previous work we have formalized the framework, relying on simplified integration methods to characterize the uncertainty distributions. In this paper we (1) provide validated constraint-based algorithms to compute these distributions, (2) discuss approximations obtained by their hybridization with Monte-Carlo methods, and (3) obtain a better uncertainty characterization, by including methods to compute expected values and standard deviations. The paper illustrates this new methodology in Ocean Color (OC), a research area which is widely used in climate change studies and has potential applications in water quality monitoring. OC semi-analytical approaches rely on forward models that relate optically active seawater compounds (OC products) to remote sensing measurements of the sea-surface reflectance. OC products are derived by inverting the forward model on a spectral-reflectance basis. Based on a set of preliminary experiments we show that the probabilistic constraint framework is able to provide a valuable characterization of the uncertainty of all scenarios consistent with the model and the measurements.
Moreover, the framework can be used to derive how measurements accuracy affects the uncertainty distribution of the retrieved OC products, which may constitute an important contribution to the OC community.

**Keywords**  Probabilistic continuous constraints · Nonlinear inverse problems · Uncertainty representation and reasoning · Ocean color remote sensing

1 Introduction

Many problems of practical interest can be formulated as nonlinear inverse problems \[33\]. Such problems aim at finding the parameters of a model, given by systems of equations, from noisy data. These are typically ill-posed problems that may have no exact solutions, multiple solutions or unstable solutions.

Classical approaches for these problems are based on nonlinear regression methods \[3\] which search for the model parameter values that best-fit a given criterion. Best-fit approaches, often based on local search methods, provide a non reliable single scenario which may be inadequate to the characterization of the parameters.

In contrast, continuous constraint programming \[7, 24, 31\] provides a framework to characterize the set of all scenarios consistent with the constraints of a problem given the uncertainty on its parameters. This is achieved through constraint reasoning, where initial intervals, representing the uncertainty on parameter values, are safely narrowed by reliable interval methods \[28\]. Nevertheless, the application of classical constraint approaches to nonlinear inverse problems \[16, 20\] suffers from the major pitfall of considering the same likelihood for all values in the intervals.

Other stochastic methods (Monte Carlo techniques) use extensive random sampling over the different scenarios to characterize the distribution of the model parameter values given the forward model and the observations. However, even after intensive computations, such characterization may be inaccurate, because a significant subset of the probabilistic space may have been missed.

In previous work \[10\], we developed an extension to the continuous constraint framework that complements the interval bounded representation of uncertainty with a probabilistic characterization of values distribution. Such information makes it possible to characterize scenarios with a likelihood value, allowing their comparison. Our main emphasis was on the formalization of the framework, which relied on a simplified integration method for computing the probability distributions. In \[11\] we applied this previous approach to two types of very simple applications (inverse and reliability problems).

In this paper we show how an enhanced version of such probabilistic constraint (PC) framework can be used as an effective tool for dealing with nonlinear inverse problems and we illustrate its main features in an Ocean Color (OC) application.

The PC framework is enhanced by providing two alternatives for integration. The first is fully based on constraint programming using reliable interval techniques for multidimensional quadrature \[8, Goldsztejn et al., Convergence analysis and adaptive strategy for the certified quadrature over a set defined by inequalities; unpublished data\]. The other is an hybrid approach that relies on constraint programming to obtain the feasible space and uses Monte Carlo Integration \[18\], sampling on this reduced space. Whereas the first outputs guaranteed results but is computationally demanding, the second only outputs approximate, if accurate,