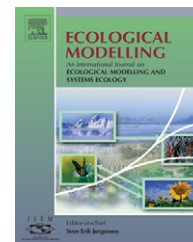


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On non-linear sensitivity of marine biological models to parameter variations

Peter C. Chu^a, Leonid M. Ivanov^b, Tetyana M. Margolina^{a,c,*}

^a Naval Postgraduate School, Monterey, CA, USA

^b University of Southern California, Los Angeles, CA, USA

^c Marine Hydrophysical Institute, Sevastopol, Ukraine

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ABSTRACT

Marine biological models are usually complex with many free parameters. Parameter prioritization (based on contribution to model output) is important for system management but difficult. A variance-based sensitivity analysis is developed in this paper using the Sobol'–Saltelli sensitivity indices, which measure the relative importance of each parameter (or group of parameters) and range these parameters along their contribution to output variability. To reduce the number of degrees of freedom, the model output is decomposed using the warping functions or irreversible predictability time. A simple three-component [nutrients, phytoplankton and zooplankton (NPZ)] model with 23 parameters for reproducing annual phytoplankton cycle of the Black Sea is taken as the example to show the usefulness and procedure of the sensitivity analysis. Single and total sensitivity indices showed strong sensitivity of the biological model to the light limitation of the phytoplankton growth. This agrees well with physical intuition. However, ranging model parameters along their contributions to model output variability does not follow exactly the physical intuition when model-related errors from large perturbations of the parameters are not small. For example, the model output becomes very sensitive to the nutrient stock parameterization for certain combinations of the light-related factors.

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1. Introduction

Ocean models, especially ocean biological models, in general, have many uncertain parameters, which should be identified from data or the physics (Lozano et al., 1996; Omlin et al., 2001; Fulton et al., 2004; Lermusiaux et al., 2006 among others). Various data assimilation methods may be used for model parameter identification: the adjoint method (Evensen et al., 1998), the non-linear optimization technique (Fasham and Evans, 1995), the weak-constraint parameter estimation (Loza et al., 2004) and others. The basic concept of these methods is to vary model parameters until the misfit between temporally varying modeled and observed

data is minimal, while the model equations are satisfied exactly.

Although robust dynamical regimes (attractors) reproduced by biological models are not very complex (most of such models demonstrate only simple periodical or quasi-periodical behavior), the parameter identification is quite a difficult problem by a number of reasons. First, data and model may be incompatible because the data contain contributions from hydrodynamic and biological processes, which may not be resolved by the model. Model error (no matter how small it is) can cause the solutions deviating far from the data. For example, Fasham and Evans (1995) could not find a single parameter set that fits the observational data well. Spitz et

* Corresponding author.

E-mail address: tmargoli@nps.edu (T.M. Margolina).

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al. (1998) could not estimate the optimal model parameters using observational data.

Second, modern data assimilation methods are on the base of statistical estimation theory, which uses the same foundation as the Kalman filtering: (1) data and model are assumed to be unbiased; (2) error variances and co-variances (dictating model-data difference) are used to correct the model state; (3) Gaussian statistics are assumed for the data errors. These conditions may not be true in biological modeling.

Third, even simple biological models with 3–10 model variables often contain 20–30 or more model parameters (e.g., Fasham et al., 1990; Oguz et al., 1996; Fennel et al., 2001; Kantha, 2004). When the number of model variables is considerably less than the number of model parameters, the parameter identification does not have a unique solution, and in general, selection of the “optimal” solution is difficult. This leads to the identifiability problem in ecological modeling, which concerns the uniqueness of the model parameters determined from the input–output data, under ideal conditions of noise-free observations and error-free model structure (Beck, 2002). The statistical method identifies the model parameters with only minimum difference between model and data but does not guarantee the absolute minimum error (Schittkowski, 2002): hyper-parameterized models may have many possible solutions.

