SPECIAL APPROACHES TO GLOBAL RECONSTRUCTION OF EQUATIONS FROM TIME SERIES

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Some problems arising during global reconstruction from time series are illustrated by reconstruction of etalon equations and modeling of real-world radiophysical systems. Efficiency of specialized approaches oriented to modeling of restricted classes of systems is demonstrated and new specific techniques are proposed.

1. Introduction

In practice, to obtain a mathematical model from general laws of nature (from "the first principles") by individualizing them with reference to the object of investigation is often impossible. Typically, numerous phenomena of different nature which details are not clear affect the process under investigation or the first principles (similar to Newton's laws in mechanics) for the field of interest are not discovered yet. In such a case, experimental data become the main source of information about an object and the problem of an *empiric* model construction arises. Its simplest example is approximation of a set of points on the plane (x, y) by a functional dependence $y = f(x)$. Since results of observations[1] are presented, as a rule, in the form of time series (sequences of observable values, measured at discrete time instants), then the problem transforms into modeling from time series. It is relevant in physics, meteorology, seismography, medicine and physiology, etc.

Here, we mean modeling of complicated (mainly, chaotic) behavior. Earlier this problem was solved with the help of statistical models [1], since complicated behavior associated only with very large numbers of degrees of freedom. However, in 1960-70s scientific community got to understand that complicated behavior can be exhibited even by simple (low-dimensional) *nonlinear* dynamical systems [2,3]. After

[1] A experimentally measured quantity is usually called "an experimental observable" or simply "an observable".

that, there appeared a significant interest to construction of dynamical empiric models in the form of

- difference equations $\mathbf{x}(t_i) = \mathbf{F}(\mathbf{x}(t_{i-1}), \mathbf{c})$, where $\mathbf{x} = (x_1, x_2, ..., x_D) \in R^D$ is a state vector, $\mathbf{F}$ is a vector-valued function, $\mathbf{c} \in R^M$ is a vector of its parameters, t_i is discrete time [4-6],
- ordinary differential equations (ODEs) $\dot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t), \mathbf{c})$ [4,7],
- delay differential equations (DDEs) [8,9],
- partial differential equations [10].

A peak of interest to the problem of global[2] reconstruction was observed in 1990s [11-36], which was followed by the appearance of reviews on this subject [37-40]. But then disadvantages of the developed approaches were shown and difficulties of empiric modeling determined to a significant extent by the use of universal structures and polynomial approximation became apparent. All that reduced, in part, attention to this research area. In the latest papers devoted to global reconstruction, one observes certain shift of focus to problems of dynamical variables and model structure selection [41-50], though there are also some works oriented to further development of universal structures and techniques [51-53].

The purpose of this work is to illustrate some difficulties arising in global reconstruction from time series and to present approaches and technologic tricks for their overcoming. In section 2 we describe a general scheme for empiric modeling and the standard approach and analyze peculiarities of its application. Our original results concerning different stages of the scheme are presented in the rest of the paer which is organized as follows. In section 3 the problem of dynamical variables selection is considered. In section 4 we demonstrate possibilities of a specialized model structure selection on the example of nonautonomous systems. A specific technique for parameter estimation, based on peculiarities of behavior of systems with delayed feedback and efficient in the case of noisy time series, is shown in

[2] The term “global” means that model equations (written down in a closed form) describe behavior of an object in the entire phase space (globally).

section 5. In section 6 we present a special method of model refinement which is based on some properties of transient processes and allows to optimize model structure by excluding superfluous terms from it. We summarize and present generalizing considerations on the problem of global modeling in section 7.

2. Typical scheme of empiric modeling and standard approach

Despite the variety of existing approaches and practical situations, it is possible to distinguish the following basic stages in the procedure of modeling from a scalar time series:

1. Organization of an experiment (if there is such a possibility) and obtaining a time series of an observable quantity η (a training time series): $\{\eta(t_i)\}_{i=1}^{N_\eta}$, where $t_i = t_0 + (i-1)\Delta t$, Δt is a sampling interval, N_η is the time series length.
2. Choice of the model equations type (stochastic or deterministic, difference or differential, etc).
3. Choice of model variables $x_1,...,x_D$. Here, one specifies the number of variables D and the kind of their relation with the observable η. As a rule, it is necessary to obtain time realizations of lacking (hidden) variables from the observable series.
4. Selection of the forms of approximating functions F_k (i.e. components of **F**), $k = 1,..,D$, which will enter right-hand sides of model equations. On the stages 2 – 4, model *structure* is specified, after that only stages of calculation remain.
5. Estimation of model parameters $c_1,...,c_M$ from a time series data.
6. Diagnostic check-up of a model, i.e. investigation of solutions to the obtained equations and their comparison with the observed process, criteria of quality being determined by modeling purposes.

Under statistical modeling, one uses, as a rule, ARMA-models [1] which are linear stochastic difference equations where subsequent values of an observable are model variables. Under nonlinear dynamics approach to modeling, one can imagine (in contrast to linear case) arbitrarily many different forms of equations. They differ from each other by both function kinds and kind of relation between dynamical variables $x_1,...,x_D$ and an observable η. Therefore, the problems of variables and

model structure selection become more difficult. This situation became easier after Takens [54] and Sauer et al [55] had shown that it is possible to obtain from a scalar time realization $\eta(t)$ of a dynamical system such vectors $\mathbf{x}(t)$ that are related to the original state vectors in one-to-one and smooth fashion. So, they "legalized" theoretically the use of sequential values of an observable $\left[\eta(t_i), \eta(t_i+\tau), ..., \eta(t_i+(D-1)\tau)\right]$ (τ is a constant delay) or its sequential derivatives $\left[\eta(t_i), \dot{\eta}(t_i), ..., d^{D-1}\eta(t_i)/dt^{D-1}\right]$ as coordinates of vectors $\mathbf{x}(t_i)$, given $D \geq 2m+1$ (sufficient but not necessary condition), where m is a dimension of the manifold which the phase orbit of an original system belongs to. Even though it does not mean that employment of different variables (e.g., obtained by integration [56]) is necessarily less effective for modeling.

The choice of variables often dictates a model structure. For example, if sequential derivatives are used for reconstruction from a scalar time series, then model equations assume the form

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= x_3, \\ &..., \\ \dot{x}_D &= F(x_1, x_2, ..., x_D), \end{aligned} \tag{1}$$

where $x_1(t) = \eta(t)$, i.e. they involve the only function F.

After the equation type and the way of dynamical variables reconstruction are chosen, one should select the forms of functions entering right-hand sides. Under global modeling, a required function F is most commonly looked for in the pseudo-linear form, i.e. linear combination of nonlinear *basis* functions f_i:

$$F(\mathbf{x}) = \sum_{j=1}^{M} c_j f_j(\mathbf{x}). \tag{2}$$

One widely uses the standard polynomial basis: $1, x_1, ..., x_D, x_1^2, x_1x_2, ..., x_D^2, ...$, i.e. representation of F in the form of the multivariate algebraic polynomial of some

order K. Coefficients c_j are estimated, as a rule, via the least-squares routine[3], i.e. by minimization of the quantity $\varepsilon^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\dot{x}_D(t_i) - F\left(\mathbf{x}(t_i)\right)\right)^2$.

Choice of dynamical variables and model structure is often oriented to construction of models in a universal form. Thus, widely exploited model ODEs (1) with a polynomial in the right-hand side are often called *standard* [17,18]. This term could be referred to all the other cases when no information on specific features of an object is incorporated into the model structure. The pretensions to universality are theoretically validated [55]. Nonetheless, all the achievements [4] in modeling of real-world objects we are aware of are isolated instances. A blunders at any of the stages of modeling scheme can become an obstacle. Choice of variables can be unfortunate. But even suitable variables can not help if the form of functions is inappropriate. Thus, the popular standard structure can not be the best one for the entire multitude of real-world systems and situations. As a rule, it provides very cumbersome equations exhibiting divergent solutions (polynomial fit is especially inefficient in high-dimensional spaces).

