ON IDENTIFICATION OF DYNAMICAL SYSTEM PARAMETERS FROM EXPERIMENTAL DATA

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Abstract. *In this paper we present a new method of numerical evaluation of unknown coefficients of a dynamical system having available information about unknown phase trajectories at some time values. The method consists in the direct integration of given dynamical system with posterior application of a quadrature rules. Using the least square method and possible Constraints we obtain a linear system for determining an unknown coefficient. A numerical example illustrates the method.*

INTRODUCTION

The problem of determination of dynamical systems coefficients from experimental data is solved for a practically important case of the linear systems with respect to their unknown coefficients . The problem often occurs in interpretation of experimental data in mathematical biology, ecology, medicine, chemical kinetics, economy etc. One of the first example of such problems (the predator-prey equations) consists of a pair of first order, non-linear differential equations frequently used to describe the dynamics of biological systems in which two species interact. They were proposed independently by Alfred J. Lotka [1] and Vito Volterra in 1926 [2]. This system can be written in the form

$$x_1'(t) = x_1 \left(a_{11} - a_{12} x_2\right)$$
$$x_2'(t) = x_2 \left(\eta a_{12} x_1 - a_{22}\right)$$

When solved for x_1 and x_2 the above system of equations yields

$$x_1 = 0, \; x_1 = 0$$

and

$$x_1 = \frac{a_{22}}{\eta a_{12}},\ x_1 = \frac{a_{11}}{a_{12}}$$

hence there are two equilibria.

The solution in the neighborhood of the first (saddle) fixed point does not have any essential physical meaning. The second (center) fixed point represents neighbourhood at which both populations uphold their current, non-zero numbers. The level of population at which this equilibrium is achieved depends on the chosen values of the parameters $a_{11}, a_{12}, a_{22}, \eta$. The value of these parameters are, generally speaking, unknown and determining of its values is confronted with serious difficulties. In general case the structure of interactions between species in the dynamical system proceeds from a real physical problem and is supposed to be known.

The method of finding the unknown parameters is based on integration of both parts of equations of the dynamical system and on applying regression methods to the obtained overdetermined system of linear algebraic equations with constraints. The least squares method is used for solution of this problem. An example of a classical model predator- prey is considered.

The proposed method could be used for approximate determination of the dynamical system parameters. The method can be easily generalized for systems with non-linear dependence on coefficients, for example for systems [3] which describe a deterministic mathematical model for the transmission dynamics of HIV infection in the presence of a preventive vaccine.

EVALUATION OF COEFFICIENTS

Let $\mathbf{x}\,(t) = (x_1(t), x_2(t), ..., x_m(t))^\intercal$ be a vector in $\mathbb{R}^m$ depending on variable t where $x_k(t) : [t_0, t_N] \to \mathbb{R}$ and $\mathbf{f}(t, \mathbf{x}(t)) = (f_1(t, \mathbf{x}), f_2(t, \mathbf{x}), ..., f_n(t, \mathbf{x}))^\intercal$ a vector in $\mathbb{R}^n$ where $f_j(t, \mathbf{x}) : [t_0, t_N] \times \mathbb{R}^m \to \mathbb{R}$

Consider a dynamical system

$$x_k'(t) = \sum_{j=1}^{n} a_{k,j} f_j(t, \mathbf{x}\,(t)),\ (k = 1, 2, ..., m) \tag{1}$$

or, in the matrix form

$$\mathbf{x}'\,(t) = \mathbb{A}\mathbf{f}(t, \mathbf{x}(t)) \tag{1$'$}$$

with initial conditions

$$\mathbf{x}\,(t_0) = \mathbf{x}_0 = (x_{1,0}, x_{20}, ..., x_{m,0}\,)^\intercal\ . \tag{2}$$

The entries a_{jk} of matrix $\mathbb{A}$ are unknown but we suppose that there is information about values of functions $x_k(t)$ at some points $t_j = t_0 + jh_j$. It may be, for example, some statistical data of the form

t_0	t_1	$\cdots$	t_i	$\cdots$	t_M
$x_k(t_0) = x_{k,0}$	$x_k(t_1) = x_{k,1}$	$\cdots$	$x_k(t_i) = x_{k,i}$	$\cdots$	$x_k(t_N) = x_{k,M}$

,

where $(k = 1, 2, ..., m)$. For the sake of simplicity we suppose that $h_j = h$ is a constant.

