Parameter Estimation of the ODE Model of Distribution of Heavy Metal in a Food Web

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Technical report

Abstract

The food consummation is an important cause of contamination of ecological systems by heavy metals. The ordinary differential equation (ODE's) are proved to be a very effective tool in both aspects of contamination the mechanism and prediction of the level of contamination. Among the multitude of the factors that affect the spreading of the pollutant through the food web the uptake rates from external medium and food and elimination rate are the more important.

In this paper we are concerned with the estimation of these rates by knowing a time series of measurements of the concentration of metals in the individuals of the system. Our approach combines the Particle Swarm Optimization (PSO) method and Levenberg-Marquardt (LM) method to minimize a proper defined cost function. Basically the PSO method is used to find a global minimum and then we apply the local search algorithm (LM) using as the starting point the point given by PSO. The numerical investigations of a linear tri-trophic models allow us to be optimistic in view of real very applications.

Contents

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1 Introduction

The fate of metals in environment and the response of organisms to the presence of metals has been debated for a long time. Presently it is largely accepted a set of principles and ecological laws [2], [3], [9].

Metal Principles.

• *Metals are naturally occurring constituents in the environment and their concentrations may vary across geographic regions.*

• *All environmental media naturally contain mixtures of metals. The metals are often introduced into the environment as mixtures.*

• *Some metals are essential in maintaining proper health of humans, animals, plants, and microorganisms.*

• *The environmental chemistry of metals strongly influences their fate and effects on human and ecological receptors.*

• *The toxico-kinetics and toxico-dynamics of metals depend on the metal, the form of the metal or metal compound, and the organism's ability to regulate and/or store the metal.*

Ecological laws.

• *Leibig' law of the minimum states: There is a minimum concentration of each substance required for life.*

• *Shelford' law of tolerance states: Every necessary condition or substance that varies in concentration in the habitat of an organism has a minimum and maximum value. When the concentration is outside these limits the population is extinguished in that habitat.*

• *Each species (in a community) has a unique, genetically-determined range of tolerances for the conditions and substances that define the boundaries of its niche in the ecosystem where it lives.*

The increase of the natural concentration in soil, water or air affect all the living organisms in the contaminated area due to the food consumption or by direct exposure.

The bioaccumulation is complex and it is influenced by multiple ways of exposure and by the capacity of the organism to assimilate and eliminate the metals.

The biodynamical models are able take into account the above mentioned metal principles and ecological laws [8]. The mathematical model consists into a set of ordinary differential equation obtained by using a mass conservation principle. Besides the prediction capability of the biodynamic model, another potential use of the model is the estimation of parameters appearing in the model. The parameter estimation is useful especially for those parameters that are very difficult to be measured directly. We discuss this problem in the sections 3 and section 4.

2 ODE Model

The base of dynamical modelling of the distribution of heavy metals in a food web is the mass balance principle. Taking into account the metals in the organism can not be created or destroyed the principle can be formulated as follows: *the rate of accumulation of a substance in an organism equals the total uptake minus total loss of the substance.*

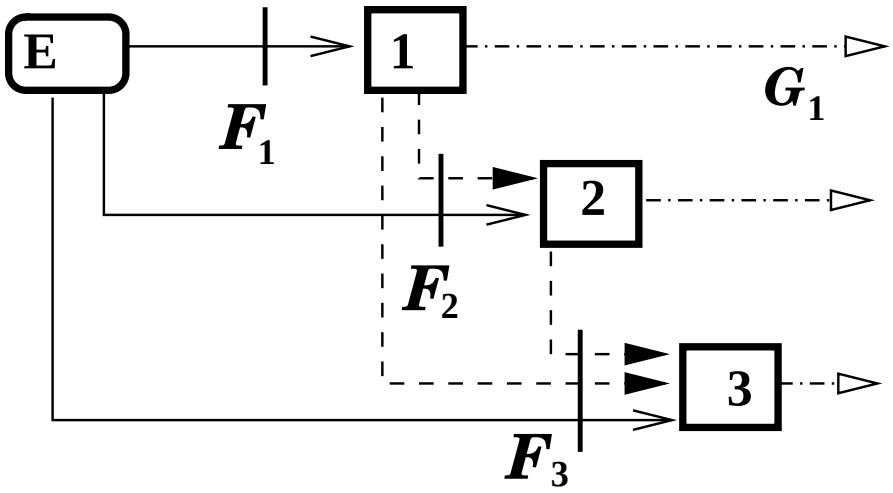

Figure 1: A schematic pathways of circulation of contaminant in a hierarchical organized food web.

