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

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ARTICLE INFO

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.

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

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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

Sobol' (1993), Saltelli et al. (1993) and Saltelli (2002), we introduce the sensitivity indices, which are quantitative measures of model output sensitivity to large variations of model parameters.

For simplicity, consider a scalar model output $y = f(a_1, a_2, \ldots, a_k)$ corresponding to a number of non-correlated model parameters $\mathbf{a} = (a_1, a_2, \ldots, a_k)$ with the joint probability density function:

$$P(a_1, a_2, \ldots, a_k) = \prod_{i=1}^{k} p_i(a_i). \tag{2.1}$$

Here, $p_i(a_i)$ is the PDF for ith parameter.

The total sensitivity of the model output relative to variations of all model parameters is estimated by the variance V

$$V(y) = \iint \cdots \int [f(a_1, a_2, \ldots, a_k) - E(y)]^2 \prod_{i=1}^{k} p_i(a_i)\, da_i$$
$$= E(y^2) - E^2(y), \tag{2.2}$$

where $E(y) = \iint \cdots \int f(a_1, a_2, \ldots, a_k) \prod_{i=1}^{k} p_i(a_i)\, da_i$.

The output variance for the fixed model parameter (a_j), should be determined by the conditional variance as

$$V_j = V(y) - E\{V(y|a_j)\} = V\{E(y|a_j)\} = U_j - E^2(y), \tag{2.3}$$

where $E(y|a_j)$ is the conditional mean:

$$E(y|a_j) = \iint \cdots \int f(a_1, a_2, \ldots, a_j, \ldots, a_k) \prod_{\substack{i=1 \\ i \neq j}}^{k} p_i(a_i)\, da_i, \tag{2.4}$$

$$U_j = \int E^2(y|a_j) p_j(a_j)\, da_j. \tag{2.5}$$

The conditional variance V_j is a good measure of the sensitivity of y with respect to the parameter (a_j). Once divided by the unconditional variance V, it is called first-order (or single) sensitivity indices

$$S_j = \frac{V_j}{V(y)}. \tag{2.6}$$

Similarly to (2.6) second-order sensitivity indices determining model output sensitivity relative to variations of two parameters a_i and a_j $(j > i)$ may be introduced by

$$S_{ij} = \frac{V_{ij}}{V(y)}, V_{ij} = V\{E(y|a_i, a_j)\} - V_i - V_j, \tag{2.7}$$

which show the joint effects of both parameters a_i and a_j on the model output.

The model sensitivity relative to variations of all the parameters excluding a_j, is represented by the conditional variance,

$$V_j^T = V\{E(y|\mathbf{a}_{-j})\} = U_{-j}(y) - E^2(y), \tag{2.8}$$

where $\mathbf{a}_{-j} = (\tilde{a}_1, \tilde{a}_2, \ldots, \tilde{a}_{j-1}, \tilde{a}_{j+1}, \ldots, \tilde{a}_k)$ is the sub-vector of $\mathbf{a}$ containing all the varying parameters other than a_j,

$$E(y|\mathbf{a}_{-j}) \equiv \int f(\tilde{a}_1, \tilde{a}_2, \ldots, a_j, \ldots, \tilde{a}_k) p_j(a_j)\, da_j, \tag{2.9}$$

$$U_{-j}(y) \equiv \int E^2(y|\mathbf{a}_{-j}) \prod_{\substack{i=1 \\ i \neq j}}^{k} p_i(\tilde{a}_i)\, d\tilde{a}_i. \tag{2.10}$$

The total sensitivity of the model output to variations of parameter a_j is written by

$$S_j^T = \frac{V - V_j^T}{V}, \tag{2.11}$$

which shows the non-additive part of model output sensitivity caused by interactions among model-related errors due to perturbations of model parameters. Following Sobol' (1993), the total output variance V is decomposed by:

$$V = \sum_{j=1}^{k} V_j + \sum_{j<i} V_{ij} + \sum_{j<i<l} V_{ijl} + \cdots + V_{12\ldots k}. \tag{2.12}$$

which shows partition of the variance between the main effects (defined by V_j) and the interaction terms (defined by V_{ij}, V_{ijl}, …). It is clear that when Eq. (2.12) holds, we can identify $V_{-j} = V\{(y|\mathbf{a}_{-j})\}$ as the sum of all terms in the right-hand side of (2.12) without terms including the subscript j.

Therefore, for the total sensitivity case, the index for the first parameter of a three-parameter model is

$$S_1^T = S_1 + S_{12} + S_{13} + S_{123}. \tag{2.13}$$

Dividing both parts of (2.12) by V, we get

$$\sum_{j=1}^{k} S_j + \sum_{j<i} S_{ij} + \sum_{j<i<l} S_{ijl} + \cdots + S_{12\ldots k} = 1, \tag{2.14}$$

which shows that any sensitivity index S_j varies between 0 and 1.

$$S_j = 1$$

for the model output depending only on the parameter a_j, and

$$S_j = 0, \quad S_j^T = 0$$

when the model output does not depend on the parameter a_j. It is also clear from Eqs. (2.11) and (2.14) that

$$\sum_{j=1} S_j \leq 1 \leq \sum_j S_j^T, \tag{2.15}$$

with equalities only when all interaction terms in (2.14) are zero.

The major advantage of variance-based non-linear analysis is that we can account for and specify the contributions of model-related errors caused by perturbations of different parameters and interactions among these errors using

second-order indices S_{ij}, S_{ijl}, ... In this case, the total model output is a non-additive function of model parameters.

Use of the sensitivity indices requires: (a) specifying the model output y in the simplest form and (b) developing a numerical technique to estimate appropriate variances of the model output. If the Monte-Carlo method (the approach used in the present study) is used to compute the conditional means and variances, the model output should be represented in the simplest form so that the sensitivity analysis would be computationally feasible.

3.   Model output representation

We suggest to use the following representations for model output. First, considering the non-negative feature of output for biological ocean models, the warping functions (Gervini and Gasser, 2004) can be used as for identification of function landmarks, such as the phytoplankton blooms. Second, IPT introduced by Ivanov et al. (1994), Chu et al. (2002a,b,c) and Chu and Ivanov (2005) to quantify the model predictability for finite-amplitude errors, is a natural measure of model sensitivity when perturbations of model parameters are not small.

3.1.   Warping functions

Following Gervini and Gasser (2004), a non-negative one-variable model output ($y(t) \geq 0$, such as phytoplankton concentration) is represented by

$$y(t) = sF\{v(t)\} + \delta(t), \tag{3.1}$$

where s is a non-negative scaling coefficient; $v(t)$ is a source of amplitude variability of the mean F; $\delta(t)$ is the random error. The function $v(t)$ generates time variability on F to shift the location of important features of the output (like the phytoplankton blooms). Representation of multi-variable model output ($y_1, y_2, \ldots, y_m$) can be found in Gervini and Gasser (2004).

The problem is to estimate the structural mean F. Clearly, the simple averaging $y(t)$ over all ensemble realizations underestimates the amplitude of local extreme values since the peaks vary from one realization to another not only in intensity but also in timing. To account for how it affects the structural mean (F), Gervini and Gasser (2004) suggest to choose $v(t)$ as

$$v(t) = w^{-1}(t), \tag{3.2}$$

where w is called the warping function, which is represented by

$$w(t) = t + \sum_{j=1}^{q} d_j \psi_j(t). \tag{3.3}$$

Here, $\mathbf{d} = (d_1, \ldots, d_q)$ is the score vector; $\{\psi_j(t)\}$ are functions constructed from a combination of B-splines and weights estimated relative to a single model output.