We suppose that system (1) – (3) has on interval $[t_0, t_N]$ a unique solution. Moreover, we suppose that the mapping $F_j : [t_0, t_N] \to \mathbb{R}$ where $F_j(t) = f_j(t, \mathbf{x}(t))$ is bounded and has a bounded second derivative with respect to t on the interval $[t_0, t_N]$, that is for all j there exist constants C such that $\left|F_j''(t)\right| \le C$ and $|F_j(t)| \le C$ for all $t \in [t_0, t_N]$.

To avoid further use of triple subscripts we introduce the following notations using the columns of the transpose

$$\mathbb{A}^{\mathsf{T}} = \begin{pmatrix} a_{1,1} & a_{2,1} & \vdots & a_{m,1} \\ a_{1,2} & a_{2,2} & \vdots & a_{m,2} \\ \cdots & \cdots & \ddots & \cdots \\ a_{1,n} & a_{2,n} & \vdots & a_{m,n} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\alpha}_1 & \boldsymbol{\alpha}_2 & \cdots & \boldsymbol{\alpha}_n \end{pmatrix}$$

of matrix $\mathbb{A}$, that is we introduce vectors $\boldsymbol{\alpha}_k = \begin{pmatrix} a_{k,1} & a_{k,2} & \cdots & a_{k,n} \end{pmatrix}^{\mathsf{T}} \overset{def}{=} \begin{pmatrix} \alpha_{n(k-1)+1} & \alpha_{n(k-1)+2} & \cdots & \alpha_{kn} \end{pmatrix}^{\mathsf{T}}$, $(k = 1, 2, ..., m)$ and also we denote by $\boldsymbol{\alpha}$ the $N \times 1$ column $\boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_m \end{pmatrix}^{\mathsf{T}}$ where $N = mn$.

Now system (1) can be rewritten in the form

$$x_k'(t) = (\boldsymbol{\alpha}_k, \mathbf{f}(t, \mathbf{x}(t)) = \sum_{j=1}^{n} \alpha_{(k-1)n+j} f_j(t, \mathbf{x}), \quad (\ k = 1, 2, ..., m) \tag{3}$$

Integration with respect to t from t_0 to t_i, $(i = 1, 2, ..., M)$ gives

$$\int_{t_0}^{t_i} x_k'(t)dt = \sum_{j=1}^{n} \alpha_{(k-1)n+j} \int_{t_0}^{t_i} f_j(t, \mathbf{x})dt. \tag{4}$$

The left hand side of (5) after integration can be written as

$$\int_{t_0}^{t_i} x_k'(t)dt = x_k(t_i) - x_k(t_0) = x_{k,i} - x_{k,0} \overset{def}{=} \Delta_{k,i}. \tag{5}$$

We evaluate the integrals in the right hand side of (4) using a quadrature rule, for example the adaptive trapezoidal rule in the form

$$\int_{t_0}^{t_i} f_j(t, \mathbf{x}(t))dt = T_i(f_j) \overset{def}{=} q_{i,j}. \tag{6}$$

We denote here

$$q_{i,j} \overset{def}{=} I_i(f_j) + R_i(f_j) \overset{def}{=} I_{i,j} + R_{ij} \tag{7}$$

where

$$I_{i,j} = \frac{h}{2}\sum_{l=1}^{i}\left[f_j(t,\mathbf{x}\,(t_l)) + f_j(t,\mathbf{x}\,(t_{l-1}))\right] \tag{8}$$

and the error functional $R_i\,(f_j)$ can be evaluated by

$$|R_{ij}| \leq \frac{1}{12}C(t_N - t_0)h^2. \tag{9}$$

Thus, we obtain the following, generally speaking, overdetermined system for finding the unknown numbers $\alpha_1, ...\alpha_N$:

$$\sum_{j=1}^{n}\alpha_{(k-1)n+j}q_{ij} - \Delta_{ki} = 0, \quad k = 1,2,...,m;\; i = 1.2,...,N \tag{10}$$