Assuming n interacting bioreceptors, one can write

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \mathcal{F}_i(\boldsymbol{x}, \boldsymbol{\lambda}) - \mathcal{G}_i(\boldsymbol{x}, \boldsymbol{\lambda}), \quad i = \overline{1,n} \tag{1}$$

where x_i denotes the concentration in the $i-$th bioreceptor, $\mathcal{F}_i$ and $\mathcal{G}_i$ are the mass fluxes that quantify the mass gain and mass loss, respectively, by the $i-$th bioreceptor. In (1), $\boldsymbol{\lambda}$ represents the vector parameter in the model.
The steady state of the system is characterized by $\boldsymbol{x}^e$ given by

$$\boldsymbol{\mathcal{F}}(\boldsymbol{x}^e, \boldsymbol{\lambda}) = \boldsymbol{\mathcal{G}}(\boldsymbol{x}^e, \boldsymbol{\lambda}) \tag{2}$$

A distinctive characteristic of the interaction in a food web is that the flux of mass is unidirectional, for a given i the mass entry flux $\mathcal{F}_i$ depends only the components $j < i$ of the state vector $\boldsymbol{x}$ and the flux of the mass loss $\mathcal{G}_i$ depends only the component x_i. Assuming the linearity of mass fluxes with respect to concentration one can write

$$\mathcal{F}_i = \mathcal{F}_i = k_i^u c_m + \sum_{j=1}^{i-1} f_i^j x_j, \quad \mathcal{G}_i = k_i^e x_i, \tag{3}$$

where:
k_i^u the rate of contaminant uptake of the individual i from external medium;
f_i^j the rate of contaminant uptake of the individual i from the individual j;
k_i^e the rate of contaminant elimination of the individual i;
c_m the concentration of the external medium.
All rates are positive numbers. On the ground we know all parameters in the model and the level of contaminant in the external medium we can calculate the evolution of the contamination level for all

individuals if we know the contaminant level for each individual at a reference time, not necessary the same reference time for all individuals,

$$\boldsymbol{x}(t_0^i) = x_0^i. \tag{4}$$

The very special structure of $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{\mathcal{G}}$ allow one to give a recursive algorithm to integrate the ODE (**??**) subject to (4). One has,

$$\begin{aligned} x_i(t) \quad &= \exp(-k_i^e\,(t-t_0^i))\left(c_{0\,i} - \frac{k_i^u c_m}{k_i^e}\right) + \frac{k_i^u c_w}{k_i^e} + \\ &+ \sum_{j=1}^{i-1} f_i^j \int_{t_0^i}^{t} \exp(-k_i^e(t-s)) x_j(s)\mathrm{d}s. \end{aligned} \tag{5}$$

If in addition we assume that

$$k_i^e \neq k_j^e, \text{if } i \neq j \tag{6}$$

the integrals can be evaluate and the solutions can be write as

$$x_i(t) = \sum_{j=1}^{i} \gamma_{i\,j} \exp(-k_j^e\,(t-t_0^i)) + w_i. \tag{7}$$

The coefficients γ and w are recursively calculate

$$\begin{aligned} \gamma_{i\,j} &= \frac{1}{k_i^e - k_j^e} \sum_{k=j}^{i-1} f_i^k \gamma_{k\,j} \exp(k_j^e(t_0^k - t_0^i)), \quad j = \overline{1, i-1} \\ w_i &= \frac{k_i^u c_w + \sum\limits_{j=1}^{i-1} f_i^j w_j}{k_i^e}, \\ \gamma_{i\,i} &= c_{0\,i} - \sum_{k=1}^{i-1} \gamma_{i,k} - w_i. \end{aligned} \tag{8}$$

The steady state is ready obtained as

$$\boldsymbol{x}^e = \boldsymbol{w} \tag{9}$$

and using (8) one can write

$$\boldsymbol{x}^e = c_w \widetilde{\boldsymbol{w}} \tag{10}$$

where $\widetilde{\boldsymbol{w}}$ is given by

$$\widetilde{w}_i = \frac{k_i^u + \sum\limits_{j=1}^{i-1} f_i^j \widetilde{w}_j}{k_i^e}, \tag{11}$$

The last two formulas allow us to draw two main conclusions.
The concentration level is increasing with respect to:
a) concentration of the external medium,
b) rates uptake from food and external medium,
and decrease with respect to elimination rate.