In many cases, change in certain parameters (non-control parameters) causes only little change in model output. Therefore, these parameters can be approximately determined and then fixed. Change in other parameters (control parameters) causes large change in model output. Thus, the control parameters have to be determined in a very accurate manner because they affect the model predictability. The question arises, how can we range model parameters according to their contributions to model output variability?

Here, a phenomenological approach may be used to detect model sensitivity to the control parameter[s]. Such an approach requires rich practical experience and, in general, often gives reasonable results if the number of control parameters is not large. If the number of model parameters is large (marine biological models are the case), such an approach may fail no matter how rich a researcher’s experience is, because model sensitivity relative to one parameter often differs from model sensitivity to a group of parameters.

Alternative methods to determine the control parameters are the first-order sensitivity function (Chu et al., 2004) and the adjoint method (Evensen et al., 1998). The traditional sensitive analysis based on the direct-perturbation method (e.g., Dickinson and Gelinas, 1976) is popular in biological oceanography. For example, Oguz et al. (1996) used this approach to verify a low-component model of annual phytoplankton cycle in the Black Sea. The direct-perturbation method pursuant to which the sensitivity of model output to change in model parameter[s] is found by comparing model integrations with the only (finite) difference in the parameter of interest. The disadvantage of the direct method is that separate model integration must be performed for each parameter of interest. That a priori assumes additive contribution from each parameter to model output.

The adjoint method (Lawson et al., 1995; Evensen et al., 1998 and others) estimates model parameters and variables

through fitting the model to data, using model equation as a constraint. However, the method requires an initial guess for unknown initial conditions and parameters. Second, a biological model cannot be taken as a ‘true model’ because of many parameterization schemes involved. Third, although Lawson et al. (1995) reported that the adjoint method worked reasonably well even for “data” with 20% noise-to-signal level, it is not clear how the optimal model parameters are determined. Pires et al. (1996) pointed out that for non-linear dynamical models and noisy data there are limitations in application of the adjoint technique, and its convergence to the optimal solution is not obvious with the presence of noise in the data.

As the exact values of control parameters of a biological model are unknown, the linear sensitivity approach assumes explicitly no interactions among forecast model-related errors caused by parameter perturbations. In many practical cases, this assumption is unrealistic, and the model regimes and transitions among regimes are controlled by parameters determined from the sensitivity analysis on finite-amplitude parameter perturbations (Nicolis, 2003).

The primary goals of the proposed study are outlined as follows: (a) develop a model-independent non-linear sensitivity analysis for marine biological models using the Sobol’–Saltelli sensitivity indices (Saltelli et al., 1993, 2000, 2005). (b) Use special metrics, such as warping functions and the irreversible predictability time (IPT) (Chu et al., 2002a,b,c) as model output. IPT is developed on the base of first passage time. (c) Demonstrate capability of this approach through the analysis of a three-component (nutrients, phytoplankton, zooplankton) model for the annual phytoplankton cycle in the Black Sea. The choice of the model is from research interests of the authors, and is not principle.

The non-linear sensitivity analysis does not find the optimal model parameters directly. It assesses the influences or relative importance of each model parameter to the model output and determines which parameters are control parameters contributing most to the output variability and, possibly, requiring additional research to reduce output uncertainty, and which parameters are non-control parameters and can be estimated approximately. Excluding the non-control parameters, we may reduce the number of model parameters that are identified from data or physics.

The rest of the paper is organized as follows. Section 2 describes the sensitivity analysis using the Sobol’–Saltelli indices. Section 3 presents model output representations for estimating the Sobol’–Saltelli indices. Section 4 shows the model output representation using the warping functions and IPT for the non-linear sensitivity analysis. Section 5 describes the simplified three-component biological model for the Black Sea phytoplankton annual cycle (hereafter, the NPZ model). Section 6 depicts the experiment design. Sections 7–10 present the results and their oceanographic interpretations. Section 11 presents the conclusions.

2. Non-linear sensitivity

A variance-based method (Saltelli et al., 2000, 2005) is developed to estimate the non-linear sensitivity of a biological model to large variations of model parameters. Following

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