In many cases the numbers $\alpha_1, ...\alpha_N$ satisfy certain Constraints. Frequently these Constraints are linear. We limit ourselves to this case. Thus system (10) must be resolved providing that the following Constraints are satisfied:

$$\sum_{j=1}^{N} c_{i,j}\alpha_j = b_i, \tag{11}$$

and system (11) in matrix form can be written as

$$\mathbb{C}\boldsymbol{\alpha} = \mathbf{b} \tag{12}$$

where $\mathbb{C}$ is an $N_1 \times N$ matrix and $N_1 \leq mn$:

$$\mathbb{C} = \begin{pmatrix} c_{1,1} & c_{1,2} & \cdots & c_{1,N} \\ c_{2,1} & c_{2,2} & \cdots & c_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ c_{N_1,1} & c_{N_1,2} & \cdots & c_{N_1,N} \end{pmatrix}$$

.

The values of entries of $\mathbb{A}$ can be found using method of least squares by minimization of the functional

$$L = \frac{1}{2}\sum_{i=1}^{M}\sum_{k=1}^{m}\left[\sum_{j=1}^{n}\alpha_{(k-1)n+j}q_{i,j} - \Delta_{k,i}\right]^2 - \sum_{i=1}^{N_1}\lambda_i\left[b_i - \sum_{j=1}^{N}c_{i,j}\alpha_j\right] \tag{13}$$

To minimize functional F we write all M equations

$$\frac{\partial L}{\partial \alpha_1} = 0, ..., \frac{\partial L}{\partial \alpha_M} = 0.$$

This is equivalent to the system

$$\boxed{\begin{array}{l}\sum_{j=1}^{n}\alpha_{(k-1)n+j}\left(\sum_{i=1}^{N}q_{i,j}q_{i,l}\right)+\sum_{i=1}^{N_1}\lambda_i c_{i,(k-1)n+l}=\sum_{i=1}^{M}\Delta_{k,i}q_{i,l},\\ \left(l=1,2,...,n\right),\left(k=1,...,m\right)\end{array}} \tag{14}$$

and we have to solve this system provided that (11) is satisfied.

Introducing the notations

$$\sum_{i=1}^{M}q_{i,j}q_{i,l}=T_{j,l};\ \sum_{i=1}^{M}\Delta_{k,i}q_{i,l}\ =p_{k,l} \tag{15}$$

we obtain the system

$$\boxed{\sum_{j=1}^{n}T_{j,l}\alpha_{(k-1)n+j}+\sum_{i=1}^{M_1}\lambda_i c_{i,(k-1)n+l}=p_{k,l}\qquad \left(\ l=1,2,...,n\right),\left(k=1,...,m\right)} \tag{16}$$

This system together with Constraints can be written in the following matrix form:

$$\boxed{\begin{pmatrix}\mathbb{T}&0&0&0&\mathbb{C}_1\\0&\mathbb{T}&0&0&\mathbb{C}_2\\\vdots&\vdots&\ddots&\vdots&\vdots\\0&0&0&\mathbb{T}&\mathbb{C}_m\\\mathbb{C}_1^{\intercal}&\mathbb{C}_2^{\intercal}&\cdots&\mathbb{C}_m^{\intercal}&0\end{pmatrix}\begin{pmatrix}\boldsymbol{\alpha}_1\\\boldsymbol{\alpha}_1\\\vdots\\\boldsymbol{\alpha}_m\\\boldsymbol{\lambda}\end{pmatrix}=\begin{pmatrix}\mathbf{p}_1\\\mathbf{p}_2\\\vdots\\\mathbf{p}_m\\\mathbf{b}\end{pmatrix}} \tag{17}$$

where

$$\mathbb{T}=\begin{pmatrix}T_{1,1}&T_{2,1}&\cdots&T_{n,1}\\T_{1,2}&T_{2,2}&\cdots&T_{n,2}\\\vdots&\vdots&\ddots&\vdots\\T_{1,n}&T_{2,n}&\cdots&T_{n,n}\end{pmatrix}; \tag{18}$$

