Probabilistic Constraints for Nonlinear Inverse Problems*
(Extended Abstract)

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The probabilistic continuous constraint (PC) framework complements the representation of uncertainty by means of intervals with a probabilistic distribution of values within such intervals. This paper, published in Constraints [8], describes how nonlinear inverse problems can be cast into this framework, highlighting its ability to deal with all the uncertainty aspects of such problems, and illustrates this new methodology in Ocean Color (OC), a research area widely used in climate change studies with significant applications in water quality monitoring.

Many problems of practical interest can be formulated as nonlinear inverse problems [20]. Such problems aim to estimate parameters from observed data based on a model of the system behavior. The model variables are divided into model parameters, $\boldsymbol{m} = (m_1, \ldots, m_n)$, whose values completely characterize the system and observable parameters, $\boldsymbol{o} = (o_1, \ldots, o_k)$, that can be measured. The model, $\boldsymbol{o} = \boldsymbol{g}(\boldsymbol{m})$, is typically a forward mapping $\boldsymbol{g}$ from the model parameters to the observable parameters. It allows predicting the results of measurements based on the model parameters.

Uncertainty arises from measurement errors on the observed data or approximations in the model specification. When the model equations $\boldsymbol{g}$ are nonlinear, the problem is a nonlinear inverse problem. Nonlinearity and uncertainty play a major role in modeling the behavior of most real systems.

Nonlinear inverse problems are typically ill-posed problems: they may have no exact solutions (no combination of parameter values are capable of predicting exactly all the observed data), solutions are not necessarily unique (different combinations of parameter values may induce the same observable values) and the stability of solutions is not guaranteed (small change in the observed data may induce arbitrarily large changes in the model parameters).

Classical approaches for these problems are based on nonlinear regression methods [2] 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 characterize the parameters.

In contrast continuous constraint programming [14,4,19], provides a framework to characterize the set of all scenarios consistent with the constraints of a problem given the uncertainty on its parameters modeled by intervals including all their possibilities. This is achieved through constraint reasoning, which

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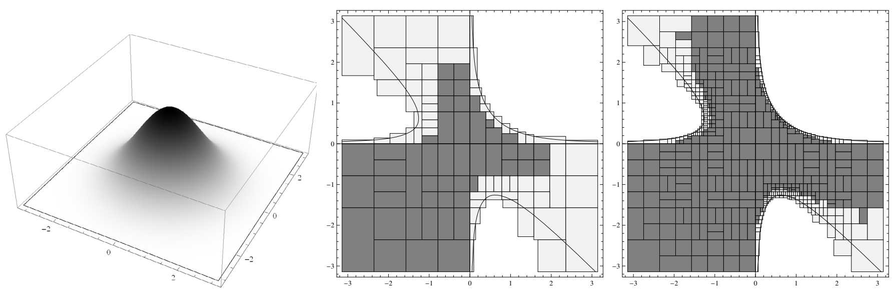
relies on branch-and-prune algorithms to obtain sets of boxes that cover exact solutions for the constraints (the feasible space). These algorithms begin with an initial crude cover of the feasible space which is recursively refined by interleaving pruning and branching until a stopping criterion is satisfied. Branching splits a box from the covering into sub-boxes. Pruning either eliminates a box from the covering or reduces it into a smaller (or equal) box maintaining all the exact solutions. Safe pruning is based on safe methods from interval analysis [16] combined within a constraint propagation algorithm [3].

Nevertheless, the application of classical constraint approaches to nonlinear inverse problems [12,10] suffers from the major pitfall of considering the same likelihood for all values in the intervals. To account for different likelihoods, stochastic Monte Carlo techniques [11,1] 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.

This is not the case of our previous work [6] where 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 probability distributions. In [7] we applied this previous approach to two types of simple applications (inverse and reliability problems).

In the present paper we a) provide a validated integration method supported on constraint-based algorithms to compute these distributions, b) study approximations obtained by their hybridization with Monte-Carlo methods, and c) obtain a better uncertainty characterization, by including methods to compute expected values and standard deviations.

The validated integration method relies on the efficiency of constraint reasoning to get a tight box covering of the region of integration, and on the efficacy of interval Taylor methods [5,9] to obtain sharp enclosures for the integrals over the obtained boxes (see figure 1).



(a) (b) (c)

Fig. 1. Given a probability distribution a), the probability of an event is computed through interval Taylor quadrature over tighter box coverings b) and c)

Although this alternative outputs guaranteed results it is computationally demanding. This justified an hybrid approach which relies on constraint programming to obtain the feasible space and then uses Monte Carlo Integration to sample on this reduced space. We show that this technique, although outputting approximate values, achieves quite accurate results even with small sampling rates and it is much faster than the previous one. Its success relies on the hybridization with constraint programming, since a pure non-naive Monte Carlo method is not only hard to tune but also impractical in small error settings.