The parameters of (3.1)–(3.3) are estimated by minimizing the mean integrated squared error,

$$\left\langle \int_{t_0}^{t_0+T} [y(t) - sF\{v(t)\}]^2 \, dt \right\rangle \to \min, \tag{3.4}$$

where $\langle \rangle$ is averaging over a statistical ensemble of the model output. Gervini and Gasser (2004) suggest a two-stage algorithm (a MATLAB routine is available on web page http://www.unizh.ch/biostat/People/gervini) to minimize (3.4), and point out that only a few functions $\{\psi_j(t)\}$ are often needed to reconstruct geometrical specificities of the model output, $y(t) \geq 0$. Therefore, only few parameters s and d_j can be used to estimate non-linear sensitivity model output for a biological model.

3.2.   IPT

The IPT is defined as a time-period when the prediction error first exceeds a pre-determined criterion (i.e., the tolerance level). The probability density function of IPT with a given initial error satisfies the backward Pontryagin-Kolmogorov-Stratonovich equation. Using IPT as a quantitative measure for prediction skill, both linear and non-linear regimes of forecast errors were found in the low-order atmospheric model (Chu et al., 2002a,b) and regional ocean circulation model (Chu et al., 2002c; Chu and Ivanov, 2005).

Following Ivanov et al. (1994) IPT (τ) is determined as a time for which difference between individual model output $\mathbf{z}$ and some reference solution $\bar{\mathbf{z}}$ (defined as a model solution with specified model parameters and initial conditions) will exceed the tolerance level (or the accepted prediction error) ε for the first time:

$$\tau = \inf_{t>0}(t| \left| \mathbf{z} - \bar{\mathbf{z}} \right| > \varepsilon). \tag{3.5a}$$

Eq. (3.5a) can be re-written using a non-dimensional tolerance level $\bar{\varepsilon}$

$$\tau = \inf_{t>0} \left(t \left| \frac{|\mathbf{z} - \bar{\mathbf{z}}|}{|\bar{\mathbf{z}}|} > \bar{\varepsilon} \right. \right). \tag{3.5b}$$

The IPT is a priori random value and depends functionally on the reference solution, as well as on perturbations in the initial conditions and model parameters.

4.   Generation of ensemble perturbations

Accuracy in estimating the non-linear sensitivity indices depends on ensemble size and structure of model parametrical space. Therefore, to generate perturbations of model parameters, it is better to get homogeneous coverage in the model parameter space. On the other hand, for any model, the ensemble size is limited due to computer capability.

The Latin hypercube (LHC) design strategy (Latin Hypercube, 2001) is used to generate appropriate perturbations. An extensive review of Latin hypercube sampling technique can be found in Helton and Davies (2003); also see Rose and Smith (1998) as an example of the ecological

applications of this technique. LHC design increases considerably the accuracy in estimating probability density functions in comparison with the classical Monte-Carlo method (Dowling et al., 1985). For the same homogeneity of coverage in model parametrical space, the Monte-Carlo method needs an ensemble with n^k components, while the LHS strategy only needs $2n(k+1)$ components. Here, n is the number of perturbations for a parameter and k is the number of model parameters.

Another computational problem is to calculate U_j and U_{-j}. Clearly, Eqs. (2.5) and (2.10) are computationally impractical. In a Monte-Carlo frame, it implies a double loop: the inner one is to compute E^2 and the outer one is to compute the integral over da_j. Saltelli et al. (1993) suggest two model parameter matrices $\mathbf{M}_1$ and $\mathbf{M}_2$,

$$
\mathbf{M}_1 = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1k} \\ a_{21} & a_{22} & \ldots & a_{2k} \\ \ldots & & & \\ a_{n1} & a_{n2} & \ldots & a_{nk} \end{pmatrix}, \quad \mathbf{M}_2 = \begin{pmatrix} a'_{11} & a'_{12} & \ldots & a'_{1k} \\ a'_{21} & a'_{22} & \ldots & a'_{2k} \\ \ldots & & & \\ a'_{n1} & a'_{n2} & \ldots & a'_{nk} \end{pmatrix}.
\tag{4.1}
$$

Two perturbed parameter matrices are used for the specific parameter a_j. The first one is constructed from $\mathbf{M}_2$ by replacing the column $[a'_{rj}]$ to $[a_{rj}]$ from $\mathbf{M}_1$, and another one from $\mathbf{M}_1$ by replacing the column $[a_{rj}]$ to $[a'_{rj}]$ from $\mathbf{M}_2$:

$$
\mathbf{N}_j = \begin{pmatrix} a'_{11} & a'_{12} & \ldots & a_{1j} & \ldots & a'_{1k} \\ a'_{21} & a'_{22} & \ldots & a_{2j} & \ldots & a'_{2k} \\ \ldots & & & & & \\ a'_{n1} & a'_{n2} & \ldots & a_{nj} & \ldots & a'_{nk} \end{pmatrix},
$$

$$
\mathbf{N}_{-j} = \begin{pmatrix} a_{11} & a_{12} & \ldots & a'_{1j} & \ldots & a_{1k} \\ a_{21} & a_{22} & \ldots & a'_{2j} & \ldots & a_{2k} \\ \ldots & & & & & \\ a_{n1} & a_{n2} & \ldots & a'_{nj} & \ldots & a_{nk} \end{pmatrix}
\tag{4.2}
$$

Either $\mathbf{M}_1$ or $\mathbf{M}_2$ is used to estimate $E(y)$,

$$
\hat{E}(y) = \frac{1}{n}\sum_{r=1}^{n} f(a_{r1}, a_{r2}, \ldots, a_{rk}) = \frac{1}{n}\sum_{r=1}^{n} f(a'_{r1}, a'_{r2}, \ldots, a'_{rk}).
\tag{4.3}
$$

Both $\mathbf{M}_1$ and $\mathbf{N}_j$ are used to estimate U_j,

$$
\hat{U}_j = \frac{1}{n-1}\sum_{r=1}^{n} f(a_{r1}, \ldots, a_{r(j-1)}, a_{rj}, a_{r(j+1)}, \ldots, a_{rk})
$$
$$
\times f(a'_{r1}, \ldots, a'_{r(j-1)}, a_{rj}, a'_{r(j+1)}, \ldots, a'_{rk}),
\tag{4.4}
$$

Thus, the computational cost associated with the full set of first-order indices S_j is only $n(k+1)$. One set of n evaluations of f is necessary to compute E, and k sets of n evaluations of f are necessary for the calculation of U_j. Additional k sets of n evaluations of f are necessary to calculate U_{-j} using both $\mathbf{M}_1$

and $\mathbf{N}_{-j}$:

$$
\hat{U}_{-j} = \frac{1}{n-1}\sum_{r=1}^{n} f(a_{r1}, \ldots, a_{r(j-1)}, a_{rj}, a_{r(j+1)}, \ldots, a_{rk})
$$
$$
\times f(a_{r1}, \ldots, a_{r(j-1)}, a'_{rj}, a_{r(j+1)}, \ldots, a_{rk}).
\tag{4.5}
$$

5. Model of annual phytoplankton cycle for the black sea

A three-component model of annual phytoplankton cycle in the Black Sea is used to illustrate the non-linear sensitivity analysis. This model has a simple configuration and may not be able to reproduce the phytoplankton behavior in summer when the mixed layer depth is shallow. If the mixed layer retreats towards the surface in the Black Sea, most of the production takes place below the mixed layer in the deep chlorophyll maximum zone.