is an $n\times n-$ matrix. The matrix $\mathbb{C}_1$ is the $n\times N_1$ matrix consisting of first n rows of $\mathbb{C}^{\intercal}$, analogously, $\mathbb{C}_2$ consists of next n rows of $\mathbb{C}^{\intercal}$ etc. so that

$$\mathbb{C}=\begin{pmatrix}\mathbb{C}_1^{\intercal}&\mathbb{C}_2^{\intercal}&\cdots&\mathbb{C}_m^{\intercal}\end{pmatrix}.$$

$$\boldsymbol{\lambda}=\begin{pmatrix}\lambda_1&\lambda_2&\cdots&\lambda_{N_1}\end{pmatrix}^{\intercal};\ \mathbf{p}_1=\begin{pmatrix}p_{11}&p_{12}&\cdots&p_{1n}\end{pmatrix}^{\intercal};...;$$
$$\mathbf{p}_m=\begin{pmatrix}p_{m,1}&p_{m,2}&\cdots&p_{m,n}\end{pmatrix}^{\intercal};\mathbf{b}=\begin{pmatrix}b_1&b_2&\cdots&b_{N_1}\end{pmatrix}^{\intercal}.$$

Relations (16) are exact. The idea of our method is to replace of $T_{j,l}$ with $I_{i,j}=\dfrac{h}{2}\sum_{l=1}^{i}\left[f_j(t,\mathbf{x}\left(t_l\right))+f_j(t,\mathbf{x}\left(t_{l-1}\right))\right]$. It is possible to prove that the error after this replacement will be of order h meaning that it will be small if h is small.

Remark 1. If the assumption of boundedness of F'' is replaced by assumption that F is Lipschitzian or is continuous with bounded variation then inequality (9) must be replaced by $|R_{ij}| \leq C(t_N - t_0)h$ (see for example [4]) and in this case we can not guarantee that the error will be small.

In what follows, we suppose that $q_{i,j}$ defined by (7) is replaced with

$$r_{i,j} = I_i(f_j)$$

(defined by (8)) and $p_{k,l}$ is replaced by $s_{k,l} = \sum_{i=1}^{M} \Delta_{k,i} r_{i,l}$. At the same time we have to replace $T_{j,l}$ by $I_{j,l} = \sum_{i=1}^{N} r_{i,j} r_{i,l}$. Thus our system can be written in the following form:

$$\boxed{\begin{pmatrix} \mathbb{I} & 0 & 0 & 0 & \mathbb{C}_1 \\ 0 & \mathbb{I} & 0 & 0 & \mathbb{C}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \mathbb{I} & \mathbb{C}_m \\ \mathbb{C}_1^{\intercal} & \mathbb{C}_2^{\intercal} & \cdots & \mathbb{C}_m^{\intercal} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_1 \\ \vdots \\ \boldsymbol{\alpha}_m \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \\ \vdots \\ \mathbf{s}_m \\ \mathbf{b} \end{pmatrix}} \tag{19}$$

where

$$\mathbb{I} = \begin{pmatrix} I_{1,1} & I_{2,1} & \cdots & I_{n,1} \\ I_{1,2} & I_{2,2} & \cdots & I_{n,2} \\ \vdots & \vdots & \ddots & \vdots \\ I_{1,n} & I_{2,n} & \cdots & I_{n,n} \end{pmatrix}; \tag{20}$$

is an $n \times n-$ matrix and

$$\mathbf{s}_1 = \begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1n} \end{pmatrix}^{\intercal}; \quad ...; \mathbf{s}_m = \begin{pmatrix} s_{m,1} & s_{m,2} & \cdots & s_{m,n} \end{pmatrix}^{\intercal};$$

.

EXAMPLE (Predator-Prey Model)

$$\left.\begin{array}{r} x_1'(t) = a_{11}x_1(t) - a_{12}x_1(t)x_2(t) + 0x_2 \\ x_2'(t) = 0x_1 + \eta a_{12}x_1(t)x_2(t) - a_{22}x_2(t) \end{array}\right\} \tag{21}$$

