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Construction of Dynamical Model Equations for Nonautonomous Systems from Time Series (Peculiarities and Special Techniques)

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Abstract

Problems, arising during global reconstruction of dynamical models from time series, and prospects of the further development of empiric modeling methods are discussed. We present a specialized approach aimed at modeling the systems being under arbitrary regular driving. Original "technical tricks" are also described: a technique for dynamical variables selection and a model structure optimization routine. All the approaches are illustrated with examples of reconstructing etalon equations and modeling real-world (radiophysical) objects.

1. Introduction

1.1. To obtain a mathematical model from "the first principles" in practice is often impossible. In more typical situations, numerous vague phenomena of different physical nature affect the process under investigation or the first principles for the field of interest, similar to Newton's laws in mechanics, are not yet discovered. In such a case, experimental data become the main source of information about an investigated system (an object of modeling) and the problem of an empiric model construction arises. Since observations of real-world processes are presented, as a rule, in the form of time series – sequences of observable values measured at discrete time instants, the problem is called "modeling from time series". It is actual in physics, meteorology, seismography, medicine and physiology, etc.

Modeling of complicated (irregular) behavior is addressed here, as well as in other contributions to this book. Earlier, this problem was treated from a statistical point of view [1] since complicated behavior was associated only with enormous numbers of degrees of freedom. In 1960-70s, it became clear that complicated behavior can be exhibited even by simple (low-dimensional) nonlinear dynamical systems [2,3]. It gave rise to appearance of methods for constructing empiric deterministic low-dimensional models in the form of difference equations (maps) [4-6] and ordinary differential equations (ODEs) [4,7]¹.

1.2. In general, the problem of empiric modeling can be formulated as follows.

- There is a system of our interest (we will call it just "an object").
- One picks out some quantities $\eta_1,...,\eta_k$, which characterize the processes occurring in the system and which can be measured experimentally (they are called observables).

An obtained time series of these quantities (i.e. the finite sequence $\{\eta(t_i)\}_{i=1}^N$, where $\eta(t_i) = (\eta_1(t_i), \eta_2(t_i), ..., \eta_k(t_i)), t_i = i\Delta t$, Δt is a sampling interval) is a main source of quantitative information about the system under investigation.

It is known that the object possesses a set of properties $\{P_1,...,P_M\}$ that are relevant for our consideration. E.g. power spectrum of its time realizations exhibits a certain structure, their correlation dimension estimates take on certain typical values, its dynamics undergoes certain bifurcations under certain conditions.

It is necessary to construct a dynamical model capable of reproducing as many of the properties $\{P_1,...,P_M\}$ as possible using the time series. According to quite a general approach, a model takes the form²

$$dx/dt = F(x(t),c),$$

 $\eta_{j}(t) = h_{j}(x(t)) + \xi_{j}(t), j = 1,...,d$
(1)

where $\mathbf{X} = (x_1, ..., x_D) \in \mathbb{R}^D$ is a state vector of the model, F is a smooth vector field, $\mathbf{c} \in \mathbb{R}^P$ is a parameter vector, $\boldsymbol{\xi}_i(t)$ are random "measurement errors", h_i are smooth functions defining relations between dynamical variables and observables (they are often called "measurement functions")³. One should find the values of parameters c, for which a

¹ Methods for construction of infinite-dimensional nonlinear models (delay differential equations [8,9] and partial differential equations [10]) are also being actively developed. But they are beyond of our scope here.

Even though the formulation (1) is given for ODEs, the further treatment would be similar for other model

types as well.

Measurement functions are important components of the model. They may also involve some parameters. In the simplest case, which is yet important and widely spread in practice, observables are suggested to coincide with dynamical variables (that is accurate to ξ_j), i.e. $h_j(\mathbf{x}(t)) = x_j(t)$. Throughout this paper, we often consider scalar time series and such a simple relation $\eta(t) = x_1(t) + \xi(t)$.

model (1) more or less accurately reproduces the time series and possesses at least some of the properties $P_1, ..., P_M$.