However, the model is able to reproduce two phytoplankton blooms observed in reality. The first one occurs during the early spring. The second bloom takes place during September–October. Both blooms are clearly identified from the climatic chlorophyll data (Chu et al., 2005) and color satellite observations (Oguz et al., 2002). This three-component model has 20 model parameters. The choice of such a model is not essential in illustrating the non-linear sensitivity analysis. More complex biological model may also apply. The well-known NPZ model originally suggested by Evans and Parslow (1985) for the North Atlantic, was modified and applied for reproducing annual phytoplankton cycle in the Black Sea. The governing model equations are

$$
\frac{dM}{dt} = \xi(t), \xi^+(t) = \max[\xi(t), 0],
\tag{5.1}
$$

$$
\frac{dP}{dt} = \left[\frac{\alpha(t, M, P)N}{j+N} - r\right]P - \frac{c(P_0 - P)Z}{K + P_0 - P} - \frac{m + \xi^+(t)}{M}P,
\tag{5.2}
$$

$$
\frac{dZ}{dt} = \frac{fc(P_0 - P)Z}{K + P_0 - P} - gZ - \frac{\xi(t)}{M}Z,
\tag{5.3}
$$

$$
\frac{dN}{dt} = -\left[\frac{\alpha(t, M, P)N}{j+N} - r\right]P + \frac{m + \xi^+(t)}{M}(N_0 - N),
\tag{5.4}
$$

Here, the model variables are phytoplankton (P), herbivore zooplankton (Z), dissolved nutrients (N), all of them expressed in terms of nitrogen specific amount (mmol/m³); the upper mixed layer depth (M). $\xi(t)$ is the time rate change of the mixed layer depth.

The model parameters are $\alpha(t, M, P)$ is the photosynthetic rate of phytoplankton, (j, r) the half-saturation and mortality rates for the phytoplankton, (c, K) the maximum grazing and half-saturation rates of herbivore zooplankton, P_0 the phytoplankton threshold, m the diffusivity, f the grazing efficiency, g the zooplankton mortality and N_0 is the nutrient stock just below the mixed layer. Among these parameters, $\alpha(t, M, P)$ and N_0, need more description.

Following Jassby and Platt's (1976) and Evans and Parslow's (1985) treatments, the photosynthetic rate of phytoplank-

i	Parameter		Unit	Model Value
Table 1 – Model parameters				
1	Nutrient stock	A_1	$mmol\,N\,m^{-4}$	0.12
2	parameterization	A_2	$mmol\,N\,m^{-3}$	−0.75
3	Initial slope of P/I curve	α_0	$(Wm^{-2})^{-1}\,day^{-1}$	0.025
4	Attenuation coefficient for seawater	k_w	m^{-1}	0.08
5	Coefficient of phytoplankton self-shading	k_c	$mmol\,N\,m^{-3}$	0.12
6	Half-saturation rate for phytoplankton	j	$mmol\,N\,m^{-3}$	0.5
7	Mortality rate for phytoplankton	r	day^{-1}	0.045
8	Phytoplankton threshold	P_0	$mmol\,N\,m^{-3}$	0.1
9	Grazing efficiency coefficient	f	day^{-1}	0.75
10	Zooplankton mortality	g	day^{-1}	0.15
11	Phytoplankton maximum grow rate		day^{-1}	2
12	Cloudiness	b	—	0.5
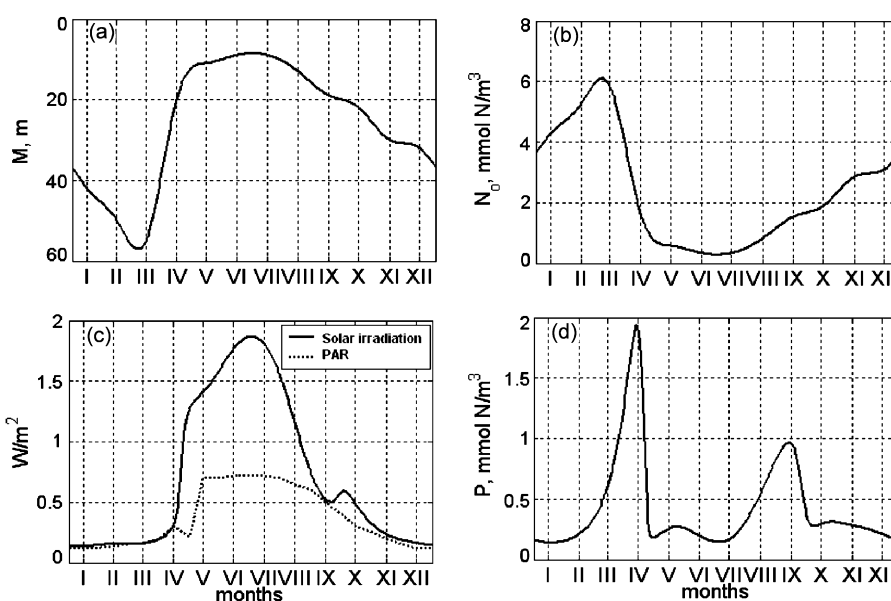
Fig. 1 – Reference solution and climatic input for the Black Sea NPZ model (5.1)–(5.5): (a) annual cycle of phytoplankton (the reference solution), (b) mixed layer depth (given by Hydrometeorology and Hydrochemistry, 1991), (c) nutrient stock below the mixed layer and (d) the solar irradiation (dashed curve) and photosynthetically active radiation (dotted curve).

ton, $\alpha(t, M, P)$ incorporates several additional parameters, namely, cloudiness (b), light attenuation by seawater (k_w) and phytoplankton self-shading coefficient (k_c), and maximum photosynthetic rate (Q).

The nutrient stock (N_0) is parameterized by

$$N_0 = A_1 z + A_2, \qquad (5.5)$$

which accounts for vertical variability of the nutrient distribution that coincides with the Black Sea climatology. Here, z is the vertical coordinate.

The model parameters (Table 1) and the depth of mixed layer M (Fig. 1a) are taken either from climatological data (Hydrometeorology and Hydrochemistry, 1991) or as traditional values generally accepted in marine biological modeling (Oguz et al., 1996; Kantha, 2004). Fig. 1b and c show the nutrient stock below the mixed layer and the solar irradiation calculated from the climatological values of M, respectively.

For the chosen model parameters and climatological input (Fig. 1a–c) the NPZ model (5.1)–(5.4) predicts the existence of a bimodal structure with occurrence of two phytoplankton blooms in April and September (Fig. 1d), that agrees well with the chlorophyll-a behavior in the Black Sea (Chu et al., 2005). Such a seasonally varying solution is treated as the reference solution for the sensitivity studies.

