Inverse estimations of the parameters: phosphorus cycle in an aquatic ecosystem

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Abstract. The phosphorus cycle in an aquatic ecosystem can be modeled by a dynamical system. Besides field measurements of the parameters, the theoretical methods can be invoked. A widely used method is finding the parameters as a minimum point of a properly defined cost function. In the paper the cost function is defined and a numerical method of minimization is presented. The numerical method is the Levenberg-Marquardt one, in which the derivatives of the cost function with respect to unknowns are evaluated as derivatives of the solution of the dynamical system with respect to the parameters.

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1 Introduction

There exist several models of phosphorus cycle in an aquatic ecosystem [2]. Each of them is obtained from the global mass balance with the proper identification of the state variable, and contains several parameters that control the rate transfer between components and the exchange mass with the exterior medium. Generally, the field measurements are used to determine the specific parameters. Most often such measurements are time consuming and are affected by errors. A very attractive alternative to that is to combine the field measurements with the inverse estimation method.

In the inverse method one tries to find the parameters such that the solution of the mathematical model fit the measured data. In the paper we present a numerical algorithm of the inverse method when the mathematical model is given by a ordinary differential equations. We firstly present two models of the phosphorus cycle.

First we take in account only two state of the phosphorus, soluble phosphorus, P_S, and phosphorus in algae, P_A. The soluble phosphorus gains mass from the exterior medium and from algae phosphorus and loses mass by drainage, while the algae phosphorus gains mass from the soluble state and loses mass by drainage (see Fig.1a).

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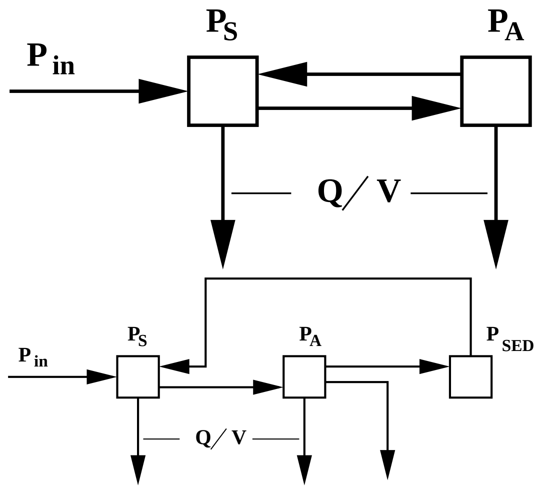


a) two state variables b) three state variables

The phosphorus cycle.

The mathematical model is given by

$$\begin{cases} \dfrac{dP_S}{dt} = (P_{in} - P_S)Q/V - (\mu - R)P_A \\ \dfrac{dP_A}{dt} = (\mu - R - Q/V)P_A \end{cases} \tag{1.1}$$

where μ represents the rate transfer between the two components that is given by

$$\mu = S(t)\frac{P_S}{P_S + K}.$$

The quantities:

- P_{in}, the input of soluble phosphorus,
- Q/V, the outflow/inflow of water= Q, the volume of system=V,
- $S(t) = S_{max}(1 + \sin(0.008603t)$, the solar radiation,

are considered to be known.

The parameters of the model subject to estimation are:

- K, the Michaelis-Menten constant,
- R, the release rate of algae phosphorus.

The second model deals with three state variables: soluble phosphorus, P_S, phosphorus in algae, P_A and phosphorus in sediment, P_{SED}. The cycle in this case is illustrated in the Fig. 1b and the corresponding mathematical model is given by

$$\begin{cases} \dfrac{dP_S}{dt} & = & (P_{in} - P_S)Q/V - \mu P_A + K_x P_{SED} \\ \dfrac{dP_A}{dt} & = & (\mu - s - Q/V)P_A \\ \dfrac{dP_{SED}}{dt} & = & f \cdot s \cdot P_A - K_x P_{SED}, \end{cases} \tag{1.2}$$

where in addition to the first model f represents the fraction of the P_A going to the exchangeable pool.

Here the parameters are:

- K,
- K_x, the release rate of sediment phosphorus,
- s, the rate of sedimentation of algae phosphorus.

2 The inverse problem

We can formulate the inverse problem as follows:

Find the parameters $\mathbf{a}$ *such that the calculated values* $\{\widetilde{\mathbf{x}}_{cal}(t_i, \mathbf{a})\}_{i=1,M}$ *obtained from the solution of the mathematical model*

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{a}) \tag{2.3}$$

"agree" to the measured datum $\{\widetilde{\mathbf{x}}_{obs}(t_i)\}_{i=1,M}$.

To solve this problem is beyond the aim of this paper, and here we only give a numerical strategy that we will hope to be useful. The general frame is the *least-squares approach.*

First we define the cost function $F(\mathbf{a})$ by

$$F(\mathbf{a}) = 1/2 \sum_i \|\widetilde{\mathbf{x}}_{obs}(t_i) - \widetilde{\mathbf{x}}_{cal}(t_i, \mathbf{a})\|^2 \tag{2.4}$$

and then we find the desired parameters as the minimizer of the cost function.

