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ADJOINT ESTIMATION OF AQUATIC ECOSYSTEM PARAMETERS

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Abstract: Modelling water ecosystem dynamics requires a thorough knowledge of the chemico-physical parameters in the constitutive equations of the chosen model. These processes are mathematically described by ordinary, in general non-linear, differential equations whose solution depends strongly on the parameter values.

We used the adjoint equation method, minimizing the square deviation between states and observations with the conjugate gradient method, in order to estimate the parameters of a logistic growth model on the basis of macroalgae data collected in the Gulf of Trieste. An extension of the method to a more complete trophic model is also discussed.

Introduction

The need for a parameter estimation procedure in an aquatic ecosystem model is due to several factors: firstly, the ecological parameters are known with a large degree of uncertainty; secondly, every model is a simplification of nature, so we must include the influence of all the other processes using a calibrated choice of the parameters (Jorgensen 1986); finally, box models are widely used in which an average of the state variables is considered, so the parameters have to be referred to the ensemble.

Usually, parameter calibration is based on trial and error procedures. This implies, in general, a large amount of computation, and, moreover, the modeller is constrained to vary only one or two parameters in each run of the model. This procedure may make the calibration of the whole system fail. All these considerations suggest the introduction of an automatic procedure.

In this paper, we are concerned with aquatic ecosystem models based on the reductionistic and deterministic approach (Platt, Mann and Ulanowicz 1981). This implies that we know the dynamic dependence among the state variables. Consequently, we are able to write a set of ordinary, in general non-linear, differential equations describing the ecological system.

In this framework, the estimation problem can be reduced to the optimal choice of parameters in the equations. The method hereafter considered is the adjoint equation method (Marcos and Payre 1988). This method requires the choice of an objective function to be minimized under the constraints of the model equations. We take as objective function a weighted sum of squares between the observed and measured data. Numerical solution of both the system and the adjoint equations, allows us to obtain an iterative solution of the optimization problem.

In what follows, a brief description of the method is outlined. Then, validation of the procedure and application to a logistic growth model are shown. Furthermore, an extension to a more complex trophic model is also reported.

The adjoint method

The adjoint method is well-known in the literature and is described both in theory and in applications within the framework of optimal control theory (Pontryagin *et al.* 1962, Lee and Markus 1967). For the sake of completeness, a short outline of the method is given here.

We consider a system of N first order differential equations in N variables, $(x_1,...,x_N) \equiv X$, all in normal form.

Moreover, the dynamic dependence of the variables X on M time independent real parameter is known, $(a_1,...,a_M) \equiv A$. This dependence may be non-linear and takes the form

$$\dot{x}_i = f_i (X,A,t), \; i=1,...,N.$$

This permits us to describe the dynamical evolution of the system with the following matrix equation:

$$\dot{X} = F(X,A,t),$$

where $(f_1,...,f_N) \equiv F$. The initial condition $X(t=0)$ determines a solution $X(A, t)$ dependent on time and on the values attributed to the parameter set.

The problem that we face at this point consists in determining the parameters A that minimize the weighted square deviation

$$J \equiv \sum_{t=0}^{T} Q \, [X(A,t) - X_D(t)]^2.$$

With X_D we denote the values of the observations, sampled over time interval (0,T). Q is a symmetric matrix that differently weights the observations in the objective J.

The adjoint equation method consists in introducing, aside to the given system of differential equation, N equations that regulate the time evolution of the Lagrange multipliers in the X adjoint space. These supplementary equations are used to calculate the gradient of the objective.

Defining the adjoint state vector with $(\lambda_1,...\lambda_N) \equiv \Lambda$, the equation that regulates their temporal equation is

$$\dot{\Lambda} = -2Q(X(A,t) - X_D(t)) - \Lambda \cdot \nabla_X F \ .$$

This system must satisfy the condition $\Lambda(T)=0$, at the limit of the integration interval. This holds because of the transversality condition applied to the extreme T of the interval time (Lee and Markus 1967).