3 Parametric Estimation

The parametric estimation problem consists in the uniquely estimation of the parameters in the ODE model from a set of observations. An observable variable can be a state variable or a given function of the state variables. The process of observations can be affected by a series of external factors. But the influence of these factors is unknown. This fact requires new parameters to quantify their effect on observations. Also there exists many situations when the reference state is only partial known or is totally unknown. Then the reference state values of the unknown variables can be considered as parameters.
For the trophic model of the distribution of the heavy metals we will restrict to the case of direct observation of the metal concentration and we will include in our analysis the cases of partial observations and of the unknown reference state.

3.1 Problem formulation

The mathematical formulation of the parametric estimation problem is given in this section.
Dynamic model parameters $\mathcal{M}(\boldsymbol{\lambda})$. By the dynamical model parameter one understand
–the ODE equations that govern the evolution of state variables
–the mathematical relations between observables and state variables
–the initial data of the state variables necessary to integrate ODE equations.

A general formulation that suits to our case can be formulated as:
(1) the ODE equations

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{A}(\boldsymbol{\lambda})\,\boldsymbol{x}(t) + \boldsymbol{B}(\boldsymbol{\lambda})\,q, \boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{A} \in \mathbb{R}^{n\times n}, \boldsymbol{B} \in \mathbb{R}^{n\times 1}, \boldsymbol{q} \in \mathbb{R}, \tag{12}$$

(2) the observables

$$\boldsymbol{y}(t) = \boldsymbol{C}(\boldsymbol{\lambda})\,\boldsymbol{x}(t), \boldsymbol{y} \in \mathbb{R}^k, \boldsymbol{C} \in \mathbb{R}^{k\times n}, \tag{13}$$

(3) the initial data

$$\boldsymbol{x}(0) = \boldsymbol{x}_0(\lambda), \tag{14}$$

(4) the constraints on parameters

$$\boldsymbol{\lambda} = \Omega \in \mathbb{R}^m. \tag{15}$$

By $\boldsymbol{\lambda}$ we denote the vector parameter. The components of λ encompass all parameters in the problem: parameters in ODE model, parameters implied in the processes of observation and the parameters associated to the reference state.
Measured values $\mathcal{O}_m$. The measured values refer to one or more times series of the measured values of the observables. Here we are not concerned in the analysis of the process of the measurement, we trust the data and our purpose is to find the best fitting parameter in accord to the measured data.

$$\mathcal{O}_m = \left\{ \boldsymbol{y}_m(t_a) \,\middle|\, \boldsymbol{y}_m(t_a)\mathbb{R}^k, a = \overline{1,N}, t_1 < t_2 < \cdots < t_N \right\}. \tag{16}$$

The fitting method The fitting method means a procedure to select a parameter $\boldsymbol{\lambda}$ from Ω that is the most "appropriate" to the measured values $\mathcal{O}_m$. A way to define the "appropriate" quality it to

introduce a cost function that measures the discrepancy between measured values of the observables and the calculated values of the observable for a given parameter. The most used cost function is the sum of squares of the difference between measured and calculated values

$$\chi^2(\boldsymbol{\lambda}) = \sum_{a=1,N} w_a \, ||\boldsymbol{y}_m(t_a) - \boldsymbol{y}(t_a;\boldsymbol{\lambda})||_k^2 \,, \tag{17}$$

where w_a are some pondered weight and $||\cdot||_k^2$ stands for usual euclidean distance in $\mathbb{R}^k$.
The solution of the parameter estimation problem is given by the global minimizer of the cost function.

$$\boldsymbol{\lambda}_{\text{sol}}: \quad \min_{\boldsymbol{\lambda}\in\Omega} \chi^2(\boldsymbol{\lambda}). \tag{18}$$

3.2 Identifiably analysis

Roughly speaking a dynamical model is identifiable if different parameters imply different values of the observables, [10], [14].