If the function F in (1) is expressed analytically in terms of elementary functions (in a closed form) and the expression holds in the entire phase space, then the model (1) is called global. Further we consider only global models.

- 1.3. The success of modeling depends on several factors. First of all, it is important to select a model structure, which is adequate to the object, that involves:
 - the number D of dynamical variables X_k (as a rule, one has to use more variables than the number of observables d),
 - the forms of the measurement functions h_j , which describe supposed relations between dynamical variables x_k and observables η_j ,
 - and the form of the function **F**.

In general, not all of the quantities, which enter a model as dynamical variables, can be measured directly or even computed from the observable values. Thus, if D > d then at least D - d of the necessary variables are not observed. Unobserved variables are often called *hidden*. During modeling, time series of all model variables (including hidden ones) need to be reconstructed somehow from the available data.

The choice of either way of hidden variables reconstruction is a particular case of the important problem of model dynamical variables selection. If there are too many observables then one should specify a subset of them to be used as model variables. If the observables are not sufficient for model construction or they cannot be used directly, then different combination of available data are employed. Very popular methods are sequential derivatives and time delays (see, e.g., [11] and [7], respectively) both of which rest upon the celebrated Takens' results and their generalizations [12]. However, different ways of obtaining hidden variables, which are based on a priori information about the system under investigation or some peculiarities of its dynamics [13], may prove to be more appropriate for modeling. Mixed situations, when one selects subset of observables and reconstructs hidden variables from their time series, are also possible.

We note that the selection of variables may affect the form of model equations. Thus, under the use of sequential derivatives [11,14-17] for modeling from a scalar time series $\{\eta(t_i)\}$, a model takes the form

$$\frac{dx_1}{dt} = x_2,$$

$$\frac{dx_2}{dt} = x_3,$$

(2)

$$dx_D/dt = F(x_1,x_2, ... x_D, c)$$

where the observable is supposed to be one of the model variables (possibly, contaminated with measurements errors) $\eta(t_i) = x_i(t_i) + \xi(t_i)$. Notice that only a single scalar-valued function F enters Eqs. (2) as opposed to the general equations (1) involving a vector-valued function F. After the form of F, or F, is chosen from either considerations, i.e. the model structure is completely specified, it remains only to estimate parameters c from a time series. A least-squares method is often exploited for this purpose d, e.g., one minimizes the quantity

$$\varepsilon^2 = \frac{1}{N_0} \sum_{i=1}^{N_0} \left(dx_D(t_i) / dt - F(\mathbf{x}(t_i), \mathbf{c}) \right)^2 \text{ to estimate parameters of the model (2).}^5$$

- 1.4. Depending on considerations determining model structure selection, one can distinguish between several typical situations arising during modeling from time series. Below, they are arranged in the order of decreasing complexity.
- 1) There is no a priori information. This situation is often referred to as the black box problem. Here, the process of modeling may be called, indeed, the reconstruction of equations from an observable time series. The structure of equations should be selected by guess or in a universal form. An example of a universal (in a sense, standard) model structure is Eqs. (2) with a polynomial on the right-hand side

$$F(x_1, x_2, ..., x_D) = \sum_{l_1, l_2, ..., l_D = 0}^{K} c_{l_1, l_2, ..., l_D} \prod_{j=1}^{D} x_j^{l_j}, \sum_{j=1}^{D} l_j \le K.$$
(3)

From a theoretical point of view, Eqs. (2) and (3) must serve well for approximation of any system (1). But many researchers, relying on experience of their practical applications, believe that polynomials are not appropriate for construction of high-dimensional models. More promising methods exploit ideas of strong approximation, in particular, neural networks and radial basis functions [19-23].

- 2) The structure of equations is known, to a significant extent, from physical considerations. Only some nonlinear functions involved in a model remain unclear. Here, the function **F** has not any longer to give a universal-form approximation of a dependence in the D-dimensional space as in the black box situation. It may now involve just a few simpler standard functions, e.g., univariate polynomials. Therefore, the modeling problem is simplified considerably provided that the model structure is adequate to the object under investigation. This situation may be called **reconstruction of nonlinear characteristics**. 6
- 3) The complete structure of model equations is written down relying on physical considerations. Only parameters values are unknown. This case seems the most simple (again, provided that the model structure is adequate to the object). The modeling problem reduces

⁴ Sometimes, a general maximum likelihood principle and its modifications are applied [18]. But they are advisable only at high noise levels and small number of model parameters to be estimated.