6. Experimental design

During numerical experiments, the NPZ model (5.1)–(5.4) is integrated with the set of twelve perturbed parameters (±50% from the climatic values, see Table 2). All the parameters are uniformly distributed within the given ranges. Homogeneous coverage in the model parameter space for matrices $\mathbf{M}_1$, $\mathbf{M}_2$, $\mathbf{N}_j$, $\mathbf{N}_{-j}$ [(4.1) and (4.2)] is required to generate statistically significant ensemble. Let n (usually $n \approx 10^3$) be the number of integrations in a statistical ensemble for one parameter. Then,

Table 2 – Ranges of parameter variation			
i	Parameter		Range of Variation
1	Nutrient stock	A_1	0.06–0.18
2	parameterization	A_2	−0.375 to −1.125
3	Initial slope of P/I curve	α_0	0.01–0.04
4	Attenuation coefficient for seawater	k_w	0.04–0.12
5	Coefficient of phytoplankton self-shading	k_c	0.06–0.18
6	Half-saturation rate for phytoplankton	j	0.25–0.75
7	Mortality rate for phytoplankton	r	0.0225–0.0675
8	Phytoplankton threshold	P_0	0.05–0.15
9	Grazing efficiency coefficient	f	0.5–1.0
10	Zooplankton mortality	g	0.075–0.225
11	Phytoplankton maximum grow rate		1–3
12	Cloudiness	b	0.25–0.75

for the NPZ model with $k = 12$, only 26,000 perturbations are generated. This is computationally feasible even for a personal computer.

There are about 20 parameters in original Evans and Parslow (1985) biological model, but only 12 parameters here for the sensitivity study. From the computational point of view, there is no restriction on the number of perturbed parameters. However, part of model parameters are fixed due to: (a) little influence on the model output (non-control parameters) and (b) little information on the range of variation for that parameter.

7. Construction of warping functions

Since the reference solution is quasi-periodic, one year is taken for constructing the warping functions for annual phytoplankton cycle. Our computations show that a two-component decomposition [i.e., $q = 2$ in (3.3)] is sufficient for the reconstruction of the mean phytoplankton annual cycle

shown in Fig. 1d from the ensemble of perturbed reference solutions (Fig. 2a). This ensemble of stochastic realizations is calculated by adding white noise to the reference solution (Fig. 1d). Here, ratio of noise-to-signal (the reference solution) is about 1. Two bell-shaped warping functions ψ_1 and ψ_2 (Fig. 2b) are computed on the base of six B-splines with equally spaced knots.

Reconstruction, using ψ_1 and ψ_2, leads to the annual phytoplankton cycle with the maxima corresponding approximately to the time of the two blooms (Fig. 2c). Some distortions of the reconstructed reference solution (1-month shift of the fall bloom and reduction of bloom peaks) observed in Fig. 2c are due to high noise added to the reference solution. However, the accuracy of the reconstruction increases with reducing the noise-to-signal ratio. The root mean square error indicates that this technique can reconstruct the two modal structures in the annual phytoplankton cycle with reasonable accuracy using only two warping functions even with large noise-to-signal ratios (Fig. 2d).
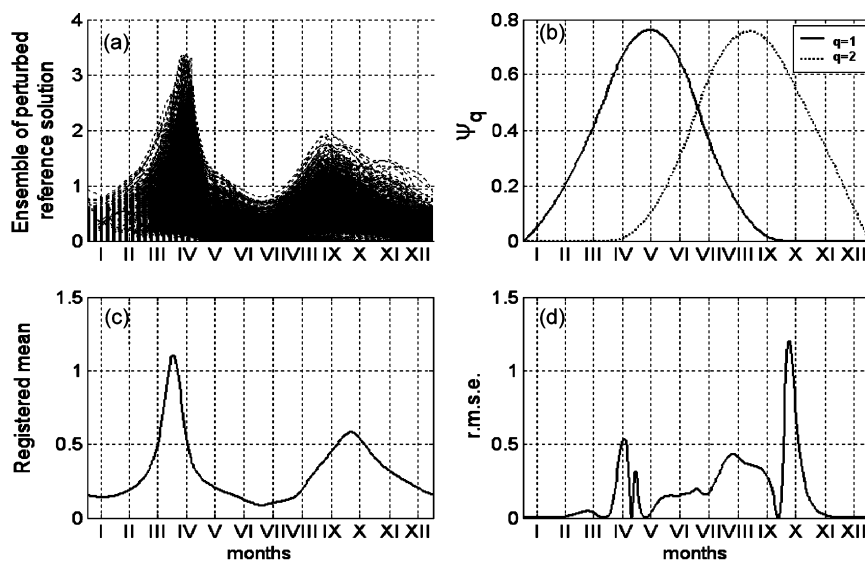
Fig. 2 – Construction and evaluation of warping functions: (a) an ensemble of perturbed reference solutions, (b) warping functions ψ_1 and ψ_2, (c) reconstructed mean and (d) the root mean square error between the reference solution and the reconstructed mean solution ψ_2 estimated by the warping function with $q = 2$.
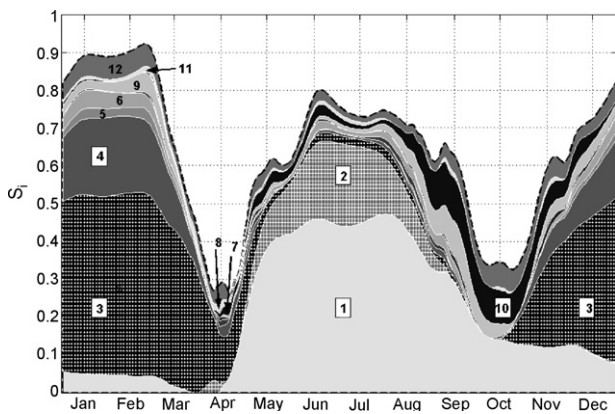
Fig. 3 – The first-order sensitivity of phytoplankton amount in upper mixed layer to variations of twelve model parameters. Labels 1, . . ., 12 correspond to parameters specified as in Tables 1 and 2.

Fig. 4 – The high order sensitivity of phytoplankton amount in upper mixed layer to variations of twelve model parameters. Labels 1, . . ., 12 correspond to parameters specified as in Tables 1 and 2.

8. Sensitivity indices for phytoplankton component

The above non-linear sensitivity analysis is directly applied to phytoplankton concentration computed by the NPZ model. The first-order sensitivity indices (S_i) for all 12 parameters (Table 2) are calculated numerically for each month within a year cycle. Fig. 3 shows the temporal variations of $\bar{S}_i = \sum_{j=1}^{i} S_j (i = 1, \dots 12)$ (indicated by bold curves in Fig. 3).

Two interesting features are important for further analysis. First, the set of influential parameters considerably varies with time. The annual phytoplankton cycle is divided into three periods: (1) prior to spring bloom, (2) between the spring and fall blooms and (3) after the fall bloom. It is expected that the phytoplankton during the first and third periods is mostly influenced by initial slope of the P/I curve α_0 (i = 3) and the light conditions (i = 4) while the phytoplankton during the second period is driven mainly by the nutrients stock under the mixed layer (i = 1, 2).

Second, the summation of the first-order indices never reaches 1. This means that the model output is not simple additive relative to parameters. Even if a possible uncertainty up to 50% in the model output is taken into account, the sum of all first indices drops evidently during the blooms. It means that the contribution of interactions among model-related errors generated by perturbations of different parameters, to model output is large. The first-order indices alone cannot fully explain the model output variance as a whole.