Seemingly, a promising way of the further development of global reconstruction methods is rejection of the pretensions to model structure universality and creation of specialized approaches oriented to some classes of objects. It is reasonable to consider sufficiently important classes which specific features are known. But development of specialized techniques for parameter estimation and

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[3] One could also employ the more general maximum likelihood principle [57]. But it is reasonable only under the high noise levels that is not our case. So, we have used the least-squares approach.

[4] Global model ODEs with polynomials are used for control [11,26], attractor characteristics estimation from short and noisy time series [30], signal classification [23,24], and confidential transmission of information [31]. Under the standard approach, there were obtained models qualitatively reproducing complex dynamics of Belousov – Zhabotinskiy reaction [21], electrochemical process of copper dissolution in sulphuric acid [19], a certain regime of vortex fluid movement [20].

model refinement seems also quite useful. All these considerations are illustrated in the next sections.

3. Dynamical variables selection: preliminary testing for single-valuedness and continuity

As it has been already mentioned, in constructing model equations in the form $\mathbf{y}(t) = \mathbf{F}(\mathbf{x}(t))$ from a time series $\{\mathbf{ç}(t_i)\}$, one forms the series of state vectors $\{\mathbf{x}(t_i)\}$, where $\mathbf{x} = (x_1, x_2, ..., x_D) \in R^D$, x_k are dynamical variables, D is a model dimension. Coordinates of vectors **x** can be obtained as sequential derivatives, time delays, etc. Then, the series of quantities to enter left-hand sides of model equations $\{\mathbf{y}(t_i)\}$ is obtained from the series $\{\mathbf{x}(t_i)\}$ according to the chosen model type: either by numerical differentiation of $\{\mathbf{x}(t_i)\}$ for ODEs $d\mathbf{x}(t)/dt = \mathbf{F}(\mathbf{x}(t))$, or just by the shift of $\{\mathbf{x}(t_i)\}$ along the time axis for discrete maps $\mathbf{x}(t_{i+1}) = \mathbf{F}(\mathbf{x}(t_i))$. Finally, the forms of approximating functions F_k are specified and their parameters are estimated.

An uncontrolled choice of the variables can make approximation of the dependencies $y_k(\mathbf{x})$ with a smooth function extremely problematic [58] or even make these dependencies non-unique. Here, we describe the method of estimating suitability and "convenience" of the chosen variables x_k for constructing a *global* dynamical model. It is based on testing the series $\{\mathbf{y}(t_i)\}$ and $\{\mathbf{x}(t_i)\}$ for single-valuedness and continuity of each dependency $y_k(\mathbf{x})$ in the entire region of an observed motion [46]. Importantly, we use local characteristics rather than averaged ones [35,59].

Our technique is based on the following consideration. If a dependency $y(\mathbf{x})$ is single-valued and continuous in a domain V, then the difference $|y(\mathbf{x}) - y(\mathbf{x}_0)|$ tends to zero when $\|\mathbf{x} - \mathbf{x}_0\| \to 0$ for each $\mathbf{x}_0 \in V$. In practice, violation of this condition may be viewed as a sign of non-single-valuedness or discontinuity of the dependency $y(\mathbf{x})$. Since the observable time series has a finite length, the above-mentioned limit, strictly speaking, cannot be found. However, it is possible to trace a tendency in variations of the quantity $|y(t_i) - y(t_j)|$ when the vectors $\mathbf{x}(t_i)$ and $\mathbf{x}(t_j)$ are made

closer and closer, down to a certain *finite* distance. Given sufficiently large amount of data N_η, high accuracy of measurements, and low noise level, this distance can be made small enough for each region of the observed motion.

The method of testing consists in the following (Fig.1a). The domain V is partitioned into identical hypercubic boxes of the size δ, all boxes containing at least two vectors are selected (they are denoted $s_1, s_2, ..., s_M$). Difference between maximal and minimal values of y inside a box s_k is called *local variation* $\varepsilon_k = \max_{\mathbf{x} \in s_k} y(\mathbf{x}) - \min_{\mathbf{x} \in s_k} y(\mathbf{x})$. Maximal local variation $\varepsilon_{\max} = \max_{1 \le k \le M} \varepsilon_k$ and its graph $\varepsilon_{\max}(\delta)$ are used as the main characteristics of the investigated dependency. The suitability of the considered variables $\mathbf{x}$ and y for global modeling is assessed in the following way.

1) If a dependency $y(\mathbf{x})$ is single-valued and continuous, the value of $\varepsilon_{\max}$ is sufficiently small for small δ and tends to zero when $\delta \to 0$ (Fig.1b, filled squares). It is not hard to show that a graph $\varepsilon_{\max}(\delta)$ is a straight line for sufficiently small δ.

2) If a single-valued and continuous dependency has a region of very steep slope (a "jump"), then $\varepsilon_{\max}$ remains rather big for sufficiently small δ, since that region is situated within one box. However, the further decrease of δ leads to the decrease of $\varepsilon_{\max}$ because the region of a jump becomes divided into several boxes. The graph $\varepsilon_{\max}(\delta)$ exhibits a "breakpoint" at the value of δ equal to the size of the region of steep slope (e.g., Fig.1b, white circles). In such a case, the dependency $y(\mathbf{x})$ is also difficult to approximate with a smooth function.

3) If $\varepsilon_{\max}$ remains rather large and does not decrease at $\delta \to 0$ (Fig.1b, filled circles), then the considered variables are not appropriate for global modeling. Such a situation can be related both with non-uniqueness of the dependency and high noise level

So, dynamical variables should be selected so that the graph $\varepsilon_{\max}(\delta)$ tend to the origin gradually, without breakpoints, and with small slope (Fig.1b, filled squares). The most important feature distinguishing the proposed approach and

providing its usefulness for global modeling is employment of local (not averaged) characteristics. Let us illustrate it by modeling a real-world radiophysical system: a nonlinear electric circuit (harmonically driven *RLC*-circuit with switched capacitors) which scheme is shown in Fig.2a. The element K is an electronic key, a microscheme comprising dozens of transistors and other passive elements which is fed from a special source of dc-potential. At small values of voltage U on the capacity C_1, the resistance of the key is very large and linear oscillations occur in the circuit RLC_1. When the voltage U achieves a threshold value U_{thr}, the resistance of the key decreases abruptly and the capacity C_2 becomes connected to the circuit. Back switching occurs approximately at the same value of U (in fact, at somewhat smaller value – hysteresis takes place). As a result, the system is nonlinear and exhibits complex dynamics (in particular, chaotic oscillations) at big values of driving amplitude [60,61].

We employ a chaotic time realization of the current I through the resistor R (see Fig.4a) as an observable time series $\{\eta(t_i)\}$. The data are recorded with the aid of a 12-bit ADC, the sampling interval is $\Delta t = 4$ μsec, the driving period is $T = 84\Delta t$, the length of the series is $N_\eta = 3 \cdot 10^4$. Six examples are considered below (three variants of the model ODEs structure for two different observables). The results of the application of the proposed method (Fig.4b,c) and of the model construction are presented. The graphs in Fig.4 are numbered in agreement with the numbers of the following examples.

1) A popular model structure

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, x_3), \\ \dot{x}_2 &= f_2(x_1, x_2, x_3), \\ \dot{x}_3 &= f_3(x_1, x_2, x_3), \end{aligned} \tag{3}$$

where $x_1(t_i) = \eta(t_i), x_2(t_i) = \eta(t_i + \tau), x_3(t_i) = \eta(t_i + 2\tau)$ are time delay coordinates, $\tau = 21\Delta t$ is the first zero of the autocorrelation function. A smoothing polynomial is constructed for numerical differentiation. All three dependencies $\dot{x}_k(x_1, x_2, x_3), k = 1, 2, 3$ are analyzed. The value of $\varepsilon_{\max}$ does not tend to zero when δ

decreases for all *k*. All graphs $\varepsilon_{\max}(\delta)$ look similarly, one of them is presented in Fig.2b with filled squares (for $k = 3$). It indicates the impossibility of constructing an efficient global model that is confirmed in practice completely.