The next step is to determine the gradient $\nabla_A J$ that permits us to calculate the new value of the parameters with the steepest descent approach:

$$A^{(k+1)} = A^{(k)} - S^{(k)} = A^{(k)} - \tau \nabla_A J.$$

The gradient is completely bound to the solution of the original system X and to that of the adjoint equations Λ by the expression

$$\nabla_A J = \int_0^T \Lambda \cdot \nabla_A F dt.$$

For example, in the case of the simple equation

$$\frac{dx}{dt} = ax,$$

the adjoint equation is

$$\dot{\lambda} = -2Q(x-x_D) - a\lambda.$$

Using this result and the gradient expression, the new value of the parameter at step k+1 becomes

$$a^{(k+1)} = a^{(k)} - \tau G(a^{(k)}) = a^{(k)} - \tau \int_0^T \lambda x dt.$$

To assure the convergence and stability of the steepest descent method, an accurate choice of the step τ with which we scale the gradient in successive approximations is very important. In fact, considering too small a value gives a slow convergence, while a large value can produce divergence of the method (Papageorgiou 1983).

Applications to the logistic growth model

Let us consider the case of the logistic model. If we define x as the biomass of the species under study, we have the following equation for the growth rate:

$$\dot{x} = r(x - kx).$$

The analytical solution of this equation is

$$x(t) = \frac{k}{1 - Ae^{-rt}} \ ,$$

where A is related to the initial condition $x(0)=x_0$ by the relation

$$A = \frac{x_0 - k}{x_0} \ .$$

Validation of the algorithm was done on synthetic logistic data both due to the nonlinearity involved in its equation and for comparison with other non-analytical methods.

The problem of fitting the two parameters r and k to synthetic and real data is tackled here with the adjoint equation method. Introducing the Lagrange multiplier λ, we obtain the adjoint equation

$$\dot{\lambda} = -(r - 2kx)\lambda - 2Q(x - x_D).$$

Here x_D are measured data, Q is a weighting function dependent on the data; while for synthetic data, Q is chosen equal to the identity matrix.

In Fig. 1 the decrement of the objective function versus the iteration number is shown. The objective is here the sum of squared deviations. The number of discretized points is 100 under a logistic curve with parameters r=1.0 and k=0.2.

Next, we consider the solution of the logistic model with added noise. The noise was increased up to 10% of the signal amplitude. The objective value eventually converges to the final values plotted in Fig. 2 versus the chosen noise.

After validation on synthetic data, we can apply this method to the parameter estimation of a logistic growth curve for macroalgae data collected in the Gulf of Trieste (Zangrandi 1990). To solve this equation on measured data, we must solve three problems:

1. selecting an appropriate initial condition; in fact it is not exactly known because of the error in the measured data;
2. choosing a convenient objective to be minimized;
3. fixing the initial values of the parameters r and k.

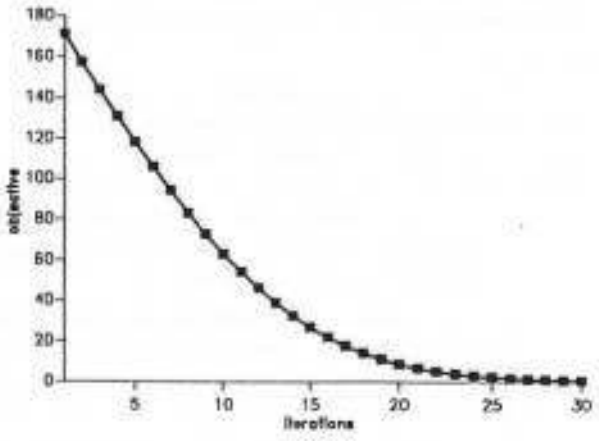

Figure 1. Objective of the logistic iterations.

The first point remains open, because the method is a deterministic one. We chose, as a first approximation, to minimize the objective on curves all originating from the measured point x_0. This seemed good because in a growth curve the experimental error is small at initial times.

The second point was solved by considering the χ^2 objective, always using the data and results of the actual iteration. This is a method for weighting the forecasts in which the experimental errors in the data are also considered. The initial values of the two parameters r and k were chosen close to the estimates obtained with a non-linear estimation.