Here $m = 2, n = 3$ and according to our notations

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \ \mathbf{f} = \begin{pmatrix} x_1 \\ x_1x_2 \\ x_2 \end{pmatrix}; \ \mathbb{A} = \begin{pmatrix} a_{11} & -a_{12} & 0 \\ 0 & \eta a_{12} & -a_{22} \end{pmatrix};$$

$$\mathbb{A}^{\intercal} = \begin{pmatrix} a_{11} & 0 \\ -a_{12} & \eta a_{12} \\ 0 & -a_{22} \end{pmatrix};$$

$$\boldsymbol{\alpha}_1 = \begin{pmatrix} a_{11} \\ -a_{12} \\ 0 \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix};\ \boldsymbol{\alpha}_2 = \begin{pmatrix} 0 \\ \eta a_{12} \\ -a_{22} \end{pmatrix} = \begin{pmatrix} \alpha_4 \\ \alpha_5 \\ \alpha_6 \end{pmatrix}; \boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_2 \end{pmatrix}$$

Constraints ($\mathbb{C}\boldsymbol{\alpha} = \mathbf{b}$) can be written as

$$\eta\alpha_2 + \alpha_5 = 0,\ \ \alpha_3 = 0,\ \ \alpha_4 = 0$$

In matrix form

$$\begin{pmatrix} 0 & \eta & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_2 \end{pmatrix} = \begin{pmatrix} \alpha_5 + \eta\alpha_2 \\ \alpha_4 \\ \alpha_3 \end{pmatrix} = \mathbf{0}$$

Thus,

$$\mathbb{C}^{\intercal} = \begin{pmatrix} 0 & 0 & 0 \\ \eta & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \mathbb{C}_1 = \begin{pmatrix} 0 & 0 & 0 \\ \eta & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ \ \mathbb{C}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and to find $\boldsymbol{\alpha}$ we must solve the system

$$\begin{pmatrix} \mathbb{I} & 0 & \mathbb{C}_1 \\ 0 & \mathbb{I} & \mathbb{C}_2 \\ \mathbb{C}_1^{\intercal} & \mathbb{C}_2^{\intercal} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_2 \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \\ \mathbf{0} \end{pmatrix}$$

where

$$\mathbf{s}_1 \begin{pmatrix} \sum_{i=1}^{M} (x_{1,i} - x_{1,0})\, I_i(f_1) \\ \sum_{i=1}^{M} (x_{1,i} - x_{1,0})\, I_i(f_2) \\ \sum_{i=1}^{M} (x_{1,i} - x_{1,0})\, I_i(f_3) \end{pmatrix};\ \mathbf{s}_2 = \begin{pmatrix} \sum_{i=1}^{M} (x_{2,i} - x_{2,0})\, I_i(f_1) \\ \sum_{i=1}^{M} (x_{2,i} - x_{2,0})\, I_i(f_2) \\ \sum_{i=1}^{M} (x_{2,i} - x_{2,0})\, I_i(f_3) \end{pmatrix}$$

$$\mathbb{I} = \begin{pmatrix} \sum_{i=1}^{M} I_i^2(f_1) & \sum_{i=1}^{M} I_i(f_2)I_i(f_1) & \sum_{i=1}^{M} I_i(f_3)I_i(f_1) \\ \sum_{i=1}^{M} I_i(f_1)I_i(f_2) & \sum_{i=1}^{M} I_i^2(f_2) & \sum_{i=1}^{M} I_i(f_3)I_i(f_2) \\ \sum_{i=1}^{M} I_i(f_1)I_i(f_3) & \sum_{i=1}^{M} I_i(f_2)I_i(f_3) & \sum_{i=1}^{M} I_i^2(f_2) \end{pmatrix}$$

and

$$
\begin{aligned}
I_i(f_1) &= \frac{h}{2}\sum_{l=1}^{i}\left(x_{1,l}+x_{1,l-1}\right), \; I_i(f_2) = \frac{h}{2}\sum_{l=1}^{i}\left(x_{1,l}x_{2,l}+x_{1,l-1}x_{2,l-1}\right), \\
I_i(f_3) &= \frac{h}{2}\sum_{l=1}^{i}\left(x_{21,l}+x_{2,l-1}\right)
\end{aligned}
$$

Numerical realization was accomplished using MathCad13.