Both alternatives allow the computation of probability distributions (both joint and marginal, conditional or unconditional) and extra information, not previously addressed in [6], such as expected values and variances. All these features are illustrated in the OC application (see figure 3 and tables 1 and 2).

OC satellite missions can provide cost-effective environmental indicators at large spatial scales by deriving optically active seawater compounds (OC products) through remote sensing measurements of the sea-surface reflectance [18]. Semi-analytical approaches [15,21,13] handle this problem as a nonlinear inverse problem where field data are used to configure a forward model [17,22] that expresses sea-surface reflectance as a function of the OC products (see figure 2).

In the paper we show how to apply the PC framework to invert the forward model and compute all OC product scenarios consistent with the model, characterized by a probability distribution conditioned by the measurement error. Such information is of extreme importance to understand the impact of measurement uncertainties on the derived OC products, providing support to: a) investigate the applicability of ocean color inversion schemes in different water types; and b) define accuracy requirements for the radiometric sensors to guarantee specified levels of uncertainty for the estimated concentrations. This is an innovative and remarkable contribution to the OC community and can be extended to different parameterizations of the semi-analytical model.

To assess the approach we studied a set of 12 simulated cases representative of different seawater types found in nature. Figure 3 shows the results obtained for the uncertainty on the model parameters given the measurements. Table 1 shows the results obtained to compute the Chla expected value and standard deviation, where the enclosures get sharper as time proceeds.

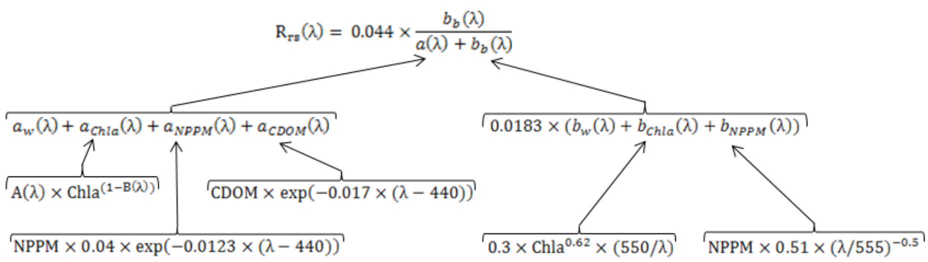
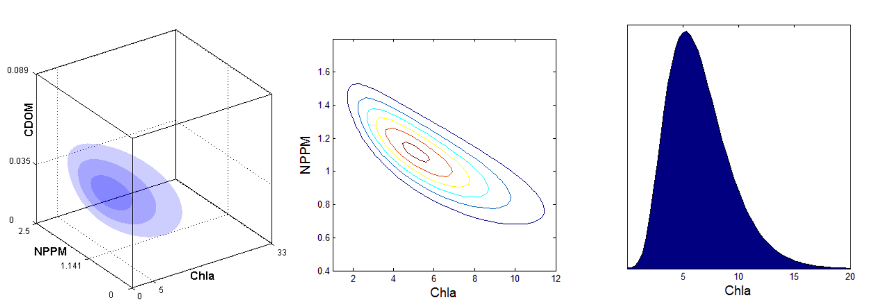


Fig. 2. The forward model is a function from the OC products ($Chla$, $NPPM$ and $CDOM$) to the remote sensing reflectance (R_{rs}) at a given wavelength (λ)



(a) (b) (c)

Fig. 3. Joint and marginal uncertainty distributions computed by the PC framework

Table 1. Interval enclosures computed for $E[Chla]$ and $STD[Chla]$

	$E[Chla]$			$STD[Chla]$		
	enclosure	midpoint	error	enclosure	midpoint	error
10 min	[6.5366, 6.7694]	6.6530	0.1164	[2.6983, 2.9418]	2.8201	0.1218
20 min	[6.5924, 6.7092]	6.6508	0.0584	[2.7716, 2.9011]	2.8364	0.0648
60 min	[6.6260, 6.6742]	6.6501	0.0241	[2.8193, 2.8753]	2.8473	0.0280
300 min	[6.6393, 6.6609]	6.6501	0.0108	[2.8400, 2.8644]	2.8522	0.0122

The hybrid approach, that combines constraint reasoning and Monte Carlo integration, is shown to provide very accurate results in a fraction of the computation time (see table 2). It was also demonstrated that this technique clearly benefits from the contribution of constraint programming to reduce the sample space into a sharp enclosure of the feasible space, combined with the efficiency of Monte Carlo integration.

Table 2. Approximations computed for $E[Chla]$ and $STD[Chla]$

	N	$E[Chla]$	$STD[Chla]$
2 min	5	6.6543	2.8627
3 min	10	6.6545	2.8631
4 min	20	6.6553	2.8629
7 min	50	6.6547	2.8629

In summary the paper overviews the Ocean Color inversion problem and discusses the preliminary results obtained with the PC framework, confirming the relevance of improving methods to control error propagation in the semi-analytical models, an important issue for decisions about the sensors used in satellite-based studies.

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