 $^{^{5}}$ N_{0} is the length of time series of model state vectors obtained from the observable one. This time series is used for parameters estimation and, therefore, is often called *training time series*.

Note, that impossibility of obtaining a "good" model is the evidence for inadequacy of physical considerations underlying the selected model structure. So, the modeling procedure can serve to compare and validate different hypotheses concerning the mechanisms of the object functioning.

just to estimation of parameters from a time series. But even in this case essential technical difficulties can arise due to the large number of free model parameters and the presence of hidden variables.

1.5. A peak of interest to the problem of global reconstruction from time series fell on 1990s (see [19-21,24-34], to mention a few works) after that the first reviews appeared (e.g., [35,36] and the book [37]). Black box techniques were mostly considered and choice of variables and approximating functions was oriented to construction of models in a general form. Thus, often employed model ODEs (2),(3) were called standard [11]. This term could be referred also to other cases where model structure contains no information about any specific features of an object. Pretentions of standards models to be always appropriate are theoretically justified. As a rule, the justifications rely on Takens' and Stone – Weierstrass' theorems.

However, practical shortcomings of the developed methods (conditioned, to a significant extent, by the use of universal structures) soon became apparent. All successes of real-world objects modeling we are aware of (e.g., [11,14,15]) seem to be exclusions rather than typical cases. Blunders at any stage of the modeling scheme can become obstacles: selected variables may turn out inappropriate, but even the variables suitable for dynamical modeling do not help if the forms of approximating functions do not correspond to them. Thus, the standard structure (2),(3) cannot be the best choice for the entire variety of real-world systems. It often leads to very bulky equations exhibiting divergent solutions.

In the recent papers addressing global reconstruction, rise of attention to the problems of model structure selection (both dynamical variables and function forms) is noticed. A part of the investigations is devoted to the development of approaches based on using a priori information on the object [38-42]. Another important direction of research involves the papers aimed at refining universal techniques [43-49].

1.6. In our opinion, main prospects of the further development of global reconstruction techniques relate to the refusal of completely general (universal) model structures and creation of specialized approaches oriented to certain classes of objects. It is reasonable to consider sufficiently important classes which specific features are known a priori. On the other hand, development of novel procedures for model refinement applicable both to universal and special structures is also of significance.

We try to justify these theses in the presented chapter where the development of special techniques for global modeling of regularly driven systems is in the center of attention (Section 3). They represent right one of the above mentioned important classes of objects. Besides, we propose certain technological tricks appropriate for arbitrary situations, namely

- a dynamical variables selection technique based on testing a time series for single-valuedness and continuity of certain dependencies (Section 2),
- a model structure optimization technique based on using transient processes properties and allowing to exclude spurious model terms (Section 4).

In conclusion we present some general considerations on the problem of global modeling from time series.

2. Dynamical Variables Selection

As it has been already mentioned, to construct model equations in the form $\mathbf{y}(t) = \mathbf{F}(\mathbf{x}(t))$ from a time series $\{\mathbf{c}(t)\}$, one forms, first of all, the series of state vectors $\{\mathbf{x}(t)\}$. Coordinates \mathbf{x}_j of a state vector \mathbf{x} (dynamical variables) can be obtained as sequential derivatives, time delays, etc. Then, the time series of quantities to enter the left-hand side of model equations $\{\mathbf{y}(t_1)\}$ is obtained from the time series $\{\mathbf{x}(t_1)\}$ according to the chosen model type:

via numerical differentiation of $\{x(t)\}$ for ODEs, since y(t) = dx(t)/dt;

• via the shift of $\{\mathbf{x}(t_i)\}$ along the time axis for discrete maps, since $\mathbf{y}(t_i) = \mathbf{x}(t_{i+1})$.