2) A standard model (1,2) with $x_1(t_i) = \eta(t_i)$. The dependency $\dot{x}_3(x_1, x_2, x_3)$ is tested. $\varepsilon_{\max}(\delta)$ decreases when δ decreases (Fig.2b, white circles) that points out to the possible single-valuedness. The result of modeling: an efficient model, which right-hand sides are algebraic polynomials, can not be obtained. Obviously, a polynomial is inappropriate to fit the dependency $\dot{x}_3(x_1, x_2, x_3)$. Another form of the approximating function is necessary here. Its choice is a difficult problem which is not a subject of the present paper.

3) Following the recommendations on the reconstruction of nonautonomous systems [33,34], we construct a model in the form

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= F(x_1, x_2, \varphi), \end{aligned} \tag{4}$$

where $x_1(t_i) = \eta(t_i)$ and φ is the phase of driving. The dependency $\dot{x}_2(x_1, x_2, \varphi)$ is tested. The time series of the phase φ is obtained as $\varphi(t_i) = \omega t_i \pmod{2\pi}$, the angular frequency ω is assumed to be known. The graph $\varepsilon_{\max}(\delta)$ (Fig.2b, filled circles) shows that the dependency is, possibly, single-valued. However, an efficient model with harmonic driving and polynomial fit can not be obtained. Again, one needs to select a special form of the function *F*.

3) A standard model (1,2) with $x_1(t_i) = \int_{t_1}^{t_i} \eta(t)dt$. This variable makes physical sense, it is the summed charge on the capacities C_1 and C_2. The time series $\{x_1(t_i)\}$ is obtained via the numerical integration of the measured time series of the current *I* (using the method of trapeziums). The value of $\varepsilon_{\max}(\delta)$ for the dependency $\dot{x}_3(x_1, x_2, x_3)$ does not decrease when δ decreases (Fig.2c, white circles) and remains large. An effective model can not be constructed.

A model (3) with $x_1(t_i) = \int_{t_1}^{t_i} \eta(t)dt$ and delayed coordinates $x_2(t_i) = x_1(t_i + \tau)$ and $x_3(t_i) = x_1(t_i + 2\tau)$, where τ is again the first zero of the ACF. All three dependencies $\dot{x}_k(x_1, x_2, x_3), k = 1, 2, 3$ are tested. The graphs $\varepsilon_{\max}(\delta)$ do not tend to the origin when δ decreases in all three cases. One of them (for k = 1) is shown in Fig.2c with filled squares. An effective model can not be constructed.

6) A model (4) with $x_1(t_i) = \int_{t_1}^{t_i} \eta(t)dt$. A graph $\varepsilon_{\max}(\delta)$ shows that the dependency $\dot{x}_2(x_1, x_2, \varphi)$ is single-valued and, moreover, varies "gradually" (Fig.2c, filled circles). A reconstructed model (4) with additive harmonic driving and bivariate polynomial of the 11th order demonstrates a chaotic attractor qualitatively similar to the experimental one (see also section 4, Fig.4) and provides an accurate forecast 5T ahead.

It is significant that an optimistic estimate according to the criterion $\varepsilon_{\max}(\delta)$ and good results of the global reconstruction are achieved only in the last (the sixth) case. The graphs for averaged over all the boxes local variation $\bar{\varepsilon}(\delta)$ are, however, practically the same for all above-mentioned choices of variables (one of them is shown in Fig.2b with the dashed line). It means that the average quantity $\bar{\varepsilon}$ does not provide all information necessary for global modeling. Therefore $\bar{\varepsilon}$ can be used in dynamical modeling only as an *additional* characteristic.

4. Model structure selection: nonautonomous systems under regular external driving

Here, we consider another cause of the standard approach inefficiency. In fact, its failure is inevitable "payment" for the generality of model structure. Probability to guess optimal model form without using a priori information or special preliminary investigation of the object is quite low. Therefore, we suggest to choose some classes of systems and modify the standard structure with reference to that classes. Here, we propose such a modification for modeling systems under regular external driving. It consists in the use of *nonautonomous* ODEs. That is function explicitly depending on

time are incorporated into the model equations. First, we consider the simplest case of harmonic additive driving. Model is suggested to be constructed in the form

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= x_3, \\ &\ldots \\ \dot{x}_D &= F(x_1, x_2, ..., x_D) + a\cos\left(\frac{2\pi}{\hat{0}}t\right) + b\sin\left(\frac{2\pi}{\hat{0}}t\right), \end{aligned} \tag{5}$$

where F is an algebraic polynomial of some order K (at $D = 2$, this is just an equation of harmonically driven oscillator). However, it is insufficient only to incorporate the driving into the last equation (5), a necessary condition for the success of modeling is to estimate driving period T from a time series with high accuracy.

Prerequisites for construction of model equations in the form (5) can be a priori information or the presence of a discrete peak in the power spectrum of an observed time series (Fig.3a). Location of the latter can also serve as a rough estimate of driving period. Given a precise value of T, parameters a and b and polynomial coefficients are easily estimated via the linear least-squares routine. But to estimate T is not so simple since it enter equation (5) in a *nonlinear* way. Therefore, it is estimated individually using a special procedure [33] (it is illustrated in Fig.3b where the graph of an approximation error versus trial value of T is shown). Importantly, error in its estimation $\Delta T = T - T_0$ (where T_0 is an unknown "truth" value) leads to a significant "phase shift" between the truth driving and its model fit if the training time series is long. The following relationships between relative error of driving approximation ε_T, and quantities $\Delta T/T_0$ and T_N/T_0 (where T_N is the duration of the observed time realization) holds

$$\varepsilon_T \approx \frac{2\pi}{\sqrt{3}} \frac{\Delta T}{T_0} \frac{T_N}{T_0}. \tag{6}$$

It follows that the driving period should be estimated more accurately for longer training time series, otherwise incorporation of explicit time dependence is useless.

A result of application of the proposed technique to modeling of the above-mentioned (section 3) harmonically driven *RLC*-circuit with switched capacitors from

the integrated time series of current I (i.e. in the case selected as the best for modeling with the help of the testing method of section 3) are presented in Fig.4. Obtained empiric model (5) with $D = 2$ and $K = 11$ (and excluded superfluous terms) behaves like the original system and provides sufficiently accurate forecast quite far ahead.

Harmonic force represents an important but sufficiently narrow class of possible ways of driving. The proposed approach to modification of standard structure can be extended to more complex and realistic situations, namely, for

1. arbitrary *way of entry* of harmonic driving;
2. arbitrary *form* of regular (i.e. periodic or quasiperiodic) driving.

For the first situation, significantly bigger than for a model (5) degree of generality can be achieved by using a polynomial F with alternating coefficients [44]:

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= x_3, \\ &\ldots \\ \dot{x}_D &= F(x_1, x_2, \ldots, x_D, t), \end{aligned} \tag{7}$$

where $x_1 = \eta$, and F reads

$$F(x_1, x_2, \ldots, x_D, t) = \sum_{l_1, l_2, \ldots, l_D = 0}^{K} \left(c_{l_1, l_2, \ldots, l_D} + a_{l_1, l_2, \ldots, l_D} \cos\omega t + b_{l_1, l_2, \ldots, l_D} \sin\omega t \right) \prod_{j=1}^{D} x_j^{l_j}, \quad \sum_{j=1}^{D} l_j \le K. \tag{8}$$

To estimate parameters of a model (7,8), one can exploit an above mentioned procedure where accurate determination of the driving period T is provided.

