II. Building of simulation models of ecosystems : non linear interaction parameters estimation

by

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Introduction

An ecosystem is evoluting under the influence of a lot of interacting variables. In order to build the *a posteriori* mathematical model simulating its evolution, some of them are chosen and supposed adequate to give a good gross description of this ecosystem. For these ones, the differential evolution equations are written.

The effect and the control of all the other ones have to be introduced in these equations by the numerical values of the interactions coefficients.

If one assumes a spatial homogeneity and neglects the hydrodynamical effects, the box model may be written as :

$$\dot{X} = F(X,\vartheta,t) \tag{1}$$

with X the state vector and ϑ the parameter vector.

Sometimes, a parameter is expressed by a constant ϑ_i multiplied by a given time fonction $Y_i(t)$. It reproduces the excitating effects of the outside ecosystems from which the considered ecosystem is demarked. So, (1) may be rewritten as

This method has the advantage to require as many minimizations and integrations as there are equations in the system (2) and thus to reduce the CPU time. Its main disadvantage is the effect of accumulation — during the integration — of systematic errors of the derivation.

2.2.- The maximum likelihood method

Using the statistical theory of the estimation Bard (1967) built another finer method of evaluating the parameters.

The error

$$u_{i,k}(\vartheta) = X_i(\vartheta, t_k) - \tilde{X}_i(t_k)$$

may be considered as a random variable distributed following a function of probability density $p[u_{i,k}(\vartheta), \varphi]$ with a known form. The statistical parameters φ are fixed from the classical hypothesis of the statistical behaviour of the error : zero mean, no correlation and covariance matrix estimated by

$$V = V(i,j) = \frac{1}{u} \sum_k u_{i,k} u_{j,k}.$$

The maximum likelihood principle is to maximize the object function

$$G_3(\vartheta, \varphi) = \ln \prod_{i,k} p(u_{i,k}, \varphi) \quad . \tag{5}$$

This maximization obtained by the method given in appendix requires the computation of $\frac{\partial G_3}{\partial \vartheta_a}$; thus the one of $\frac{\partial X_i}{\partial \vartheta_a}$.

This one is obtained by integrating the system of the sensitivity equations of the state variables with regard to the parameters :

$$\frac{\partial}{\partial \vartheta_a} \dot{X}_i = \left(\frac{\partial \dot{X}_i}{\partial \vartheta_a}\right) = \frac{\partial F_i}{\partial \vartheta_a} + \sum_j \frac{\partial F_i}{\partial X_j} \frac{\partial X_j}{\partial \vartheta_a} \tag{6}$$

In the maximization processus, the two systems (2) and (6) have to be integrated for every iteration of the ϑ value. The advantage of this method is to make an optimization of a statistically significant function of the state variables themselves (and not of their derivatives). Its disadvantage is obviously an important increase of the CPU time.

So, the adopted strategy is firstly to use the gradient method for a gross estimation of the parameters and then to use these values as the initial values for the maximum likelihood method.

3.- Theoretical application

These two methods were tested with a theoretical model containing the same analytical interaction forms that the previously mentioned ones.

Suppose the system :

$$\dot{X}_1 = \exp(0.1\ Y_1)\ \left[\frac{\vartheta_1\ X_3}{\vartheta_2 + X_2} - \frac{\vartheta_1\ X_2}{\vartheta_3 + X_1}\right] \tag{7a}$$

$$\dot{X}_2 = \vartheta_4\ X_3 + \vartheta_5\ \left[\frac{X_1\ X_3}{\vartheta_6 + X_3} - X_2\ Y_1\right] \tag{7b}$$

$$\dot{X}_3 = \vartheta_7 + \vartheta_8\ [X_1\ X_2 - \vartheta_9\ X_2\ X_3]\ Y_2 \tag{7c}$$

with $X = (X_1, X_2, X_3)$ the state vector, $\vartheta = (\vartheta_1, \vartheta_2, \ldots, \vartheta_9)$ the parameter vector, $Y = (Y_1, Y_2)$ the excitating vector and $X(0) = (10, 0.5, 2.5)$ the initial conditions.

The system (7) is integrated between $t = 0$ et $t = 100$ and sampled at some $t_k (k = 1, \ldots, 15)$. The parameter vector ϑ is then estimated from the information of the "observed" series $\tilde{X}(t_k)$ and $\tilde{Y}(t_k)$ by the first and second methods. The theoretical, initial and estimated values of the components of ϑ are given in Table 6.16.