Contribution of interactions between model-related errors generated by perturbations of different parameters is estimated by the difference,

$$S_j^{\text{int}} = S_j^T - S_j.$$

Fig. 4 shows the temporal variation of $S_i^{\text{int}} = \sum_{j=1}^{i} S_j^{\text{int}}$. Although, we can still conclude higher significance of some factors, such as the initial slope α of the I/P curve and the parameters defining the nutrient stock (A_1, A_2) below the mixed layer, the interpretation of this plot is questionable. Therefore, instead of analyzing the temporally varying model
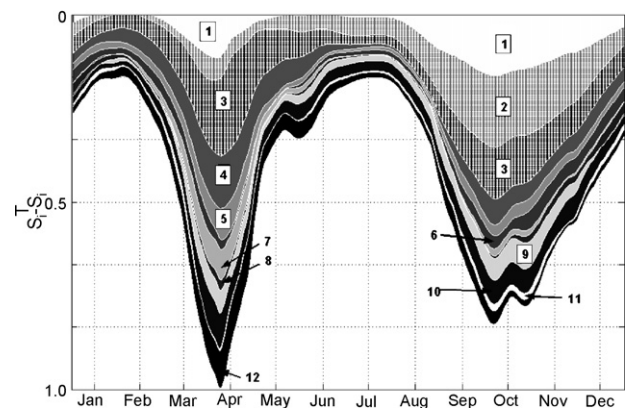
output, we use the scale parameters and scores of the corresponding functions as described above.

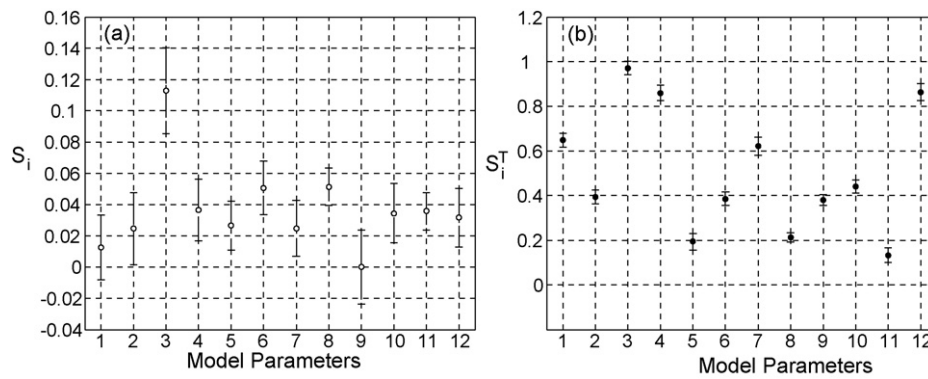## 9. Sensitivity indices for scale (s) and score vector (d_1, d_2)

Section 7 shows that the model output (phytoplankton concentration) can be represented only by two warping functions (ψ_1, ψ_2). Therefore, the model output sensitivity is reduced to the sensitivity of a scale s and a score vector (d_1, d_2) relative to variations of model parameters.

9.1. Sensitivity of d_1

The first component of score vector (d_1) in general, determines the spring-bloom landmark and fixes the position of the spring bloom. Therefore, joint analysis of the single (Fig. 5a) and total (Fig. 5b) sensitivity indices for d_1 identifies the main factors responsible for the generation of this bloom. The indices (Fig. 5a and b) are computed with 95% confidence interval using the bootstrap technique (Efron and Tibshirani, 1993) with a bootstrap sample dimension of 10^3.

It is obvious from Fig. 5a and b that the single indices are very small as comparing to the total indices. This implies high importance of parameter interactions. The single indices for d_1 show that the initial slope α_0 of the P/I curve (i = 3) has a significant effect (about 0.12) while all the other parameters are non-significant (Fig. 5a). This result seems to be correct only for small perturbations of model parameters.

In contrast to this, the total indices for d_1 give more information about model sensitivity and factors determining it. Fig. 5b indicates that the parameter α_0 (i = 3) still retains the leading role with the total index of about 1, however, other parameters, such as the light attenuation coefficient of the seawater (i = 4) and cloudiness (i = 12) become important too. The total indices for these parameters are up to 0.85–0.87. The light attenuation coefficient and cloudiness are related mostly to the light limitation of the phytoplankton growth.

Fig. 5 – (a) Single and (b) total sensitivity indices for the first score vector component (d_1). Bars show 95% confidence interval computed by the bootstrap technique.

Less important but still influential is the mortality rate of the phytoplankton ($i = 7$) and the parameter A_1 determining the nutrient stock below the mixed layer ($i = 1$). The total indices for these parameters reach 0.61–0.65. The model solution is not sensitive to the choice of second parameter A_2 in Eq. (5.4) ($i = 2$), half-saturation rate for phytoplankton ($i = 6$), crazing efficiency coefficient ($i = 9$) and zooplankton mortality ($i = 10$). The weakest sensitivity is also for the coefficient of plankton self-shading ($i = 5$), phytoplankton threshold ($i = 8$) and phytoplankton maximum growth rate ($i = 11$).

Our method estimates relative importance of each model parameters on the spring bloom generation and identifies their contributions using non-dimensional numbers $\eta_i = S_i^T / \max_i(S_i^T)$ as follows

$0.85 \leq (\eta_3, \eta_4, \eta_{12}) \leq 1.00$ for highly significant,

$0.60 \leq (\eta_1, \eta_7) \leq 0.65$ for significant,

$0.38 \leq (\eta_2, \eta_6, \eta_9, \eta_{10}) \leq 0.45$ for low significant,

$0.15 \leq (\eta_5, \eta_8, \eta_{11}) \leq 0.25$ for not significant.

Sensitivity enhancement of the spring bloom (phytoplankton growth) to the light limitation is intuitively understandable. However, ranging model parameters along their contributions to model output variability does not follow exactly the physical intuition.

More biological insight can be obtained using the second-order indices S_{ij} (Fig. 6). These indices show that the sensitivity of model output depends strongly on interactions among model-related errors caused by different model parameters. For example, the model-related error due to uncertainty of initial slope of the P/I curve ($i = 3$) is amplified through interaction with error caused by uncertainty of phytoplankton threshold ($i = 8$) (large value of S_{38} in Fig. 6), and is diminished due to uncertainty of grazing efficiency coefficient ($i = 9$) (small value of S_{39} in Fig. 6). However, the model output is very sensitive to uncertainty in determination of parameter pairs $(i,j) = (2,3)$, $(2,10)$, $(4,6)$, $(5,10)$ and $(11,12)$. In general, we may conclude that the generation of the spring bloom depends strongly on light-related model parameters and weakly on different phytoplankton ratios.
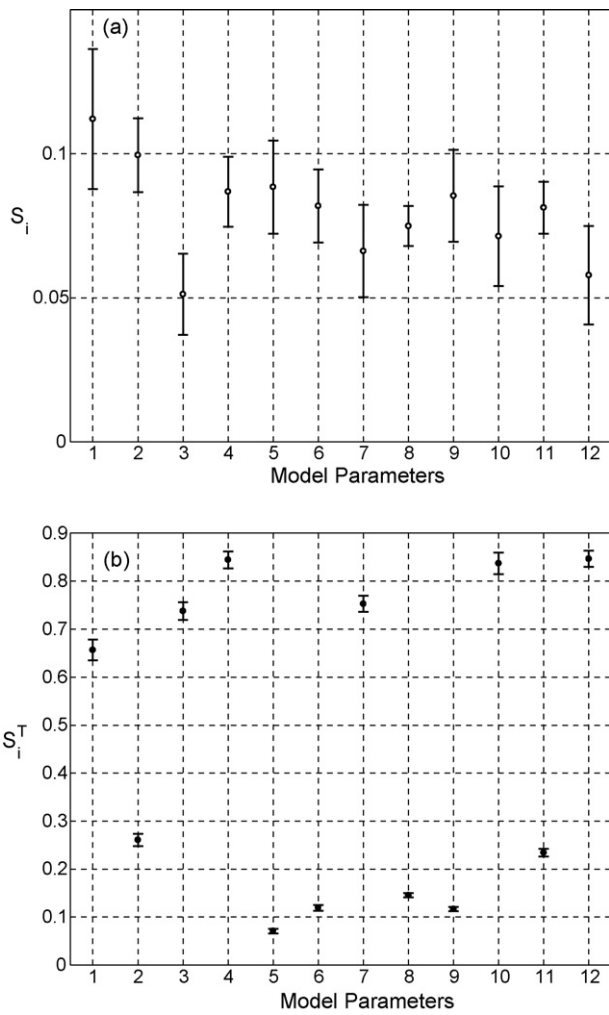
9.2. Sensitivity of d_2