To illustrate of efficiency and advantages of the structure (7,8), we present a numerical example: reconstruction of equations from chaotic time series of Toda oscillator when driving is not only additive. Original equation read

$$\begin{aligned} \dot{u}_1 &= u_2, \\ \dot{u}_2 &= -0.45u_2 + (5 + 4\cos t)(e^{-u_1} - 1) + 7\sin t. \end{aligned} \tag{9}$$

Time series is obtained here (and in all numerical examples presented below) by numerical integration of original equations with the help of Runge-Kutta routine. The best model (7,8) is achieved at $D = 2$, $K = 9$, it exhibits chaotic attractor practically

identical to the original one (Fig.5a,b). Such results can not be achieved with models (5) (Fig.5c). Standard models (1,2) demonstrate, as a rule, globally unstable orbits (Fig.5d). Prediction times for the best models (7,8), (5) and (1,2) are equal to $7T$, $1.5T$ and $0.15T$, respectively.

For the second situation (arbitrary regular driving), we propose to use the structure of equations (7) involving time dependence but not necessarily harmonic:

$$F(x_1, x_2, ..., x_D, t) = f(x_1, x_2, ..., x_D) + g(t), \qquad (10)$$

where f is a n algebraic polynomial, and function $g(t)$ describes the driving and involves also free parameters. Two approaches to the specification of $g(t)$ are possible. The first one is to guess a special formula on the basis of *a priori* information. The second approach is more universal and can be used in the absence of detailed knowledge of the form of driving which is approximated as

$$g(t) = a_0 + \sum_{j=1}^{k_1} a_{1,j} \cos\left(\frac{2\pi j t}{T_1} + \varphi_{1,j}\right) + ... + \sum_{j=1}^{k_m} a_{m,j} \cos\left(\frac{2\pi j t}{T_m} + \varphi_{m,j}\right) \qquad (11)$$

Here, $m = 1$ for the periodic case, while quasiperiodic driving is described as the sum of $m > 1$ trigonometric polynomials with different periods T_m and different orders k_m. Procedure of estimating parameters of the model (7,10) also rests on the least-squares technique. But, since here several free parameters can enter the expression for the driving g *in a nonlinear way*, it is reasonable to use one of well-known iterative methods for the solution to the nonlinear least-squares problem (we use a modified Levenberg – Marquardt routine [62]).

Efficiency of the approach was verified in numerical experiments (reconstruction of equations from time series of Toda oscillator under different forms of driving: pulse periodic, periodic with subharmonics, quasiperiodic [63]). We note that efficient models with trigonometric polynomials (11) can be achieved for very large number of harmonics (that is necessary to describe uneven driving signal). This is an important advantage of the proposed approach, since instability of models (1,2)

with algebraic polynomials of high orders seems the main reason for the standard approach failures.

The considered stages (dynamical variables and model structure selection) are the key ones in modeling. However, efficient specialized techniques for parameter estimation and model refinement are also useful. Techniques of such a sort are presented in the following two sections

5. Model parameters estimation: quick determination of delay time from noisy time series

Here, we describe a technique of parameter estimation for DDEs. The technique is based on some specific properties of time realizations of delayed feedback systems [47,48]. We consider one of the most popular first-order DDE as an object of investigation

$$\varepsilon_0 \dot{x}(t) = -x(t) + f(x(t-\tau_0)), \qquad (12)$$

where τ_0 is the delay time, f is a nonlinear function, and parameter ε_0 characterizes inertial properties of the system. In general case, Eq. (12) is a mathematical model of an oscillating system composed of a ring with three ideal elements: nonlinear, delay, and inertial ones. In a radiophysical version of the ring (Fig. 6), an amplifier with the transfer function f plays the role of nonlinear device, a delay line provides a delay τ_0, and a filter defines the parameter ε_0. We develop a technique for estimating τ_0, f, and ε_0 from the time series.

The proposed method of estimating τ_0 exploits the features of extrema shape and location in the temporal realization $x(t)$ of the system (12). The peculiarities of extrema location in time are clearly illustrated by $N(\tau)$ plot in Fig. 7. To construct it one has to define for different τ values the number N of pairs of extrema in $x(t)$, that are separated in time by τ. If N is normalized to the total number of extrema, then for sufficiently large extrema number, it can be used as an estimation of probability to find a pair of extrema in $x(t)$ separated by the interval τ. Let us explain the qualitative features of $N(\tau)$ for various values of parameter ε_0.

In the absence of inertial properties ($\varepsilon_0 = 0$) differentiation of Eq. (12) gives

$$\dot{x}(t) = f'(x(t-\tau_0))\dot{x}(t-\tau_0). \qquad (13)$$

From Eq. (13) it follows that if $\dot{x}(t-\tau_0) = 0$, then $\dot{x}(t) = 0$. Thus, for $\varepsilon_0 = 0$ every extremum of $x(t)$ is followed within the time τ_0 by the extremum. As the result, $N(\tau)$ shows a maximum for $\tau = \tau_0$ in Fig. 7(a).

In the presence of inertial properties ($\varepsilon_0 > 0$), which corresponds to real situations, the most probable value of the time interval between extrema in $x(t)$ shifts from τ_0 to larger values. This effect can be explained using the ring system shown in Fig. 6: the filter introduces a certain additional delay in the system. As the result, the extrema in $x(t)$ can be found most often at the distance $\tau_0 + \tau_s$ apart (Fig. 7b). For instance, the computational investigation of Eq. (12) with quadratic nonlinear function $f(x) = \lambda - x^2$ allows us to obtain an estimation $\tau_s \approx \varepsilon_0/2$ for large values of the parameter of nonlinearity λ.

For $\varepsilon_0 > 0$ the extrema in $x(t)$ are close to quadratic ones and therefore $\dot{x}(t) = 0$ and $\ddot{x}(t) = 0$ at the extremal points. It can be shown that in this case there are practically no extrema in $x(t)$ separated in time by τ_0. To prove this, let us differentiate Eq. (12) with respect to t:

$$\varepsilon_0\ddot{x}(t) = -\dot{x}(t) + f'(x(t-\tau_0))\dot{x}(t-\tau_0). \qquad (14)$$

If for $\dot{x}(t) = 0$ in a typical case $\ddot{x}(t) = 0$, then, as it can be seen from Eq. (14), for $\varepsilon_0 \neq 0$ the condition $\dot{x}(t) \neq 0$ must be fulfilled. Thus, there must be no extremum separated in time by τ_0 from a quadratic extremum and hence $N(\tau_0) \to 0$. For $\tau \neq \tau_0$, the derivatives $\dot{x}(t)$ and $\dot{x}(t-\tau)$ can be simultaneously equal to zero, i.e., it is possible to find extrema separated in time by τ. The proposed method of τ_0 determination does not need significant time of computation because only operations of comparing and adding can be used for the extrema definition and $N(\tau)$ construction.

To recover the parameter ε_0 and the nonlinear function *f* of system (12) from the chaotic time series we plot in a plane a set of points with coordinates $\left(x(t-\tau_0), \varepsilon_0 \dot{x}(t) + x(t)\right)$. According to Eq. (12), which can be written in the form

$$\varepsilon_0 \dot{x}(t) + x(t) = f(x(t-\tau_0)) \tag{15}$$

the constructed set of points reproduces the function *f*. Since the parameter ε_0 is a priori unknown, one needs to plot $\varepsilon \dot{x}(t) + x(t)$ versus $x(t-\tau_0)$ under variation of ε, searching for a single-valued dependence in the plane $\left(x(t-\tau_0), \varepsilon \dot{x}(t) + x(t)\right)$, which is possible only for $\varepsilon = \varepsilon_0$. As a quantitative criterion of single-valuedness in searching for ε_0 we use the minimal length of a line $L(\varepsilon)$, connecting all points ordered with respect to $x(t-\tau_0)$ in the plane $\left(x(t-\tau_0), \varepsilon \dot{x}(t) + x(t)\right)$. The minimum of $L(\varepsilon)$ is observed at $\varepsilon = \varepsilon_0$. The set of points constructed for the defined ε_0 in the plane $\left(x(t-\tau_0), \varepsilon_0 \dot{x}(t) + x(t)\right)$ reproduces the nonlinear function, which can be approximated if necessary. In contrast to methods presented in [8,35] which use only extremal points or points selected according to a certain rule for the nonlinear function recovery, the proposed technique uses all points of the time series. It allows one to estimate the parameter ε_0 and to reconstruct the nonlinear function from short time series even in the regimes of weakly developed chaos.