Definition 3.1 *The dynamical model $\mathcal{M}(\lambda)$ is globally identifiable at $\boldsymbol{\lambda} \in \Omega$ if there exists a finite time $t_1 > 0$, such that if $\boldsymbol{y}(t,\boldsymbol{\lambda}) = \boldsymbol{y}(t,\widetilde{\boldsymbol{\lambda}})$, $\widetilde{\boldsymbol{\lambda}} \in \Omega$ for any $t \in [0,t_1]$, then $\boldsymbol{\lambda} = \widetilde{\boldsymbol{\lambda}}$.*

The eigenvalues and the eigenvectors of $\boldsymbol{A}(\boldsymbol{\lambda})$. It is easily two show that the eigenvalues of the matrix $\boldsymbol{A}(\boldsymbol{\lambda})$ are given by

$$\alpha_{(i)} = -k_i^e, i = \overline{1,n}.$$

The components of a right eigenvector $\boldsymbol{r}^{(k)}$ can be recursively calculated as follows

$$\begin{aligned} r_i^{(k)} &= 0, && 1 \le i \le k-1, \\ r_i^{(k)} &= \frac{1}{\alpha_{(k)} - \alpha_{(i)}} \sum_{j=k}^{i-1} a_{i\,j} r_j^{(k)}, && k+1 \le i \le n \end{aligned}$$

Similarly for left a eigenvector $\boldsymbol{l}^{(k)}$ one has

$$\begin{aligned} l_i^{(k)} &= \frac{1}{\alpha_{(k)} - \alpha_{(i)}} \sum_{j=i+1}^{k} a_{j\,i} l_j^{(k)}, && 1 \le i \le k-1 \\ l_i^{(k)} &= 0, && k+1 \le i \le n, \end{aligned}$$

For each $k = \overline{1,n}$ one can choose $r_k^{(k)}$ and $l_k^{(k)}$ such that the matrices $\boldsymbol{R}$ of the right eigenvectors and $\boldsymbol{L}$ of the left eigenvectors given by

$$R_{i\,j} = r_i^{(j)}, L_{i\,j} = l_j^{(i)}$$

satisfy

$$\boldsymbol{A} = \boldsymbol{R}\boldsymbol{\Lambda}\boldsymbol{L}, \boldsymbol{R}\boldsymbol{L} = \boldsymbol{I},$$

where $\boldsymbol{\Lambda}$ stands for the diagonal matrix of the eigenvalues, $\Lambda_{ii} = \alpha_{(i)}$.

There are several methods to tackle the identifiably of a linear dynamical system. One of them uses the Laplace transform and the identifiably problem is reduced to the study of the injectivity of the transfer function. Denote by $\hat{\psi}(s)$ the one side Laplace transform of the function ψ, *i.e.*

$$\hat{\psi}(s) = \int_0^\infty \mathrm{e}^{-st}\psi(t)\mathrm{d}t$$

In the space of Laplace transform the dynamical model $\mathcal{M}(\lambda)$ given by (12), (13) and (14) takes the form

$$\begin{array}{l} s\hat{\boldsymbol{x}}(s) = \boldsymbol{x}_0 + \boldsymbol{A}(\lambda)\hat{\boldsymbol{x}} + \boldsymbol{B}(\lambda)\boldsymbol{q}(s) \\ \hat{\boldsymbol{y}}(s) = \boldsymbol{C}(\lambda)\hat{\boldsymbol{x}}(s), \end{array} \tag{19}$$

that allows us to write

$$\hat{\boldsymbol{y}}(s,\boldsymbol{\lambda}) = \boldsymbol{C}(\lambda)\left(s\boldsymbol{I} - \boldsymbol{A}(\lambda)\right)^{-1}\left(\boldsymbol{x}_0(\lambda) + \boldsymbol{B}(\lambda)q(s)\right). \tag{20}$$

Using the left and right eigenvectors one has

$$\left(s\boldsymbol{I} - \boldsymbol{A}(\lambda)\right)^{-1} = \boldsymbol{R}\left(s\boldsymbol{I} - \boldsymbol{\Lambda}\right)^{-1}\boldsymbol{L}$$

or component-wise

$$\left(s\boldsymbol{I} - \boldsymbol{A}(\lambda)\right)^{-1}_{ij} = \sum_k \frac{r_i^{(k)} l_j^{(k)}}{s - \alpha_{(k)}}.$$

Then, we can write

$$\hat{\boldsymbol{y}}(s,\boldsymbol{\lambda}) = \sum_k \frac{\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\boldsymbol{l}^{(k)}, \boldsymbol{x_0}\right)}{s - \alpha_{(k)}} + \sum_k \frac{\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{s - \alpha_{(k)}} q(s),$$

where for any quantity Ψ

$$\left(\boldsymbol{\Psi}, \boldsymbol{r}^{(k)}\right) = \sum_{j=1}^n \Psi_{\bullet j} r_j^{(k)},\ \left(\boldsymbol{l}^{(k)}, \boldsymbol{\Psi}\right) = \sum_{j=1}^n \Psi_{j\bullet} l_j^{(k)}$$