The second component of score vector, d_2, determines the fall-bloom landmark. The single sensitivity indices (Fig. 7a) of d_2 show that the nutrient stock parameterization ($i = 1, 2$) is the most important for reproducing the fall phytoplankton bloom ($S_1 = 0.12$ and $S_2 = 0.10$). On the contrary, the total sensitivity indices identify six most important model parameters for reproducing the fall phytoplankton bloom (Fig. 7b). They are the nutrient stock parameterization ($i = 1$), the initial slope of the P/I curve ($i = 3$), the attenuation coefficient for seawater ($i = 4$), the mortality rate for phytoplankton ($i = 7$), the zooplankton mortality ($i = 10$) and the cloudiness ($i = 12$). The reference solution, in general, is insensitive to perturbations of parameters with $i = 2, 5, 6, 8, 9$ and 11. Significant total effect for the fall-bloom landmark also depends on the parameters for the nutrient distribution below the mixed layer as well as photosynthesis.

The sensitivity indices S_{ij} (Fig. 8) show the important effect of interactions among model-related errors generated by uncertainty inserted into the following pairs of model parameters $(i,j) = (1,3)$, $(1,4)$, $(1,12)$, $(1, 6-11)$, $(3,4)$, $(3,11)$, $(6,9)$, $(7,10)$, $(8,9)$ and $(9,11)$. Again, note that interactions among model related errors can lead to increasing or decreasing
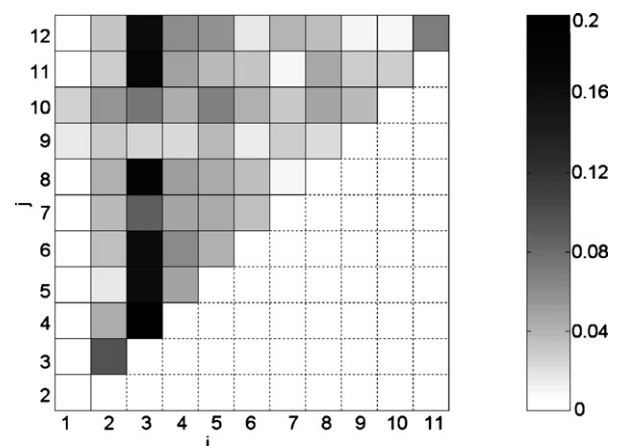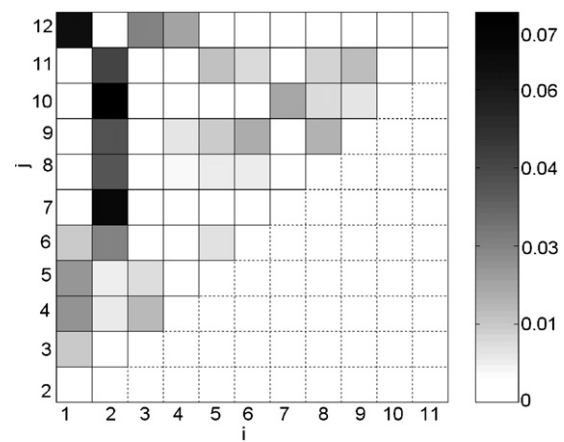

Fig. 6 – Second-order indices S_{ij} for the first component of the score vector d_1.

Fig. 8 – Second-order indices S_{ij} for the second component of the score vector d_2.

Fig. 7 – (a) Single and (b) total sensitivity indices for the second score vector component (d_2). Bars show 95% confidence interval computed by the bootstrap technique.

model output sensitivity to uncertain model parameters. For example, the reference solution is insensitive to perturbations inserted into model parameters pairs $(i,j) = (1,7)$, $(1,8)$, $(1,9)$, $(1,10)$, $(1,11)$. The large value of single sensitivity

index for A_1 indicates high influence of A_1 on the reference solution.

9.3. Sensitivity of the scale coefficient s

The single sensitivity indices of the scale coefficient (s) demonstrate no one parameter (or several parameters) dominating the model output (Fig. 9a). Although S_1 and S_2 are larger than other indices, their values are quite small (<0.11). However, the total sensitivity indices (Fig. 9b) and second-order indices S_{ij} (Fig. 10) indicate high sensitivity of the scale coefficient (s) to interactions among model-related errors caused by uncertainty inserted in different pairs of model parameters. The model parameters are decomposed into two groups with respect to model output sensitivity. The first group contains model parameters relative to which α has maximum sensitivity: nutrient stock parameterization ($i = 1, 2$), initial slope of P/I curve ($i = 3$) and attenuation coefficient for seawater ($i = 4$). The second group includes model parameters causing minimum sensitivity of model output: from plankton self-shading ($i = 5$) to cloudiness ($i = 12$). The second-order indices S_{ij} (Fig. 10) show that the model output is strongly sensitive to interactions among model-related errors induced by pairs of model parameters: $(1,2)$, $(1,3)$, $(1,4)$, $(1,10)$ and $(2,3)$.
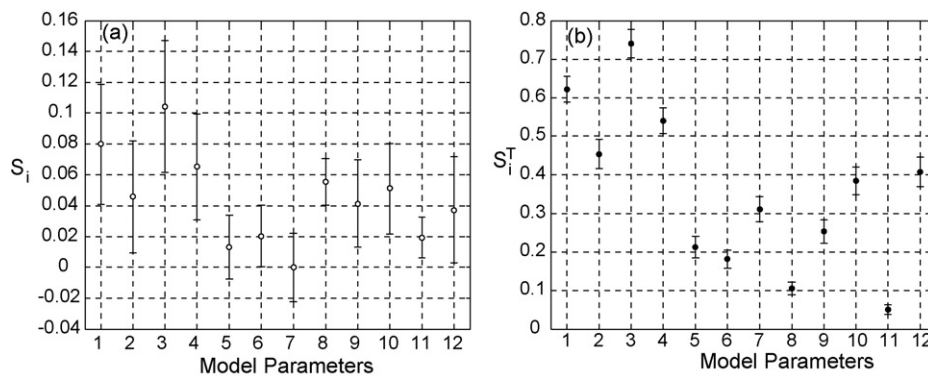
Fig. 9 – (a) Single and (b) total sensitivity indices for the scaling coefficient s. Bars show 95% confidence interval computed by the bootstrap technique.
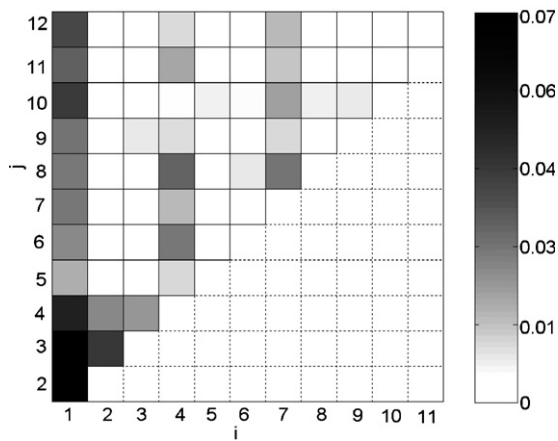
Fig. 10 – Second-order indices S_{ij} for the scaling coefficient s.