To test the efficiency of the proposed technique we apply the method to a time series produced by the Mackey-Glass equation

$$\dot{x}(t) = -bx(t) + \frac{ax(t-\tau_0)}{1 + x^c(t-\tau_0)}, \tag{16}$$

which can be converted to Eq. (12) with $\varepsilon_0 = 1/b$ and the function

$$f(x(t-\tau_0)) = \frac{ax(t-\tau_0)}{b(1 + x^c(t-\tau_0))}. \tag{17}$$

The parameters of the system (16) are chosen to be $a = 0.2$, $b = 0.1$, $c = 10$, $\tau_0 = 300$ to produce a dynamics on a high-dimensional chaotic attractor.

Fig.8 illustrates the reconstruction of the system parameters. To construct the $N(\tau)$ plot we use 10000 points of the time series of $x(t)$. The time series exhibits about

600 extrema and $N(\tau)$ is normalized to their total number. The time derivatives $\dot{x}(t)$ are estimated from the time series by applying a local parabolic approximation. The absolute minimum of $N(\tau)$ takes place exactly at $\tau = \tau_0 = 300$, where $N(300) = 0$. $L(\varepsilon)$ is normalized to the most uncorrelated point set. To reduce the computation time one can choose a large initial step of ε variation and then to reduce it in the neighborhood of minimum $L(\varepsilon)$. Thus, in Fig.8b the step of ε variation is 1 and in the inset this step is reduced to 0.1. The minimum of $L(\varepsilon)$ takes place exactly at $\varepsilon = \varepsilon_0 = 1/b = 10$. The recovered nonlinear function (Fig.8c) coincides practically with the true function (17). Note, that for the construction of the $L(\varepsilon)$ plot and for the recovery of the function f we use only 1000 points of the time series.

To investigate the robustness of the method to perturbations we apply it to the data produced by adding a zero-mean Gaussian white noise to the time series of Eq. (16). We found out that the method is still efficient for a noise level of 10%.

As another example, we consider an experimental time series from an electronic oscillator with delayed feedback. For the case when the filter (see Fig.6) is a low-frequency first-order RC-filter this oscillator is given by

$$RC\dot{V}(t) = -V(t) + f(V(t-\tau_0)), \tag{18}$$

where $V(t)$ and $V(t-\tau_0)$ are the delay line input and output voltages, respectively; R and C are the resistance and capacitance of the filter elements. Eq. (18) is of form (12) with $\varepsilon_0 = RC$. In our experiment the nonlinear device has a quadratic transfer function. The proposed method allows us to define accurately the parameters of the system.

The procedure of the delay time estimation from the $N(\tau)$ plot considered with systems like (12) can be successfully applied to time series gained from a more general class of time-delay systems

$$\dot{x}(t) = F(x(t), x(t-\tau_0)). \tag{19}$$

Time differentiation of Eq. (19) gives

$$\ddot{x}(t) = \frac{\partial F(x(t), x(t-\tau_0))}{\partial x(t)}\dot{x}(t) + \frac{\partial F(x(t), x(t-\tau_0))}{\partial x(t-\tau_0)}\dot{x}(t-\tau_0). \tag{20}$$

Similarly to Eq. (14), Eq. (20) implies that in the case of quadratic extrema derivatives $\dot{x}(t)$ and $\dot{x}(t-\tau_0)$ do not vanish simultaneously, i.e., if $\dot{x}(t)=0$, then $\dot{x}(t-\tau_0)\neq 0$.

In principle, it is possible to extend the proposed method of τ_0 definition from time series to high-dimensional time-delay systems having the following form

$$x^{(n)}(t)+a_1x^{(n-1)}(t)+...+a_{n-1}\dot{x}(t)=F(x(t),x(t-\tau_0)), \tag{21}$$

where $x^{(n)}(t)$ is the derivative of order n and $a_1,...a_{n-1}$ are the coefficients. Differentiation of Eq. (21) with respect to t gives

$$x^{(n+1)}(t)+a_1x^{(n)}(t)...+a_{n-1}\ddot{x}(t)=\frac{\partial F(x(t),x(t-\tau_0))}{\partial x(t)}\dot{x}(t)+\frac{\partial F(x(t),x(t-\tau_0))}{\partial x(t-\tau_0)}\dot{x}(t-\tau_0). \tag{22}$$

The condition $\dot{x}(t-\tau_0)\neq 0$ for $\dot{x}(t)=0$ will be satisfied if the left-hand side of Eq. (22) does not vanish. In general, a probability to obtain zero in the left-hand side of Eq. (22) is very small and therefore, the $N(\tau)$ plot qualitatively must have a shape similar to that inherent in the case of first-order delay-differential equations like (12) and (19).

The proposed method of estimation of the parameter ε_0 and the nonlinear function can be also applied to a variety of nonscalar time-delay systems. For instance, the dynamics of an electronic oscillator with delayed feedback containing two identical in-series *RC*-filters is described by the second-order delay-differential equation

$$\varepsilon_0^2\ddot{V}(t)+2\varepsilon_0\dot{V}(t)=-V(t)+f(V(t-\tau_0)), \tag{23}$$

where $\varepsilon_0=RC$. Plotting $\varepsilon^2\ddot{V}(t)+2\varepsilon\dot{V}(t)+V(t)$ versus $V(t-\tau_0)$ under variation of ε, we can estimate the parameter ε_0 by the location of the minimum of $L(\varepsilon)$ and recover the function *f*. Thus, the proposed technique of parameter estimation can be successfully applied to a wide class of time-delay systems.

6. "Technologic trick": model structure optimization using transients

Usually, global models are constructed from time realizations of established motion corresponding to an attractor in phase space. Such an approach seems reasonable when the problem of predicting future behavior of an object after establishing of oscillations is addressed. However, for modeling object dynamics in wide region of phase space, success is more probable when one uses time realizations of transient processes (when a phase orbit has not yet settled down onto an attractor). In this section we will show how this property of transients (to explore wider region of phase space) can be used to refine a model (to optimize its structure).

To detect a part of a time series which is the optimal for modeling, we compare performance of global models obtained from different parts of a time series (some of them involves a transient while the others do not). Let us use etalon differential equations of Van der Pol – Toda oscillator as an object of modeling:

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= (1 - x_1^2)x_2 - 1 + \exp(-x_1). \end{aligned} \tag{24}$$

Reconstruction is performed form a chaotic scalar time series of the x_1-coordinate with a transient (a phase orbit is shown in Fig.9a). Models of the form (1) with $D = 2$ are constructed in two variants differing from each other by the form of a function $F(x_1, x_2)$. In the first case, a bivariate algebraic polynomial of some order K is employed:

$$F(x_1, x_2) = \sum_{i,j=0}^{K} c_{ij} x_1^i x_2^j, \; i + j \le K. \tag{25}$$

In the second case, F is given by

$$F(x_1, x_2) = (\lambda - x_1^2)x_2 + f_K(x_1), \tag{26}$$

where $f_K(x_1)$ is a univariate algebraic polynomial of the order K, which approximates exponential function. To assess a model quality, right-hand side reconstruction error σ is calculated. This quantity compare functions entering right-hand sides of an object F_0 and a model F:

$$\sigma = \iint_S \left(F(x_1, x_2) - F_0(x_1, x_2)\right)^2 dx_1 dx_2, \tag{27}$$

where S is an integration domain containing the phase orbit (hence, much larger than the domain of an attractor). The lower is σ, the better is a model.