Assume that the "command" is a constant function and it equals to q. This implies

$$q(s) = \frac{q}{s}.$$

By rewriting the two terms in the transfer function for the observables one can write

$$\hat{\boldsymbol{y}}(s,\boldsymbol{\lambda}) = -\frac{q}{s}\sum_k \frac{\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{\alpha_{(k)}} + \sum_k \frac{\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\left(\boldsymbol{l}^{(k)}, \boldsymbol{x_0}\right) + \dfrac{\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{\alpha_{(k)}} q\right)}{s - \alpha_{(k)}}.$$

It is clear that two transfer functions are equal if they have same poles and same residuals. We split the parameter vector in two parts. One part denoted by $\boldsymbol{k}^e$ that keeps the rates of elimination k_i^e and another part denoted by $\boldsymbol{\lambda}_e$ that keeps the remainder components of $\boldsymbol{\lambda}$. $\boldsymbol{\lambda}$ can be represented as $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_e, \boldsymbol{k}^e)$. We introduce the vector function $\boldsymbol{F} : \Omega \to \mathbb{R}^{n+1}$ by

$$F_k(\boldsymbol{\lambda}) = \left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\left(\boldsymbol{l}^{(k)}, \boldsymbol{x_0}\right) + \frac{\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{\alpha_{(k)}} q\right),\ a = \overline{1,n}$$
$$F_{n+1}(\boldsymbol{\lambda}) = q \sum_k \frac{\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right)\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{\alpha_{(k)}}.$$

Proposition 3.1 *Assume that:*
(a) *for any vector parameter* $\boldsymbol{\lambda}$ *in* Ω *the components* k_i^e *satisfy*

$$0 < k_1^e < k_2^e \cdots < k_n^e.$$

(b)

$$\left(\boldsymbol{C}, \boldsymbol{r}^{(k)}\right) \neq 0, (\forall) k \in \{1, 2, \cdots, n\}$$

(c) $F(\boldsymbol{\lambda})$ *is an one to one map with respect to* $\boldsymbol{\lambda}_e$.
Then the dynamical system $\mathcal{M}$ *is global identifiable on* Ω.

Proof: Suppose that there exists two different $\boldsymbol{\lambda}$ and $\widetilde{\boldsymbol{\lambda}}$ in Ω such that

$$\hat{\boldsymbol{y}}(s, \boldsymbol{\lambda}_1) = \hat{\boldsymbol{y}}(s, \boldsymbol{\lambda}_2).$$

By (b), it results that

$$k_i^e = \widetilde{k_i^e},\ i \in \overline{1,n}$$

and

$$F_a(\boldsymbol{\lambda}_e, \boldsymbol{k}^e) = F_a(\widetilde{\boldsymbol{\lambda}}_e, \boldsymbol{k}^e).$$

Since F is an one to one function in $\boldsymbol{\lambda}_e$, it results that

$$\boldsymbol{\lambda}_e = \widetilde{\boldsymbol{\lambda}}_e$$

which contradicts the supposition.

In the following, we present some applications.

The top level identification. Assume that the initial state, the uptake rates and the elimination rates are all known up to level $n-1$. Then the parameter in the problems are the initial state $x_{0\,n}$, the uptake rates from the food, the uptake rates from external medium and the elimination rates. The problem is to uniquely estimate the parameter from the observation of the $x_n(t)$.
In this case

$$C = (0, 0, \cdots, 0, 1), B = (k_1^u, \cdot, k_n^u)^{\mathrm{T}}$$
$$\boldsymbol{\lambda} = \{x_{0\,n}, a_{n\,1}, a_{n\,2}, \cdots, a_{n\,n-1}, k_n^u, k_n^e\}$$

$$\Omega = \{\boldsymbol{z} \in \mathbb{R}^{n+2} | z_{n+2} > k^e_{n-1}, z_i \leq 0, i = \overline{1, n+1}\}$$

One observes that:
(a) for $k \leq n-1$ the left eigenvectors $\boldsymbol{l}^{(k)}$ for $k \leq n-1$ do not depend on the parameters of the problem and $l^{(k)}_n = 0$. Consequently

$$\left(\boldsymbol{l}^{(k)}, \boldsymbol{x_0}\right) + \frac{\left(\boldsymbol{l}^{(k)}, \boldsymbol{B}\right)}{\alpha_{(k)}} q = \psi_k, k = \overline{1, n-1}$$

are known quantities and, *assume that*, different from zero.
(b) For any k, the components of $r^{(k)}_j$, with $j \leq n-1$ do not depend on $\boldsymbol{\lambda}_e$.
We analyse the injectivity of the function $\boldsymbol{F}$. Let

$$\boldsymbol{F}(\boldsymbol{\lambda}_e, \boldsymbol{k}^e) = \boldsymbol{F}(\widetilde{\boldsymbol{\lambda}}_e, \boldsymbol{k}^e).$$