The agreement between the re-computed with the estimated parameters values of $X(t)$ and the "observed" ones is excellent and the difference between them is of the order of one percent. The agreement between the theoretical and estimated values of ϑ are good, except for its fourth and fifth components.

It is sure that one optimum is reached. But a same optimum can also be found for a set of parameter vectors ϑ of which every component varies inside a wider range as the system sensitivity with regard to it is weaker.

It is probably the case of ϑ_4 and ϑ_5 (paradoxical furthermore for the first one because its initial value is accidentally its

Table 6.16

Parameters	Theoretical values	Initial values	Estimated values
ϑ_1	1.5	1	1.36
ϑ_2	210	1	192
ϑ_3	120	1	122
ϑ_4	1	1	0.248
ϑ_5	3.3	1	0.81
ϑ_6	555	1	566
ϑ_7	10	1	8.9
ϑ_8	0.005	1	0.003
ϑ_9	1.3	1	1.45

theoretical one !) for which the sensitivity of (7) should be weak near the optimum in the accuracy limits of the used methods.

4.- Practical application

For example, a simple model simulating the evolution of the primary production at a quite representative central point of the Ostend Bassin de Chasse between 22nd April and 29th July 1971 is fitted from the data of fifteen observation days well distributed on this period [Podamo Jo (1971), Pichot (1973)].

Suppose x_1 the primary production (mg N/m^2.day) , x_2 the incident light (J/cm^2.day) , x_3 the water temperature (°C) , x_4 the nutrient concentration (mg N/m^3) , x_5 the phytoplankton biomass (mg N/m^3) .

The primary production is measured *in vitro* in mg C/m^2.h . Using a C/N report equal to 8 and a report between the *in situ* primary production per day and the *in vitro* one per hour equal to 12 as noticed by Podamo Jo (1973), one has

x_1 *in situ* (mg N/m^2.day) = 1.5 x_1 *in vitro* (mg C/m^2.h) .

The phytoplankton biomass is supposed given by its chlorophyl a concentration which is converted in mg N/m^3 by using a C/chlorophyl a report equal to 45 .

The primary production behaves like the product of functions of the incident light, of the water temperature, of the nutrient concentration and of the phytoplankton biomass, *i.e.*

$$x_1 = K_1 \, f_1(x_2) \, f_2(x_3) \, f_3(x_4) \, f_4(x_5) \quad . \tag{8}$$

4.1.- The temperature effect

By extension of the Van 't Hof law, the water temperature is supposed to generate an activity following an exponential relation and to double the production for every 10 °C increase.

So, one chooses :

$$f_2(x_3) = \exp\left(\frac{\ln 2}{10} x_3\right) = \exp(0.07 \, x_3) \quad . \tag{9}$$

4.2.- The incident light effect

Steeman-Nielsen (1960) showed that the primary production depends on the incident light following a Monod relation and the saturation level is usually reached for a lighting of 336 $J/cm^2.d$.

Now the data indicate that the light energy available for the photosynthesis (losses by reflexion and useful fraction of the light spectrum) overtop this level. So it seems that the light does not control the primary production and that (8) becomes :

$$x_1 = K_2 \exp(0.07 \, x_3) \, f_3(x_4) \, f_4(x_5) \quad . \tag{10}$$

4.3.- The nutrient effect

It seems obvious [Sen Gupta (1969)] that the phosphates are in supersaturation and they do not control the phenomenon. Thus one considers as nutrient, the sum of nitrogenous components, *i.e.*

$$x_4 = [NO_2] + [NO_3] + [NH_4] \quad .$$

If for a first approximation, the primary production is supposed to depend linearly on x_5 , the productivity defined by

$$x_6 = \frac{x_1}{\exp(0.07\ x_3)\ x_5}$$

only depends on x_4 . The regression between x_6 and x_4 gives

$$x_6 = -\ 0.00027\ x_4 + 0.28655$$

with $r = 0.4322$.

This negative correlation is hardly significant and only shows up the decrease of the mean stock of the nutrients in function of the development of the production.

If one supposes a Monod relation between x_6 and x_4 , one has

$$x_6 = \frac{a\ x_4}{b + x_4}$$

or, in a linear form

$$\frac{x_4}{x_6} = \frac{1}{a}\ x_4 + \frac{b}{a} .$$

But the correlation between $\frac{x_4}{x_6}$ and x_4 is not at all significant. It could indicate that this relation is not valid here and that the productivity has well reached its saturation level.