A procedure of searching for an optimal for modeling part of the time series (*reconstruction window*) consists in following. A certain length of a window (M points) is specified. A reconstruction window can be denoted as $\{\eta(t_i)\}_{i=m}^{m+M-1}$, where m is the number of its initial point. The initial point of the original time series coincides with the initial point of a reconstruction window for $m = 0$. When m increases, a reconstruction window moves along a time series into the region of an attractor. Models are constructed for different values of m. Optimal location of the reconstruction window corresponds to minimum on the graph $\sigma(m)$of above-mentioned criteria of quality versus.

Graphs $\sigma(m)$ in Fig.9b show that the best results for a model (1,25) are obtained with the use of the transient (the curve 1, small m). For a model (1,26) the results are better by an order of magnitude (the curve 2), but they are almost independent on the location of the reconstruction window. It can be explained as follows. The first model structure (1,25) includes variety of "superfluous" terms, e.g., the terms x_1x_2, $x_1x_2^2$, $x_1^2x_2^2$, etc, which are not relevant for the original equation (24). Theoretically, model coefficients corresponding to superfluous terms should vanish. But in practice their estimated values differ from 0 due to truncation errors and impossibility of accurate approximation of exponential function by a finite power series. Superfluous terms can become significant outside of reconstruction window and lead to essential differences between an object and a model. For a model (1,25) involving superfluous terms, σ depends essentially on m (Fig.9b) that is induced by essential dependence of "superfluous coefficients" on m (Fig.10). For a model (1,26), the use of a transient does not have advantages because model refinement is due to the absence of superfluous terms rather than extension of the explored region in the phase space.

Let us look again at Fig.10a where graphs for necessary terms are grouped on the left and for superfluous terms – on the right. The superfluous coefficients are

obviously less stable than the necessary ones, the instability appearing close to the beginning of the time series (in the region of a transient). Resting on these considerations, we propose a procedure of model structure refinement based on sequential excluding of terms with the less stable coefficients from the model. The degree of stability (reliability) of some coefficient a can be defined as the ratio of its mean value to its standard deviation $m_1 = \dfrac{\langle a \rangle}{\sqrt{\left\langle \left(a - \langle a \rangle\right)^2 \right\rangle}}$, where angle brackets designate average over the ensemble of values of a, obtained at different m.

Thus, to optimize a model structure, the less stable coefficient (with smallest m_1) is found and a corresponding term is excluded from the model, reconstruction procedure is repeated for the simplified structure and so on until exclusion of a new term leads to model deterioration. In Fig.10b a dependence of the model error σ on the number of excluded terms obtained during reconstruction from time series of the system (24) starting from the model structure (1,25). The proposed procedure are shown to allow for essential enhancement of the model quality.

7. Conclusions

To construct dynamical models means to follow the path pointed by an optimistic outlook of determinism. There is neither guarantee that the path will lead out to the highway, nor assurance that such a highway always exists. But even if a dynamical model of an object is possible, one needs accuracy and "technological purity" to achieve a success. An error at any stage of the empiric modeling scheme presented in section 2 can make obtaining an efficient dynamical model impossible. Let us remember, by way of an analogy, how at the early stage of microelectronics underestimation of the role of dust particles and foreign microinclusions turned, e.g., production of a diode into art and did not allow to do with confidence such things that nowadays are being done routinely. So, let us hope for the absence of principal and overwhelming obstacles on the way of empiric modeling.

However, we believe that to progress in this field, one needs to develop not only original technical tricks but also (this is, possibly, the main thing) new

approaches oriented to sufficiently narrow classes of systems. For the latter, a special preliminary analysis of time series and attraction of a priori information are necessary. Our work shows prospects and necessity of such a "specialization". The main results are following:

1. the proposed technique for preliminary investigation of times series of dynamical variables (section 3) allows to find variants which are the most suitable for modeling. Its advantage is in the use of local characteristics which reveal even small regions of non-uniqueness or discontinuity in dependencies between dynamical variables and quantities to enter left-hand sides of equations. However, even good choice of variables does not guarantee a success: one needs to succeed in the choice of functions form and model parameters estimation;
2. the proposed modifications of the standard structure of model equations (section 4) allow to obtain efficient models of nonautonomous systems in the case of arbitrary regular driving, while the standard approach does not give satisfactory results;
3. a special way of estimating delay time for DDEs reconstruction is proposed (section 5). It is based on peculiarities of time realizations of delayed feedback systems and efficient even when dealing with highly noisy data;
4. employed model structure often turns out very cumbersome. Therefore, it is rather important to delete "superfluous" terms (which carry only distortions) from the model. To detect such terms, we propose a special procedure which uses reconstruction from different parts of a transient process realization.

All the presented approaches are demonstrated by constructing models from numerical solutions of etalon equations and from time realizations of real-world (radiophysical) systems.

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Figure captions

Fig.1. (a) Illustration for a technique of testing a dependency $y(\mathbf{x})$ for single-valuedness and continuity in the case $D = 2$. (б) Possible appearance of graphs $\varepsilon_{\max}(\delta)$ for different variants of dynamical variables.

Fig.2. (a) The scheme for the circuit with switched capacitors: $C_1 = 0.1\,\mu F$, $C_2 = 4.4\,\mu F$, $L = 0.03\,H$, $R = 10\,\Omega$, $U_{thr} = -0.2\,V$, $U_0 = 2.344$ V, driving frequency equals 2.98 *kHz*, sampling frequency equals 250 *kHz*. (b) The graphs $\varepsilon_{\max}(\delta)$ for different variants of the model structure (for the dynamical variable $x_1 = I$): 1) for a dependency $\dot{x}_3(x_1, x_2, x_3)$ of a model (3), filled squares, 2) for a dependency $\dot{x}_3(x_1, x_2, x_3)$ of a model (1), white circles, 3) for a dependency $\dot{x}_2(x_1, x_2, \varphi)$ of a model (4), filled circles. The graphs $\bar{\varepsilon}(\delta)$ look similar for all the examples (the graph for the first one is shown with the dashed line). (c) The graphs $\varepsilon_{\max}(\delta)$ for different variants of the model structure (when the dynamical variable x_1 is an integral of the current *I*): 1) for a dependency $\dot{x}_1(x_1, x_2, x_3)$ of a model (3), filled squares, 2) for a

dependency $\dot{x}_3(x_1, x_2, x_3)$ of a model (1), white circles, 3) for a dependency $\dot{x}_2(x_1, x_2, \varphi)$ of a model (4), filled circles.

Fig.3. (a) Typical appearance of the power spectrum for harmonically driven chaotic systems: there is a pronounced peak. (b) Approximation error for a model (5) versus trial value of driving period *T*.

Fig.4. (a) Projection of an experimental orbit for the circuit with switched capacitors (shown in Fig.2a) onto the plane summed charge – current. (b) A corresponding projection for the best reconstructed model, i.e. a model (5) with $D = 2$ and $K = 11$.

Fig.5. (a) Projection of attractor of Toda oscillator (9). (b-d) Projections of phase orbits for a model (7,8) ($D = 2$, $K = 9$), a model (5) ($D = 2$, $K = 10$) and a standard model ($D = 4$, $K = 6$), respectively.

Fig. 6. Radiophysical model of time-delay system.

Fig.7. Number *N* of pairs of extrema in a realization of Eq. (12) separated in time by τ, as a function of τ. $N(\tau)$ is normalized to the total number of extrema in time series. (a) $\varepsilon_0 = 0$, (b) $\varepsilon_0 > 0$.

Fig.8. (a) Normalized number *N* of pairs of extrema in the time series of Eq. (16) separated in time by τ for $\tau = 1,\ldots,400$. (b) Length *L* of a line connecting points ordered with respect to $x(t-\tau_0)$ in the plane $\left(x(t-\tau_0), \varepsilon\dot{x}(t) + x(t)\right)$ as a function of ε. The inset shows $L(\varepsilon)$ in the neighborhood of the minimum. (c) The recovered nonlinear function.

Fig.9. (a) A phase orbit of the system (24). (b) Model error σ (27) versus the location *m* of reconstruction window for a model (1,25) (the curve 1) and a model (1,26) (the curve 2) with polynomials of 7th order.