On has

$$\sum_{k=1}^{n} F_k(\boldsymbol{\lambda}_e, \boldsymbol{k}^e) = x_{0\,n} + F_{n+1}(\boldsymbol{\lambda}_e, \boldsymbol{k}^e),$$

which implies that

$$x_{0\,n} = \widetilde{x}_{0\,n}.$$

For any $k \leq n-1$,

$$r^{(k)}_n(\boldsymbol{\lambda}_e, \boldsymbol{k}^e)\psi_k = r^{(k)}_n(\widetilde{\boldsymbol{\lambda}}_e, \boldsymbol{k}^e)\psi_k,$$

that leads to

$$\sum_{j=k}^{n-1} a_{n\,j} r^{(k)}_j = \sum_{j=k}^{n-1} \widetilde{a}_{n\,j} r^{(k)}_j.$$

Taking into account that $\left(r^{(k)}_j\right)^{k=1,n-1}_{j=k,n-1}$ is a non-singular matrix one obtains

$$a_{n\,j} = \widetilde{a}_{n\,j}, j = \overline{1, n-1}.$$

Finally from

$$F_n(\boldsymbol{\lambda}_e, \boldsymbol{k}^e) = F_n(\widetilde{\boldsymbol{\lambda}}_e, \boldsymbol{k}^e)$$

and the previous results one gets

$$k^u_n = \widetilde{k}^u_n.$$

3.3 Lvenberg-Marquardt Minimization Method

The most used method for finding the minimizer is the Levenberg-Marquardt method. Mainly, the method consists in the following steps [12]:
1) an initial guess $\boldsymbol{\lambda}$ is updated by a correction δ
2) that solves the linear algebraic system of equation

$$(\alpha + \gamma I)\,\delta = \beta \tag{21}$$

3) if for the new values $\boldsymbol{\lambda} + \delta$

$$\chi^2(\boldsymbol{\lambda} + \delta) < \chi^2(\boldsymbol{\lambda})$$

then the correction is accepted and
4) a new value $\boldsymbol{\lambda} = \boldsymbol{\lambda} + \delta$ is considered and the parameter γ is multiplied by a fractional unit,
5) if for the new values $\boldsymbol{\lambda} + \delta$,

$$\chi^2(\boldsymbol{\lambda} + \delta) > \chi^2(\boldsymbol{\lambda}),$$

then the correction is not accepted and a new correction δ is calculated by increasing the parameter γ.
The matrix α and vector β are given by:

$$\alpha_{ln}(\boldsymbol{\lambda}) = \sum_a \sum_i \frac{\partial y_i(t_a, \boldsymbol{\lambda})}{\partial \lambda_l} \frac{\partial y_i(t_a, \boldsymbol{\lambda})}{\partial \lambda_n} \tag{22}$$

$$\beta_n(\boldsymbol{\lambda}) = \sum_a \sum_i \left(\boldsymbol{y}_{m\,i}(t_a) - \boldsymbol{y}_i(t_a; \boldsymbol{\lambda})\right) \frac{\partial y_i(t_a, \boldsymbol{\lambda})}{\partial \lambda_n} \tag{23}$$

As one can see the method requires the derivatives of the solution $\boldsymbol{x}(t; \boldsymbol{\lambda}; \boldsymbol{x}_0)$ of the equation (12) with respect to parameters. For a fixed parameter λ_l the derivatives are calculated as solution of the *sensitivity* equations

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \boldsymbol{x}}{\partial \lambda_l} = \boldsymbol{A}(\boldsymbol{\lambda}) \frac{\partial \boldsymbol{x}}{\partial \lambda_l} + \frac{\partial \boldsymbol{A}(\boldsymbol{\lambda})}{\partial \lambda_l} \boldsymbol{x} + \frac{\partial \boldsymbol{B}(\boldsymbol{\lambda})}{\partial \lambda_l} \boldsymbol{q} \tag{24}$$

subject to the initial condition

$$\left. \frac{\partial \boldsymbol{x}}{\partial \lambda_l} \right|_{t=0} = \frac{\partial \boldsymbol{x}_0}{\partial \lambda_l} \tag{25}$$