So x_4 does not control the productivity; it is comprehensive because the weakest measured concentration is yet fifteen times higher than a half-saturation constant cited by Eppley (1969b) for the natural marine entrophic communities. Equation (10) becomes :

(11) $$x_1 = K_3 \exp(0.07\ x_3)\ f_4(x_5) .$$

4.4.- The phytoplankton biomass effect

A linear relation between the production and the phytoplankton is the clearest because the photosynthesis is directly proportional to the amount of the chlorophyllian pigments.

Nevertheless various tests showed that a quadratic form of x_5 improves the behaviour and reduces the standard error of the simulation. The form fitted by previously described first method is finally the

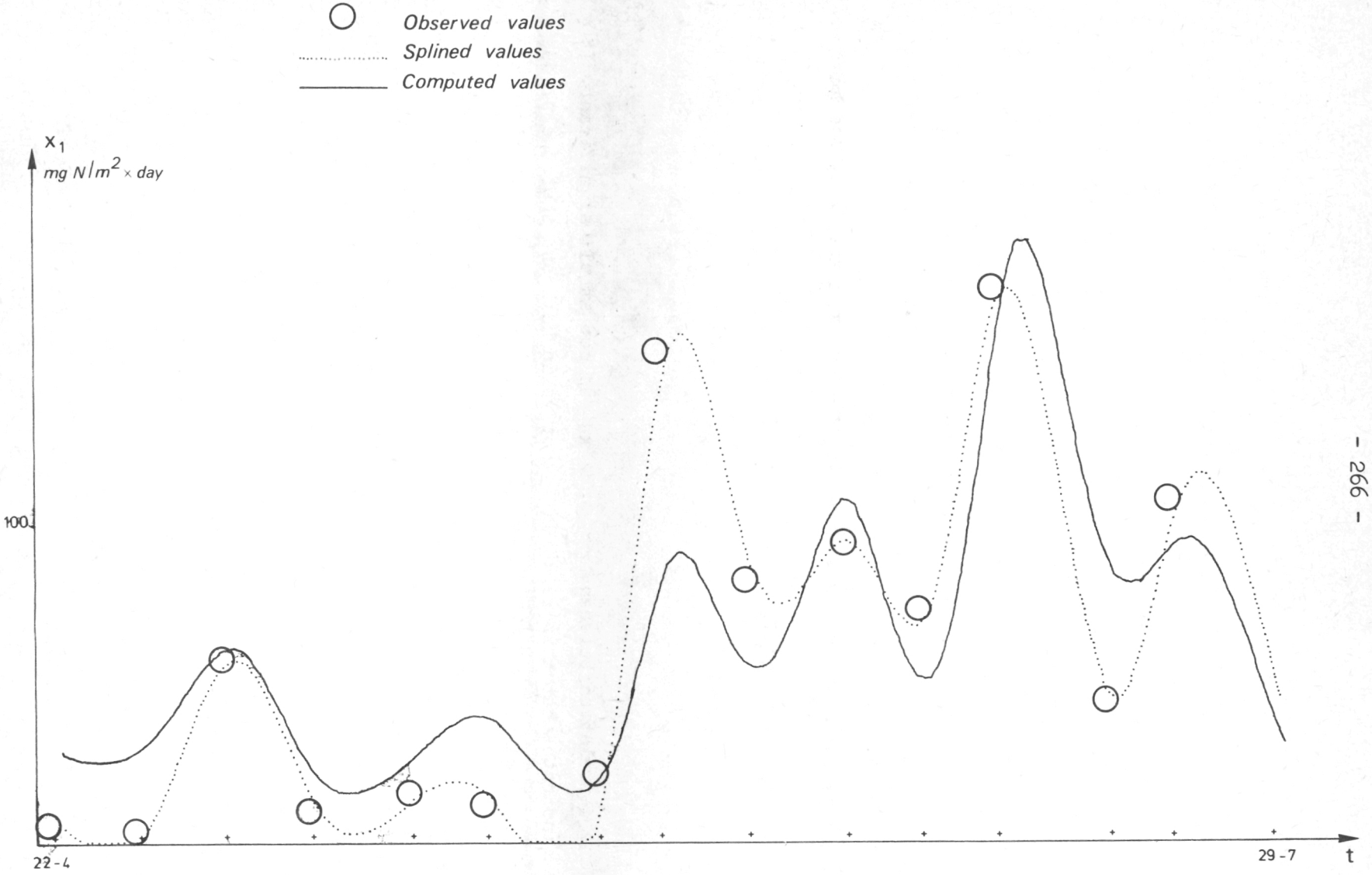


fig. 6.43.- Primary production (Ostend, Bassin de Chasse, 1971).

following one :

$$(12) \qquad x_1 = \exp(0.07\, x_3)\, [0.1028 \times 10^{-2}\, x_5^2 + 0.1338\, x_5] \,.$$

Figure 6.43 gives the curve of the observed (or exactly splined on the observed values) primary production and the one of the computed production. The two curves have the same order of magnitude and present all the same fluctuations.