Fig.10. Results of reconstruction of the system (24) from a scalar time series. (a) Dependencies of coefficients (corresponding to presented near the graphs polynomial terms) of a model (1,25) on the location *m* of reconstruction window. (b) Model error σ versus the number of excluded terms, a "starting" model structure being (1,25).

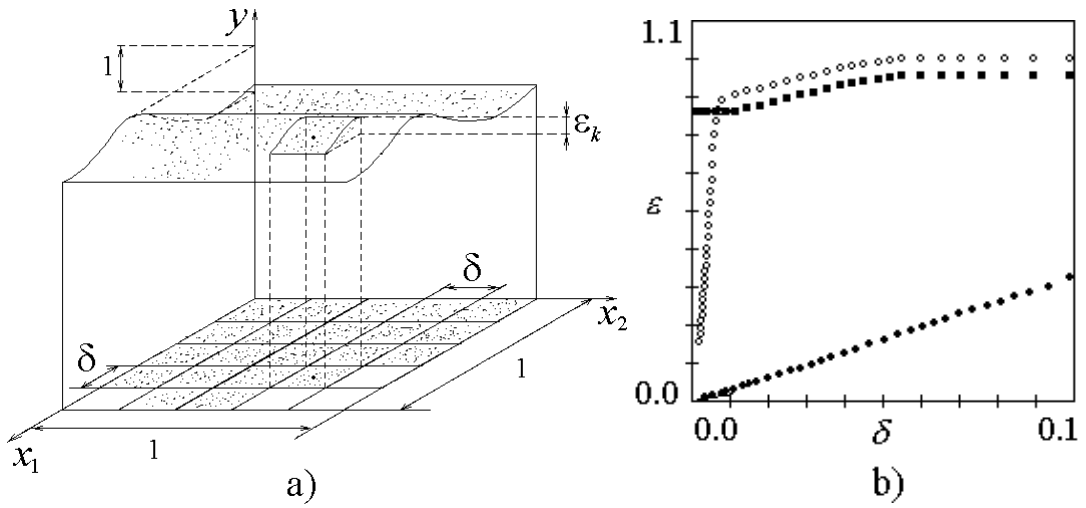

Fig.1.

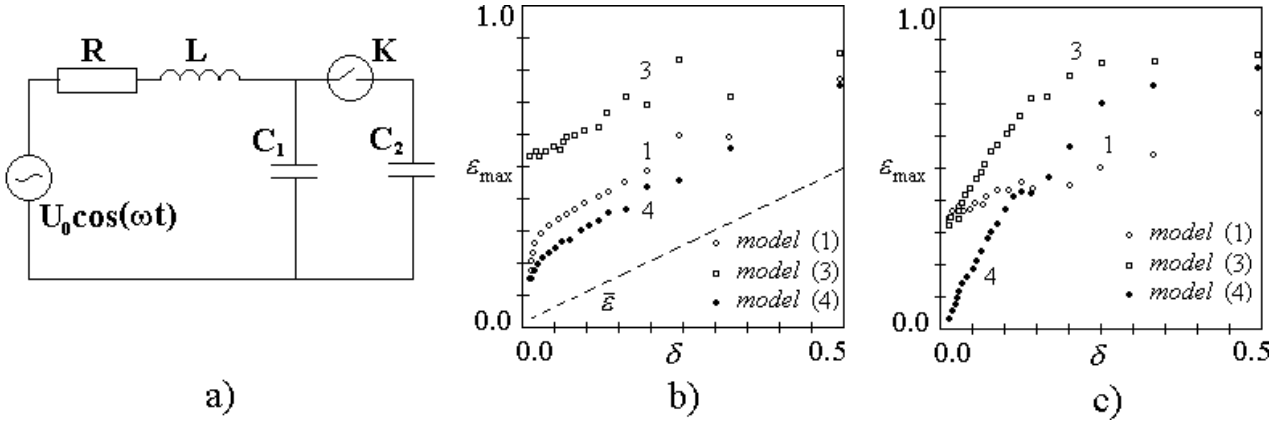

Fig.2.

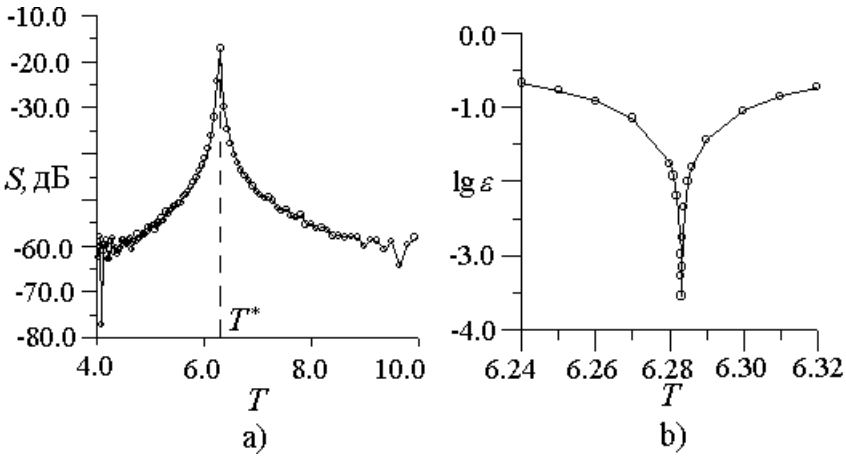

Fig.3.

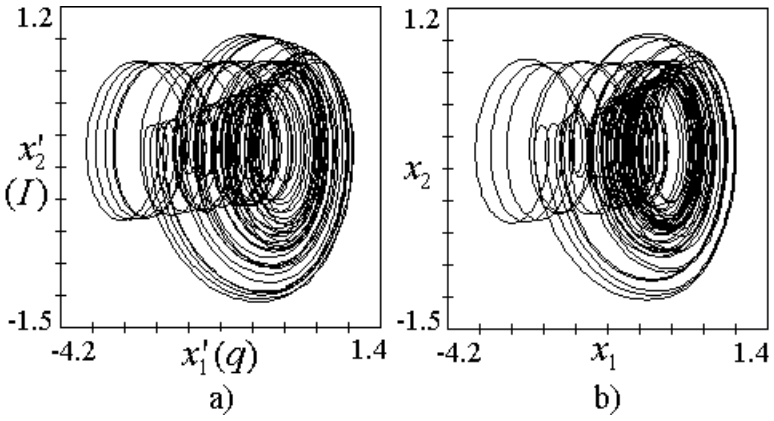

Fig.4.

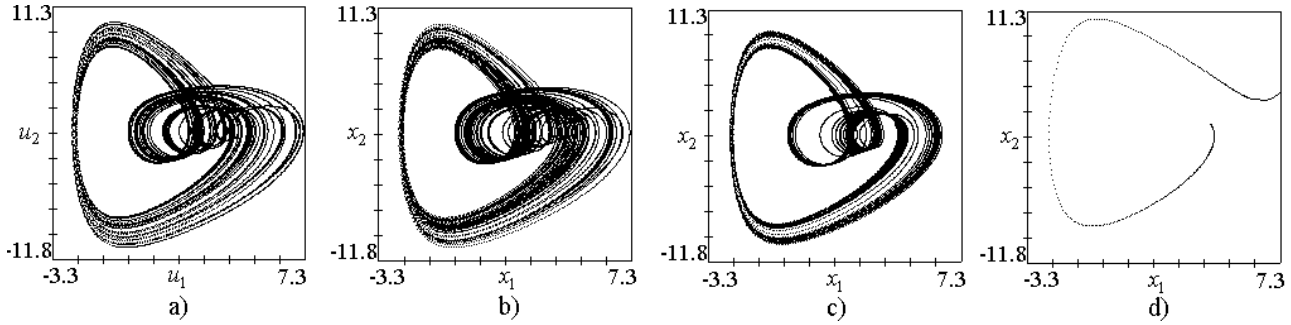

Fig.5.