The results are shown in Figures 3 and 4 for two different sets of eleven data points. The solid line is the logistic model estimated with the conjugate gradient approach previously analyzed, while the asterisks are the measured data. It is interesting to note the differences in the parameter estimation among a non-linear least squares estimator, applied to the known solution of the logistic equation, the steepest descent method with a quadratic objective, and the same with a χ^2 objective.

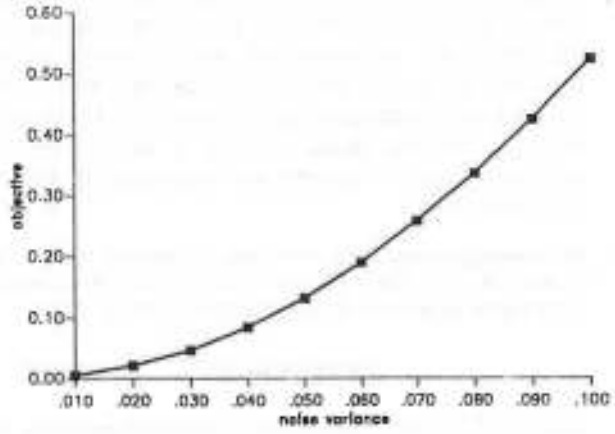

Figure 2. Objective for different noise variances.

Table 1. Parameters and objectives for data in Figure 3.

Method	r	k	obj.
LSE	.110	8.459	
SCG	.128	8.391	0.784
WCG	.139	8.276	3.020

The estimate is better in the second set of data, Fig. 4, where χ^2 is only 1.501, and the parameters are r=0.134 and k=8. 440.

An ecological system

The adjoint method is appropriate in those fields not analyzable with static methods because we do not know the solution of the equations modelling the biological system. This is the usual situation even in the case of simple but important deterministic systems.

Another application was the study of a simple ecological system, taking into account the interactions among the nutrient (N), phytoplankton (P) and zooplankton (Z):

$$\begin{cases} \dot{N} = -\dfrac{NP}{k_N+N} \\ \dot{P} = \dfrac{NP}{k_N+N} - r_P P - \dfrac{PZ}{k_P+P} \\ \dot{Z} = \dfrac{PZ}{k_P+P} - r_Z Z \end{cases}$$

In this case, the four parameters to be estimated are k_N, k_P, r_P, and r_Z.

Denoting the three Lagrange multipliers by λ, μ, ν, and using the sum of squares as objective, we obtain

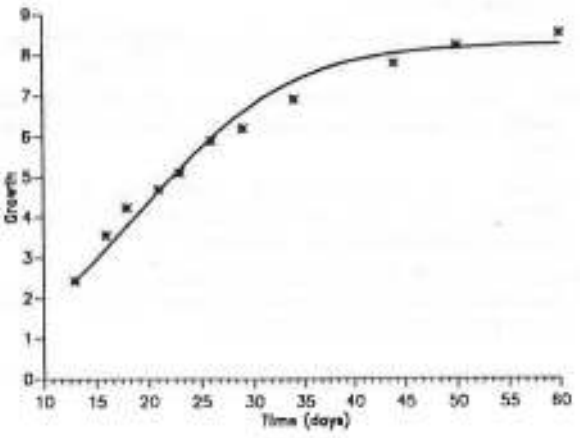

Figure 3. Steepest descent estimation for a logistic model.

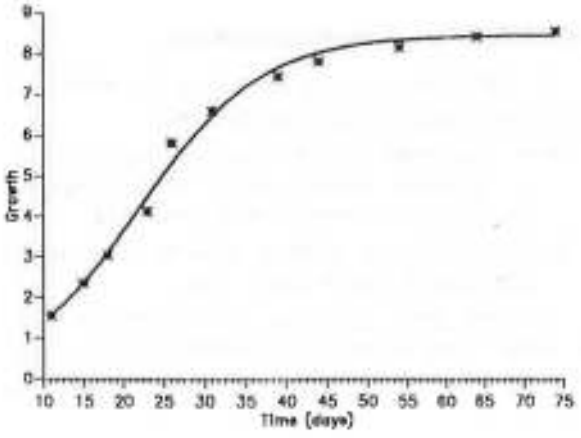

Figure 4. Estimation for a second set of biological data.