The proposed model shows that the Bassin de Chasse primary production depends on the water temperature following an exponential law and on the phytoplankton biomass following a quadratic one. In this one, the term x_5^2 non negligeable with regard to the classical linear term perhaps indicates an autocatalytic effect of the primary production. The incident light and the nutrients are indispensable for the primary production, but they are in supersaturation and do not have any influence on this phenomenon.

5.- Conclusions

The present work may be summarized in the following items :

1) It is necessary, in order to build the simulation model of an ecosystem, to find the interactions coefficients from the information provided by the data of that given ecosystem.

2) To this purpose, a gradient method and a maximum likelihood one are proposed. They are connected because the gross parameters given by the first one are used as initial conditions for the second one.

3) A theoretical example shows that these methods properly work but stresses the interest of a sensitivity pre-analysis of the system.

4) The first method is applied for a practical example. In this one, the primary production of the Ostend Bassin de Chasse is given with an exponential function of the water temperature and a quadratic function of the phytoplankton biomass.

6.- Appendix

6.1.- Estimation of the derivatives

The first problem here is to evaluate the derived functions $\dot{\tilde{X}}_i(t_k)$ from $\tilde{X}_i(t_k)$. One cannot use the finite difference formulas because the time intervals between the measures are not generally constant and not small enough to ensure a good accuracy. On the other hand, the spline functions of the interpolation are well adapted to this problem. The spline function of order r which interpolates $\tilde{X}_i(t)$ at the points t_k is the unic function $S_i^r(t)$ defined by :

1) $S_i^r(t)$ is a polynomial of order $2r - 1$ for t between (t_k, t_{k+1}) with $k = 0,\ldots,\ell-1$.

2) $S_i^r(t)$ is a polynomial of order $r - 1$ out of (t_0, t_ℓ) .

3) The derivatives $S_i^{r(s)}(t)$ are continuous for $s = 2r - 2$.

4) $S_i^r(t_k) = \tilde{X}(t_k)$.

The third condition involves that the successive polynomials are connected at t_k and also the derivatives up to the order $2r - 2$. A discontinuity may occur in t_k only for the derivatives of order $2r - 1$.

Another interesting property of the spline function of interpolation is to minimize

$$\ell_r(f) = \int_0^{t_k} [f^{(r)}(t)]^2 \, dt \ .$$

In the case $r = 2$, this will ensure the $S_i^r(t)$ functions to pass through the t_k points and to be as smooth as possible.

For the building of this function, Laurent (1972) proposes the "transport of relations" method which ensures very good results. This general method (for any r and ℓ) avoids the difficulties of the classical method of decomposition in basic polynomials and only requires to solve ℓ linear systems of order $2r$.

6.2.- Minimization

Using the first three terms of the Taylor expression of the function $G_2(\vartheta)$ in a neighbourhood of the minimum ϑ^* , one gets immediately :

(13) $$\vartheta^* = \vartheta - G^{-1}(\vartheta^*)\, g(\vartheta)$$

with G the Hessian of G_2 with regard to ϑ

$$g = \text{grad}_\vartheta\, G_2$$

and the necessary condition that G is positive definite to ensure $G(\vartheta^*)$ minimum. One get the iterative process :

$$\vartheta_{i+1} = \vartheta_i - h_i\, H_i\, g_i$$

with $$g_i = g(\vartheta_i)\ ,$$

H_i the approximation of $G^{-1}(\vartheta^*)$, h_i the stepsize in the $H_i\, g_i$ direction.

Choice of the direction

In the Newton method $H_i = G^{-1}(\vartheta_i)$. It assures $G(\vartheta_i)$ to be positive definite but it is not always verified, except if ϑ_0 is chosen in a very close neighbourhood of ϑ^* . In the case of problems with which one deals here, the parameters initial guesses may be far from the minimum and this method fails.