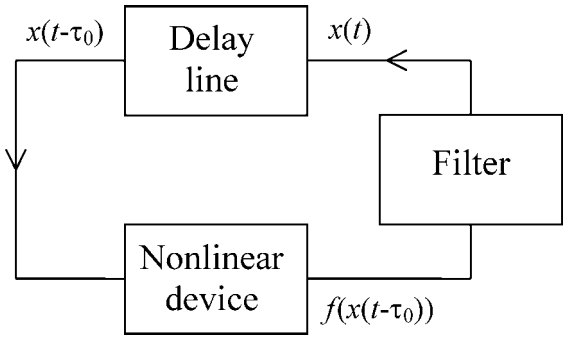

Fig. 6.

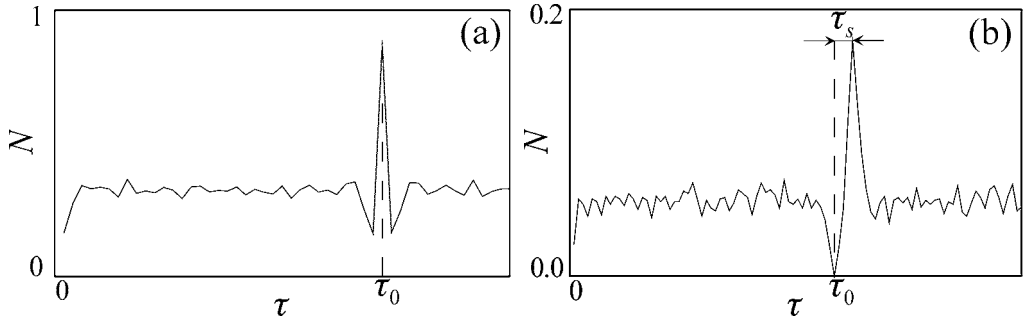

Fig.7.

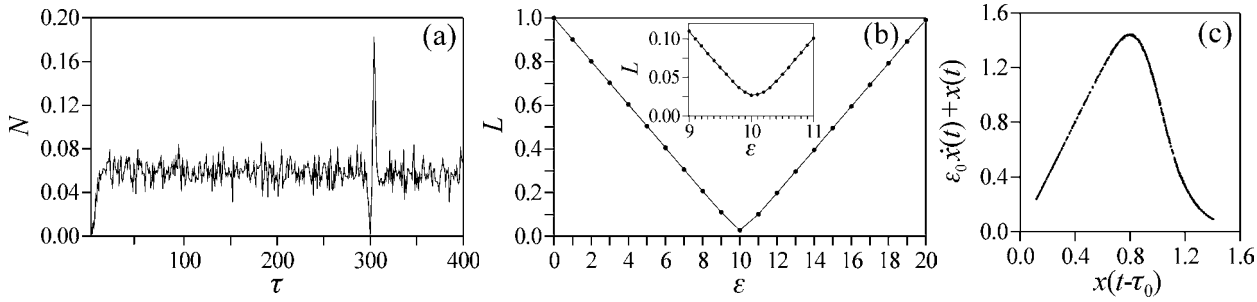
(a)
N
τ
(b)
L
ε
(c)
$\varepsilon_0 \dot{x}(t)+x(t)$
$x(t-\tau_0)$

Fig.8.

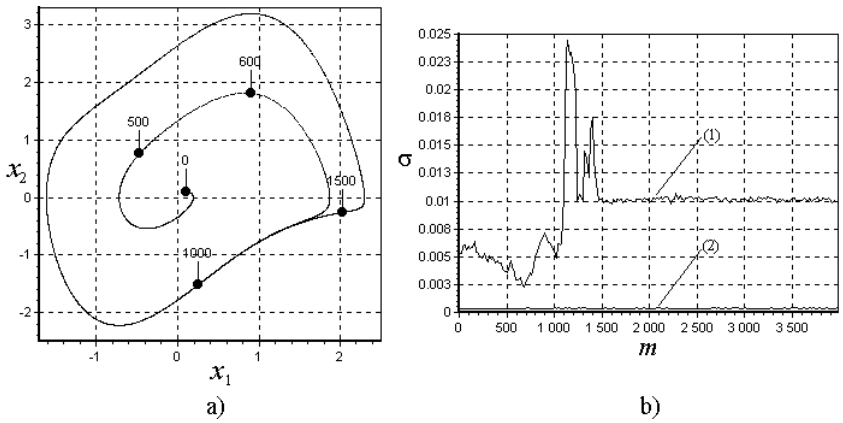
600
500
0
1500
1000
x_2
x_1
a)
σ
(1)
(2)
m
b)

Fig.9.

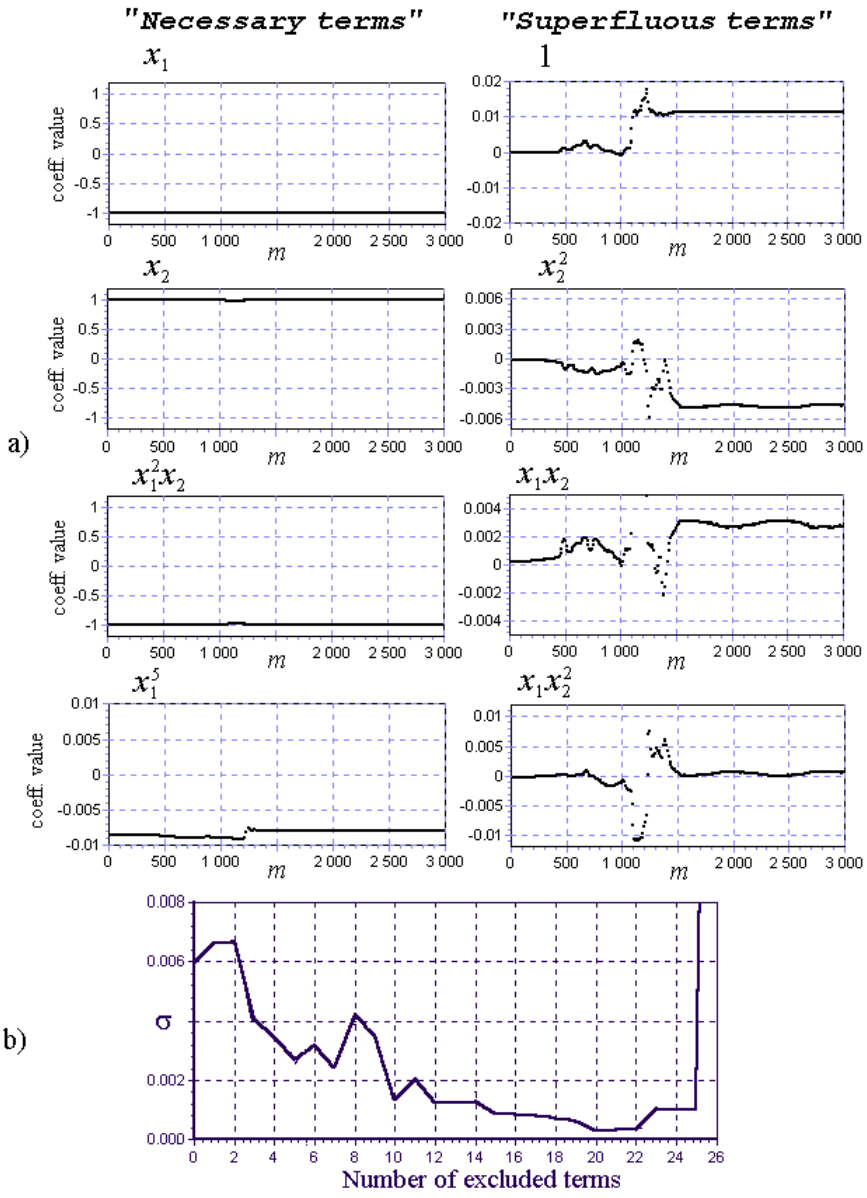
"Necessary terms"
"Superfluous terms"
a)
b)
coeff. value
m
σ
Number of excluded terms

Fig.10.