10. Sensitivity Indices of IPT

The warping functions are good metrics for the non-linear sensitivity analysis if the model output can be represented by few warping functions. This only happens when the reference solution presents the periodical or quasi-periodical attractor. For more complex dynamical regimes, such as chaotic attractor, large number of the warping functions are needed for decomposition of model output. To overcome this difficulty, IPT (represented by τ) is used to quantify model non-linear sensitivity. Clearly, smaller values of IPT correspond to higher sensitivity and vice versa.

Analyzing the functional dependence, $\tau = \tau(\bar{\varepsilon})$, we can understand the sensitivity of the reference solution to perturbations of various intensities. The tolerance level $\bar{\varepsilon}$ controls intensities of model-related errors caused by perturbations in model parameters.

The IPT, in general, is a non-smooth function in 12-dimensional parametrical space $(a_1, \ldots, a_{12})$. Fig. 11 shows the IPT computed in the model parameter sub-space (a_1, a_2) for two tolerance levels with high "ridge" and deep "valleys". IPT depends strongly not only on magnitude but also on direction of the perturbation vector.

The analysis of the IPT landscapes between $\varepsilon = 0.07$ (Fig. 11a) and $\varepsilon = 0.2$ (Fig. 11b) demonstrates that the model-related errors do not grow in dependently for tolerance levels
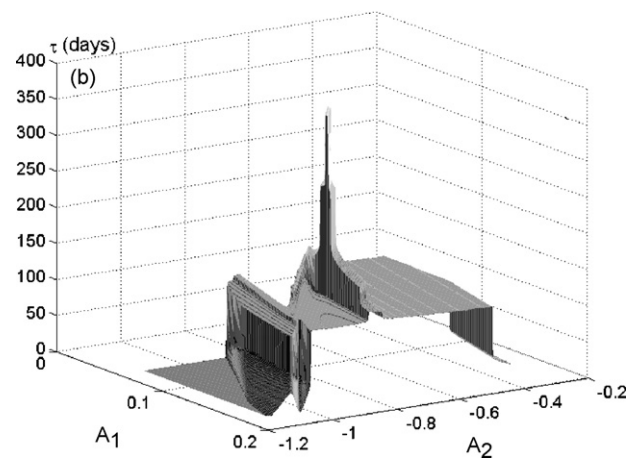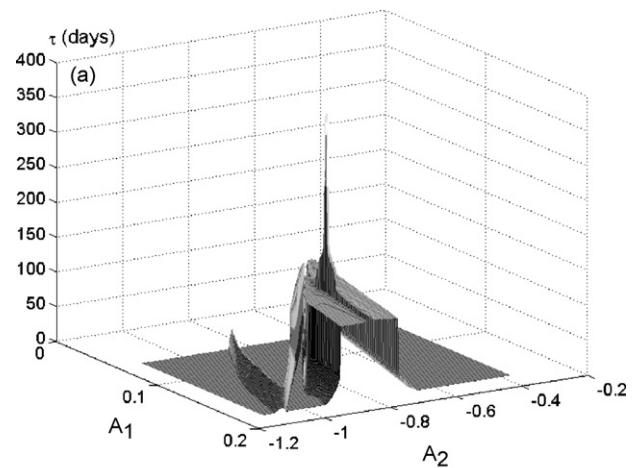

Fig. 11 – IPT for the NPZ model (5.1)–(5.4) in the model parameter phase sub-space (A_1, A_2) with the tolerance level: (a) $\varepsilon = 0.07$ and (b) $\varepsilon = 0.2$.

larger than 0.15–0.20. It indicates that the errors interact among themselves, and the total effect from the parameter perturbations on model output is non-linear. For small tolerance levels (as an example, $\varepsilon = 0.07$), the single indices (S_i) are small (Fig. 12a). Maximum value for the indices is 0.15. It indicates weak sensitivity of the model output to the choice of model parameters. However, the total indices (S_i^T) show
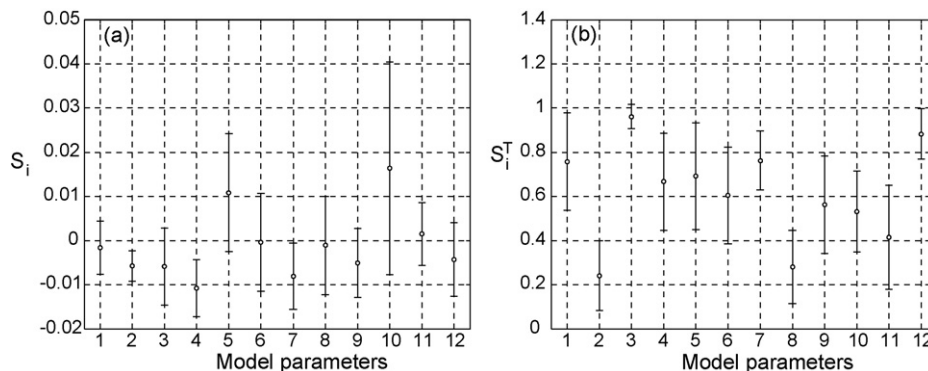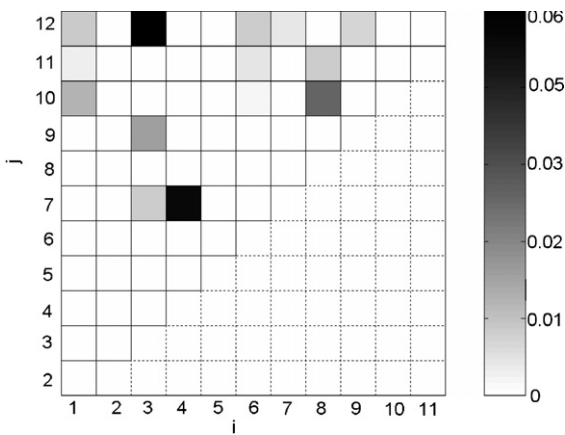