This problem can be solved, by example, using the Levenberg-Marquardt method for the unconstrained optimization problem [3]. If there exist constrains on the parameters (in many cases there exist !), this method can be used by a suitable transformation. The gradient of the cost function required by this method is obtained from the time evolution of the derivatives of the solution $\mathbf{x}(t, \mathbf{a})$ with respect to parameters. As it is known these derivatives are the solutions of the linear ordinary differential equations

$$\frac{d}{dt}\nabla_{\mathbf{a}}\mathbf{x} = \nabla_{\mathbf{x}}\mathbf{f}(\mathbf{x}, \mathbf{a}) \cdot \nabla_{\mathbf{a}}\mathbf{x} + \nabla_{\mathbf{a}}\mathbf{f}(\mathbf{x}, \mathbf{a}) \tag{2.5}$$

The evaluation of the cost function and its gradient requires numerical integration of the equations (2.3, 2.5).

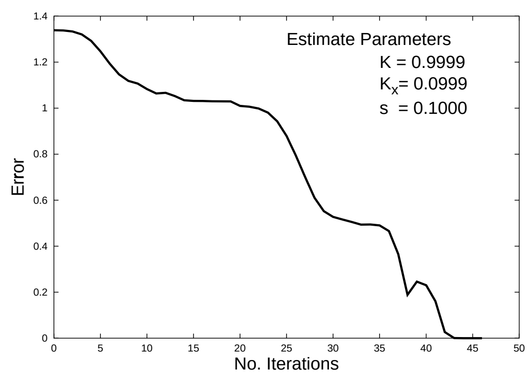
3 Numerical tests

We test our method, considering as "measured" datum the solution of the (2.3) obtained by given values of the parameters $\mathbf{a}_0$, and next we try to recover these values.

In the first test we consider the extended model (1.2). The parameters $\mathbf{a} = (K, K_x, s)$ satisfy the constraints

$$0.5 \leq K \leq 1.5, 0 \leq K_x \leq 1, 0 \leq s \leq 1,$$

as "measured" datum having the soluble and algae phosphorous $\widetilde{\mathbf{x}}_{obs} = (P_S, P_A)$ considered at several moments of time $\{t_i\}_{i=1,M}$. The input values of the parameters were $\mathbf{a}_0 = (1, 0.1, 0.1)$ and the estimated values were $(0.9999, 0.0999, 0.1)$. The Figure 3 illustrates the history of convergence of the method.



The values of the parameters and the history of the convergence per iteration. $\tilde{\mathbf{x}}_{obs}(t_i) = \tilde{\mathbf{x}}_{cal}(t_i, \mathbf{a}_0)$, $\mathbf{a}_0 = (1, 0.1, 0.1)$.

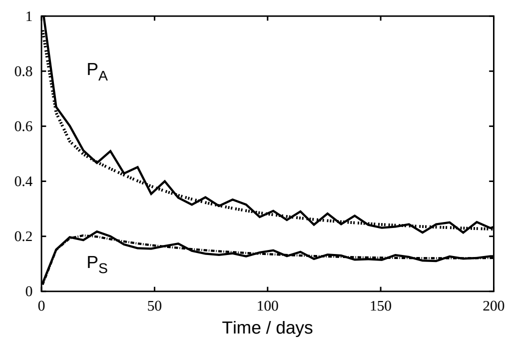
In the second test, the response of the method to the random error in measured data was analyzed. The input datum was the same as in the first test, except that $\mathbf{x}_{obs}(t_i)$ was given by

$$\widetilde{\mathbf{x}}_{obs}(t_i) = \widetilde{\mathbf{x}}_{cal}(t_i, \mathbf{a}_0) + \mathbf{b}_i,$$

where $\mathbf{b}_i$ simulate the errors. The Table 1 contains the results obtained for three cases of the magnitude of the "errors". As it is expected, small errors in the input datum led to a better estimation of the parameters.

$\|\mathbf{b}_i\|$	Estimated Parameters (K, K_x, s)
$\leq$ 10%	(0.9696, 0.1018, 0.0880)
$\leq$ 5%	(0.9848, 0.10019, 0.0936)
$\leq$ 1%	(0.9969, 0.10011, 0.0986)

Table 1. The response of the method to random errors in measured datum



Time evolution of two components of the soluble phosphorous in the extended model. The input values are affected by errors (solid lines) and by the calculated values (dashed lines).

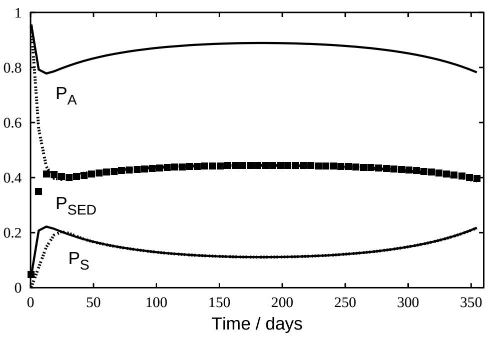
4 Conclusions

1) The main advantage of the inverse estimation of the parameters is given by its flexibility.

2) It is very important to investigate the qualitative properties of the solution (boundedness, stability, parameter dependency) of the mathematical model in order to

- set proper bounds on parameters
- obtain a correct solution.

3) The Levenberg-Marquardt algorithm in conjunction with the gradient of the solution is an effective method in the inverse problem.



Simplified Model (solid lines) versus Extended Model (dashed lines).

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