the adjoint equations

$$\begin{cases} \dot{\lambda} = -2(N-N_D) + \dfrac{k_N P}{(k_N+N)^2}(\lambda-\mu) \\ \dot{\mu} = -2(P-P_D) + \dfrac{N}{k_N+N}(\lambda-\mu) + \dfrac{Zk_P}{(k_P+P)^2}(\mu-\nu) + r_P\mu \\ \dot{\nu} = -2(Z-Z_D) + \dfrac{P}{k_P+P}(\mu-\nu) - r_Z\nu . \end{cases}$$

where for simplicity Q was made equal to the identity matrix. Considering an interval of time [0,T], we obtain the following components for the gradient:

$$\begin{cases} \dfrac{\partial J}{\partial k_N} = \displaystyle\int_0^T (\lambda-\mu)\frac{NP}{(k_N+N)^2}\,dt \\ \dfrac{\partial J}{\partial k_P} = \displaystyle\int_0^T (\mu-\nu)\frac{ZP}{(k_P+P)^2}\,dt \\ \dfrac{\partial J}{\partial r_P} = \displaystyle\int_0^T \mu P\,dt \\ \dfrac{\partial J}{\partial r_Z} = \displaystyle\int_0^T \nu Z\,dt \end{cases}$$

In Figure 5 are reported the synthetic data corresponding to the parameter choice: $k_N=1.$, $k_P=1.$, $r_P=.05$, $r_Z=.05$.

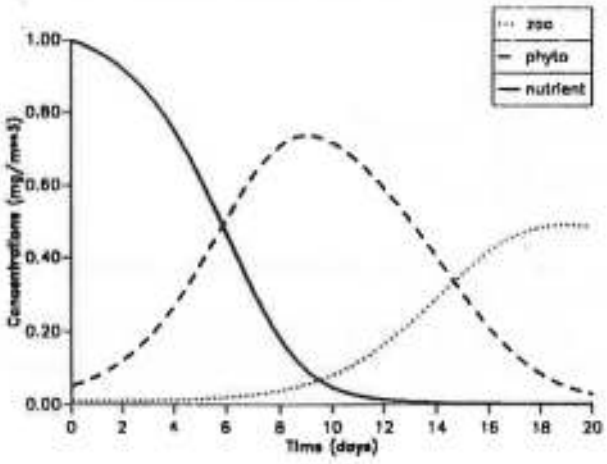

Figure 5. Evolution of the ecological system.

The effectiveness of the method is limited by two factors influencing the convergence time:

1) the determination of the optimal value of r, *i. e.* the gradient scaling, which in a completely automatic procedure must be calculated;
2) the considerable number of steps for attaining convergence when r is very small.

Thus, one great advantage of the method arises only when a long series of data sampled at a common point over a long time period is available, both for the precise estimate of the parameters and the speed of convergence. This is the case of the above synthetic example in which 200 points are considered. To accelerate the convergence rate we resorted to the conjugate gradient method, instead of the steepest descent estimation considered above.

These two optimization paths coincide except for the evaluation of the search direction s. The former method simply equalizes s to the gradient, while the conjugate gradient algorithm at the i^{th} iteration step is

$s^{(i)} = G(a^{(i)}) - [\,G(a^{(i)})s^{(i-1)}]\,/\,G(a^{(i-1)})$.

Using this estimate we obtain at convergence the following values of the parameters: $k_N=.9973$, $k_P=.9991$, $r_P=.0499$, $r_Z=.0500$, starting from the initial values $k_N=1.1$, $k_P=.9$, $r_P=.15$, and $r_Z=.06$.

Future developments

The applications of the method are in principle extensive. On the other hand, it requires a large amount of synoptic data. Our objective is to apply this method to biological data measured in different parts of the Adriatic Sea, so as to obtain a preliminary estimate of the coefficients. To achieve this goal, an extension to a more box model will probably be required. Moreover, the analysis of analogous sets of data in a Lotka-Volterra-like scheme might require a more complex analysis in terms of parameters dependent on known time functions.

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