Fig. 12 – (a) Single and (b) total sensitivity indices for the IPT with the tolerance level of $\varepsilon = 0.07$. Bars show 95% confidence intervals computed by the bootstrap technique.
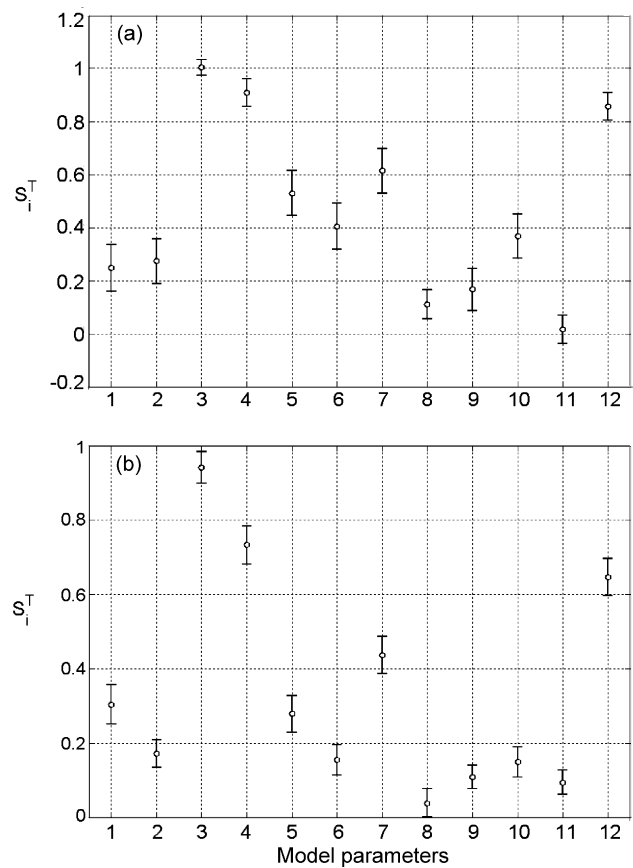
Fig. 13 – Second-order indices S_{ij} for the IPT with the tolerance level of $\varepsilon = 0.07$.

at least seven influential parameters (Fig. 12b): the nutrient stock parameterization ($i = 1$), the initial slope of P/I curve ($i = 3$), the attenuation coefficient for seawater ($i = 4$), the coefficient of phytoplankton self-shading ($i = 5$), the half-saturation rate for phytoplankton ($i = 6$), the mortality rate for phytoplankton ($i = 7$) and the cloudiness ($i = 12$). Obviously, the biological NPZ model (5.1)–(5.4) is not good enough for long-term prediction with high accuracy because it is difficult to identify the seven parameters from data with appropriate accuracy. The model produces the right type of attractor but cannot reproduce such fine details as the phase of oscillations. Note that interactions among the model-related errors caused by different parameter perturbations do not add to the general prediction error (Fig. 13). In this regime, the model sensitivity can be analyzed by a tangent model, i.e., through the first-order sensitivity functions.

For intermediate values of $\bar{\varepsilon}$ ranging from 0.1 to 0.5, the total sensitivity indices identify the model parameters with maximum contribution to model output sensitivity (Fig. 14a and b). The reference solutions are most sensitive to the choice of the initial slope of P/I curve ($i = 3$), the attenuation coefficient for seawater ($i = 4$) and the cloudiness ($i = 12$).

The sensitivity of model output to variations of the nutrient stock parameterization ($i = 1, 2$) and different phytoplankton ratios is weak. However, the second-order indices S_{ij} (Fig. 15) show that the contribution of the nutrient stock parameterization to the model output sensitivity can be amplified considerably through interactions among appropriate model-related errors. For example, the model-related errors corresponding to the perturbations of A_1 and A_2 strongly interact with the errors caused by perturbations in α_0 and k_w. These interactions are non-linear and do not exist for small tolerance levels (see Figs. 12b and 13).

Thus, a model of the Black Sea phytoplankton cycle with higher accuracy than the NPZ model, requires high accurate model parameters. It is hard to estimate these parameters with necessary accuracy from existing biological observations. A less accurate model, such as the NPZ model, which is able to reproduce the main events (spring and fall blooms), may be successfully constructed because only few parameters need to be identified.

Fig. 14 – The total sensitivity indices for the IPT on the tolerance level: (a) $\bar{\varepsilon} = 0.2$ and (b) $\bar{\varepsilon} = 0.5$. Bars show 95% confidence intervals computed by the bootstrap technique.
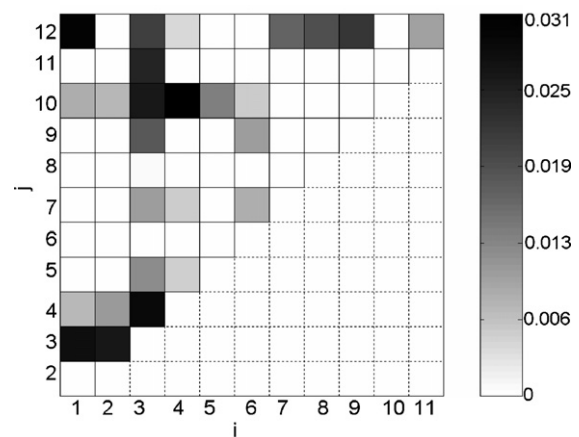
Fig. 15 – Second-order indices S_{ij} for the IPT with the tolerance level of $\varepsilon = 0.2$.

11. Conclusions

The present study has developed a variance-based method for the analysis of non-linear sensitivity of marine biological models to large variations of model parameters. This approach utilizes the Sobol'–Saltelli's sensitivity indices as a measure of model sensitivity and special scalar model output decom-

posed through the warping functions or represented by the irreversible predictability time.

The method does not identify directly the optimal parameters from model-data fitting but ranges the parameters relative to their influence to model output. It determines the control parameters, which contribute most to output variability. Additional research is required to increase knowledge of the control parameter in order to reduce output uncertainty. The insignificant parameters are held constant or even eliminated from the model.

Many methods currently in use have some sort of sensitivity aspect for linear and non-linear biological models. The variance-based method developed here, can be used to investigate non-linear sensitivity of model output to large variations of model parameters.

Large values of the sensitivity indices S_{ij} show the amplification of the model output variance due to perturbations of both ith and jth model parameters. Here, output variances corresponding to perturbations of appropriate parameters are not additive. Contrarily, small values of the indices S_{ij} show no such amplification of the model output variance when two parameters are perturbed simultaneously.

The simplified three-component model of annual phytoplankton cycle in the Black Sea is chosen to illustrate the technique and to understand some generic features of model sensitivity to large perturbations of model parameters. This model has very simple configuration and may fail to reproduce the phytoplankton behavior in summer when the mixed layer depth is shallow. However, the model reproduces the bi-modal behavior of phytoplankton observed in the Black Sea and can be a useful tool for the demonstration of capability of the non-linear sensitivity analysis.

The single and total sensitivity indices demonstrate that the model predicted spring bloom (in April–May) is most sensitive to the choice of the initial slope of the photosynthesis/irradiation curve. As far as the parameter interactions are concerned, the light attenuation of the seawater, cloudiness, the mortality rate of the phytoplankton and the nutrient stock parameter become influential as compared to the initial slope of the P/I curve, the light attenuation coefficient of the seawater and cloudiness. These factors are mostly related to the light limitation of the phytoplankton growth. Of course, this result is intuitive from the physical point of view.

However, ranging model parameters along their contributions to model output variability does not show straightforward result. The intuition is also useless when we try to understand and to estimate contributions of interactions among model-related errors caused by perturbations of different parameters to model output variance. For example, this is not a priori clear when model-related error caused by uncertainty in the nutrient stock parameterization is amplified considerably by interactions with uncertainty in the light-related factors.

Acknowledgments

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