The algorithm of the method follows [12]:
1. `initial guess` $\boldsymbol{\lambda}$, `initial` γ
2. `solve`

$$(\boldsymbol{\alpha}(\boldsymbol{\lambda}) + \gamma \boldsymbol{I})\, \boldsymbol{\delta} = \boldsymbol{\beta}(\boldsymbol{\lambda})$$

if $\chi^2(\boldsymbol{\lambda} + \boldsymbol{\delta}) < \chi^2(\boldsymbol{\lambda})$
3. **then** $\boldsymbol{\lambda} = \boldsymbol{\lambda} + \boldsymbol{\delta}, \gamma = 0.1 \times \gamma$
else $\gamma = 10 \times \gamma$
4. **go to 1**
In applying the Levenberg-Marquatdt one encounter two main difficulties
1) the stability of the integration algorithm.
2) the minimizer found by the method is a local minimum not a global one.

3.4 Particle Swarm Optimization Method

The particle swarm optimization method is a probabilistic optimization method that mimics the strategies of a birds flock foraging for pray. A number of particles are placed in the search space of the problem and for each particle one evaluates the cost function at the current position. Each

particle moves in space according to its velocity. The velocity of a particle is evaluated by a strategy that combines the history of the particle, the history of the swarm and some random perturbation. The history retains the best position of the particle and the best position of the swarm. The best position is evaluated with respect to cost function. The method was firstly introduced by Kennedy and Eberhart, [7],
see [11] for an overview of the method.
Let Ω be the domain of the parameters and χ^2 the cost function (18). One considers M "particles" in Ω, $\{\mathcal{P}\}_{i=1,M}$. The position and the velocity of the particle $\mathcal{P}_i$ at "moment time s" are denoted by $\boldsymbol{\lambda}_i(s) \in \Omega$ and $\boldsymbol{v}_i(s)$, respectively. One introduces the vector $\boldsymbol{p}(s)_i$ that counts for the "best position" of the particle $\mathcal{P}_i$ up to the moment s,

$$\chi^2(\boldsymbol{p}(s)_i) \leq \chi^2(\boldsymbol{\lambda}(t)_i),\ s \geq t$$

and the vector $\boldsymbol{g}(s)$ that counts the best position of the swarm up to the moment s,

$$\chi^2(\boldsymbol{g}(s)) \leq \chi^2(\boldsymbol{\lambda}(t)_i), s \geq t,\ i = \overline{1, M}.$$

The strategy is to define a law of motion $\{\boldsymbol{\lambda}_i(s), \boldsymbol{v}_i(s)\}_{s\geq 0}$ such that

$$\boldsymbol{\lambda}^{PSO} := \lim_{s\to\infty} \boldsymbol{g}(s)$$

is the solution of the minimization problem.
Here is the algorithm.
1. `randomly initialization of`:
`position`, $\{\boldsymbol{\lambda}_i(0)\}_{i=1,M}$, `and velocity`, $\{\boldsymbol{v}_i(0)\}_{i=1,M}$, **set** $s = 0$
2. `update the best position of the particle` $\mathcal{P}_i$, $\boldsymbol{p}_i$ `and the best position of the swarm` $\boldsymbol{g}$

$$\boldsymbol{p}_i(n) :: \chi\left(\boldsymbol{p}_i(s)\right) = \min_{k=1,s}\{\chi(\boldsymbol{\lambda}_i(k))\}$$

$$\boldsymbol{g}(s) :: \chi\left(\boldsymbol{g}(s)\right) = \min_{k=1,s;i=1,M}\{\chi(\boldsymbol{\lambda}_i(k))\}$$

`update position and velocity using the law of motion`

$$\boldsymbol{v}_i(s+1) = \omega\boldsymbol{v}_i(s) + \alpha_1\phi_1(\boldsymbol{p}_i(s) - \boldsymbol{\lambda}_i(s)) + \alpha_2\phi_2(\boldsymbol{g}(s) - \boldsymbol{\lambda}_i(s))$$

$$\boldsymbol{\lambda}_i(s+1) = \boldsymbol{\lambda}_i(s) + \boldsymbol{v}_i(s+1)$$

4. set $s = s + 1$ `and` **go to 2**
The parameters in algorithm are:
M the number of particles in swarm,
ω inertia factor,
α_1 self-confidence factor,
α_2 swarm-confidence factor,
ϕ_1, ϕ_2 uniformly distributed random numbers in [0,1].