In the Davidson Fletcher Powel method (1963), this necessary condition is satisfied by a matrix serie H_i . It is positive definite, computed from any initial H_0 and converging to $G^{-1}(\vartheta^*)$. H_i becomes H_{i+1} by

$$H_{i+1} = H_i + A_i + B_i$$

where A_i and B_i are matrices computed from H_i , g_i , H_i^T and g_i^T such as A_i assures the convergence of H_{i+1} to $G^{-1}(\vartheta^*)$ and B_i makes H_{i+1} definite positive. In the case of a quadratic function G_2 , the convergence occurs in n interactions, n being the dimension of ϑ .

Choice of the stepsize

When the direction $H_i\, g_i$ is chosen, one has to define a distance on this direction where the minimum occurs. The stepsize is roughly evaluated by a finite difference formula :

$$s = 2 \frac{Y_{est} - Y(0)}{Y'(0)}$$

with $Y(h) = G_2(\vartheta_i - h\, H_i\, g_i)$

and Y_{est} a given estimation of the minimum of G_2 .

If $s > 1$, it is set equal to 1 to agree with (13). Y and Y' are computed at points s , $2s$, $4s$, ... , s_1 , s_2 . When $Y'(s_2) = 0$ or $Y(s_2) > Y(s_1)$, the minimum s_3 is found by a cubic interpolation between $[Y(s_1),Y'(s_1)]$ and $[Y(s_2),Y'(s_2)]$. This procedure is repeated until a good accuracy is reached.

One assumes there is no local minimum in the $H_i\, g_i$ direction if

$$s_2\left(\sum_{i=1}^{n} |H_i\, g_i|\right) > 10^{10} .$$

6.3.- Integration (Extrapolation method)

In order to integrate a differential system $y' = f(x,y)$ with initial value $y_0 = y(x_0)$, the classical method is to divide $[x_0,x]$ by a stepsize h and to use one of the finite difference formulas (for instance the midpoint rule) to compute the approximation $T(h,x)$ of the integral $y(x)$. The accuracy is a function of h and $T(h,x)$ converges to the solution $y(x)$ when h tends to zero.

In the extrapolation method, some approximations $T(h_i,x)$ are computed and the true solution $T(0,x)$ is extrapolated from these values.

Burlisch and Stoer (1966) proposes a rational extrapolation

$$\hat{T}_m^i(h) = \frac{p_0^i + p_1^i h^2 + \ldots + p_r^i h^{2r}}{q_0^i + q_1^i h^2 + \ldots + q_v^i h^{2v}}$$

with $r = \frac{m}{2}$

$v = m - 2$

$\hat{T}_m^i(h_k) = T(h_k,x)$ $\qquad k = i,i+1,\ldots,i+m$

$h_k = \frac{h_0}{2k}$, strictly decreasing sequence.

The coefficient p^i is not computed but the extrapolated values $T_m^i = \hat{T}_m^i(0)$ are computed by a recurrent process starting with

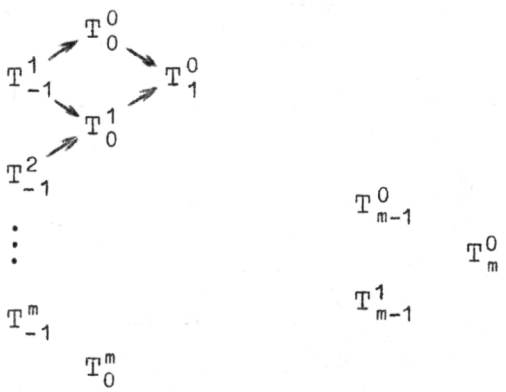
$$T_{-1}^i = 0$$

$$T_0^i = T(h_i, x)$$

$$\vdots$$

$$T_k^i = T_{k-1}^{i+1} + \frac{T_{k-1}^{i+1} - T_{k-1}^i}{(\frac{h_i}{h_{i+k}})^2 \left[1 - \frac{T_{k-1}^{i+1} - T_{k-1}^i}{T_{k-1}^{i+1} - T_{k-2}^{i+1}}\right]}$$

This scheme gives a rhombus rule illustrated by the following tableau



The initial stepsize and the wanted accuracy EPS are given at the beginning of the computation. This one runs for $m = 1,2,\ldots$ until $|T_m^0 - T_{m-1}^0| < \text{EPS}$. m is bounded by 20 to avoid a too large CPU time.

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