Let us generate 120 points of solution of the system (21) with the coefficients $a_{11} = 1.8, a_{12} = 0.25, a_{22} = 0.7, \eta = 0.1$ $(a_{21} = 0.025)$ by means of direct solution of the initial value problem with $x(0) = 100,\ y(0) = 10$ by the Runge-Kutta method. These points are considered further as "experimental data".

Application of the proposed method gives us the following set of estimated parameters: $\widetilde{a}_{11} = 1.839,\ \widetilde{a}_{12} = 0.256,\ \widetilde{a}_{21} = 0.026,\ \widetilde{a}_{22} = 0.715$. We see that the values of coefficients are close enough to original values.

Further, the initial value problem was solved with the new coefficients and old initial conditions. Comparison of the "experimental Data" with the estimated solutions are presented in figures 1 and 2. One can see that the estimated values of predators and preys are close enough to the original "experimental data". Divergence of the graphs is stipulated by the errors of the trapezoidal rule used at the stage of numerical integration. Application of the quadrature formulae of higher orders allows to achieve more accurate results.

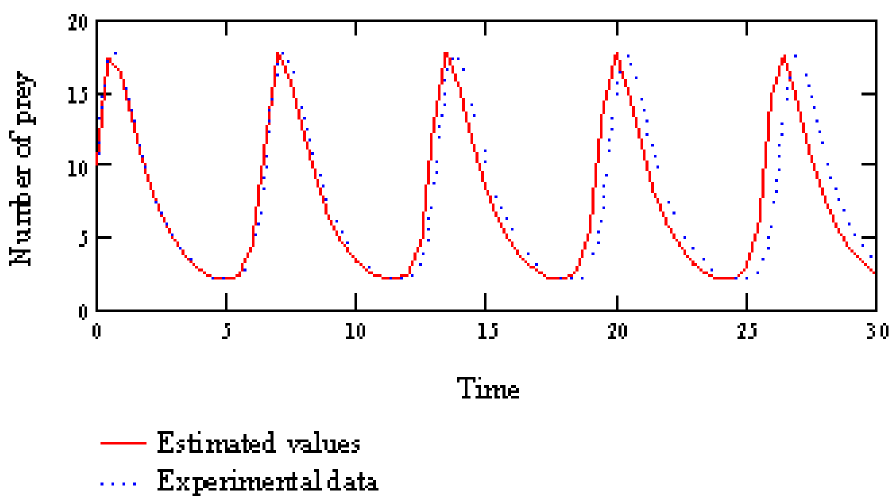

Figure 1

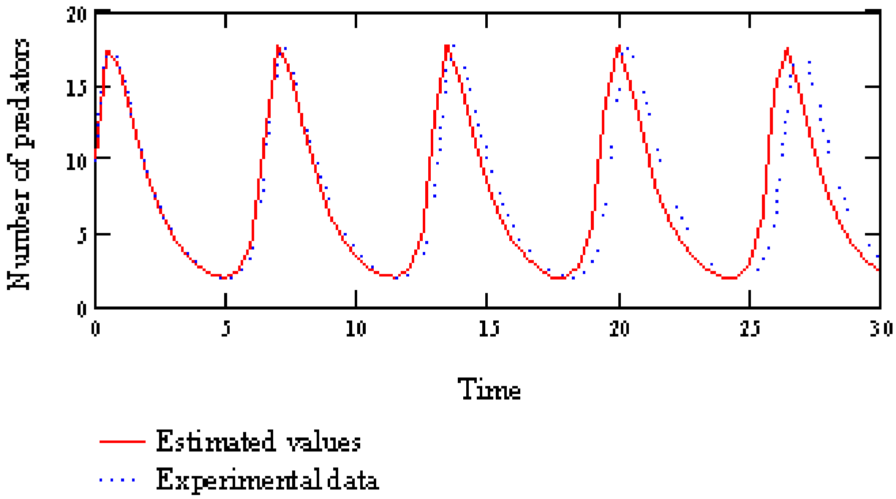

Figure 2

CONCLUSION

1. The Method of identification of unknown parameters of a given dynamical system from experimental data is formulated on the basis of least squares method.

2. The error functional is estimated as a value of order h - the step in statistical data.

3. Example of predator-prey model identification is considered as an example of general theory and it is shown that obtained parameters give accurate interpretation of the experimental data.

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