4 Numerical Simulation

As application of the parameter identification we consider the case of an arctic aquatic system. The trophic chain includes: sea water, phytoplankton, zooplankton, polar cod and harp seal. The structure of the food web and the parameter are given in the figure 2 and table 4, respectively.

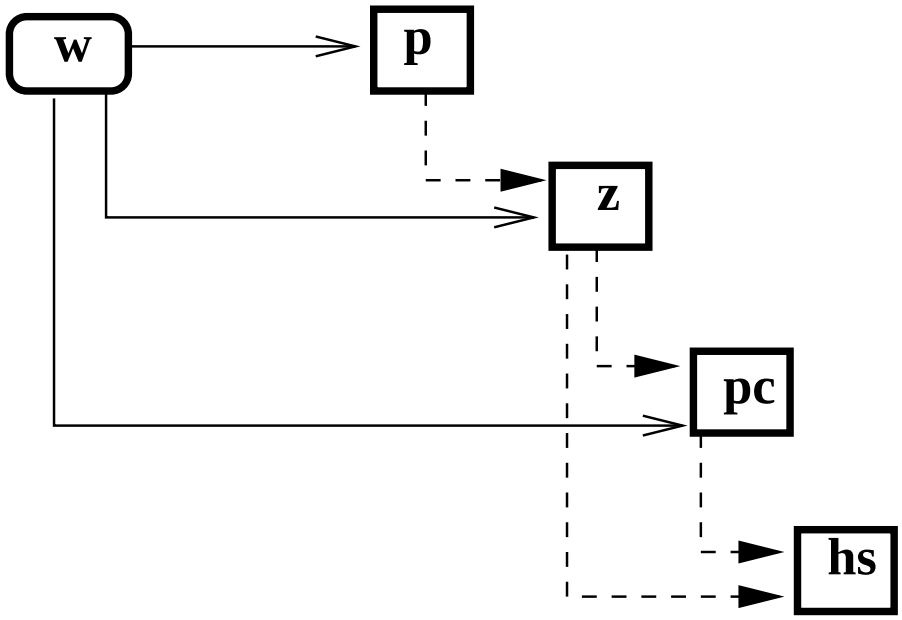

Figure 2: Aquatic system: water, phytoplankton, zooplankton, polar cod, harp seal. The arrows indicate the pat-ways of contamination with radionucleids.??????????????????????????????????????

Table 1: The parameters in the system for ^{239}Pu contaminant [4].

Level	uptake rate k^u from water	uptake rates $f = p \times \alpha \times K$ from food	elimination rates k^e
Level 1	$x_1 = w_1$ equilibrium with water		
Level 2	$k_2^u = 18.7$	$f_2^1 = \alpha_2^1 K_2^1$ $\alpha_2^1 = 0.01\, K_2^1 = 0.105$	$k_2^e = 0.05$
Level 3	$k_3^u = 0.01$	$f_3^2 = \alpha_3^2 K_3^2$ $\alpha_3^2 = 0.01\, K_3^2 = 9\mathrm{e}-3$	$k_3^e = 0.01$
Level 4	$k_4^u = 0.0$	$f_4^j = p_j \alpha_4^j K_4^j$ $\alpha_4^2 = \alpha_4^3 = 0.01\, K_4^2 = K_4^3 = 0.018$ $\alpha_4^1 = K_4^1 = 0, p_1 = 0, p_2 = p_3 = 0.5$	$k_3^e = 5\mathrm{e}-5$

α – assimilation efficiency, K – food consumption rates, p – feeding preference factor

The steady values of the distribution of the contaminant are calculated by (8) and for the parameters given by (4) one obtains

	zooplankton	polar cod	harp seal
w/c_w	$2.47\text{e}+3$	$2.3\text{e}+1$	$4.44\text{e}+3$

To test the method of parameter estimation we generate a set of observables and then we try do recover the parameters from observations.

Table 2: The top level identification problem

$n = 3$, true parameter

$x_{0,3}$	k_3^u	f_3^1	f_3^2	k_3^e
0	0	$9\text{e}-5$	$7\text{e}-5$	0.005

PSO, parameters

$M = 20, \alpha_1 = 2.5, \alpha_2 = 1, \omega \in I(n)$

$\boldsymbol{g}$

0	0.07	0	0.001	0

LM method $\boldsymbol{\lambda}_0 = \boldsymbol{g}$

0	0.0	$9\text{e}-5$	$7\text{e}-5$	0.005

ne can see that the best results are obteined by hybrid method.

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