Finally, the form of the function F is specified and its parameters are estimated.

Voluntary dynamical variables selection can make approximation of the dependencies

 Y_j (\mathbf{x}) with a smooth function extremely problematic [48,49] or even make these dependencies many-valued. Here, we describe the method for assessing suitability and convenience of the selected variables X_i , X_D for constructing a global dynamical model. It is based on testing the time series $\{\mathbf{y}(t_i)\}$ and $\{\mathbf{x}(t_i)\}$ for single-valuedness and continuity of each dependency Y_j (\mathbf{x}) in the entire region of an observed motion. It is crucial here that we use local characteristics rather than the averaged ones as in [34,50].

2.1. Description of Technique

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 many-valuedness or discontinuity of the dependency $y(\mathbf{x})$. Since the length of an observable time series is finite, the abovementioned limit cannot, strictly speaking, be found. However, it is possible to trace a tendency in variations of the quantity $|y(t_1) - y(t_j)|$ when the vectors $\mathbf{x}(t_j)$ and $\mathbf{x}(t_j)$ are made closer and closer, down to a certain *finite* distance. Given sufficiently large amount of data N, high accuracy of measurements, and low noise level, the distance $||\mathbf{x}(t_i) - \mathbf{x}(t_j)||$ can be made sufficiently small for each local region of observed motion.

The technique of testing consists in the following (Fig.1,a). The domain V containing the set of vectors $\{\mathbf{x}(t_i)\}_{i=1}^{N_0}$ is partitioned into identical hypercubic boxes of the size δ . All

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boxes containing at least two vectors are selected. Let us denote them $S_1, S_2, ... S_M$. The difference between the largest and the smallest values of y inside a box S_k is called *local variation* $\mathcal{E}_k = \max_{\mathbf{x} \in S_k} y(\mathbf{x}) - \min_{\mathbf{x} \in S_k} y(\mathbf{x})$. The largest local variation $\mathcal{E}_{\max} = \max_{1 \le k \le M} \mathcal{E}_k$ and its graph $\mathcal{E}_{\max}(\mathcal{S})$ are used as the main characteristics of the investigated dependency. Suitability of the considered quantities \mathbf{x} and \mathbf{y} for global modeling is assessed using the following considerations [44].

- 1. If a dependency $y(\mathbf{x})$ is single-valued and continuous, \mathcal{E}_{\max} is sufficiently small for small δ and tends to zero for $\delta \to 0$ (Fig.1,b, filled circles). It is not hard to show that the plot \mathcal{E}_{\max} (δ) 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 \mathcal{E}_{max} remains rather big for sufficiently small δ since that region is situated typically within one box. However, further decrease in δ leads to decrease in \mathcal{E}_{max} because the region of the jump becomes divided into several boxes. The graph \mathcal{E}_{max} (δ) exhibits a "kink" at the value of δ roughly equal to the size of the steep slope region (e.g., Fig.1,b, white circles). In such a case, the dependency y(x) is also difficult to approximate with a smooth function.
- 3. 3) If \mathcal{E}_{max} remains large and does not diminish for $\delta \to 0$ (Fig.1,b, filled squares) then the considered variables are not appropriate for global modeling. Such a situation may be related both to non-uniqueness of the dependency and high noise level.
- 4. To summarize, dynamical variables should be selected so that the graph $\varepsilon_{\text{max}}(\delta)$ tend to the origin without kinks and with slight slope (Fig.1b, filled circles). The most important feature distinguishing the proposed approach and providing its usefulness for global modeling is the employment of local (rather than averaged) characteristics. Let us illustrate this thesis by modeling a real-world nonlinear nonautonomous system.

note that the presence of outliers in real-world data is not compulsory.

It may be easily shown that the averaged over all boxes local variation $\overline{\mathcal{E}}$ does not allow detecting small regions of non-uniqueness. Certainly, the use of only the largest value \mathcal{E}_{max} makes the technique too sensitive to outliers. To apply the technique successfully in such a situation, it is possible to exclude "atypical" data points from the time series before testing. One can also exclude small fraction of data points giving the largest local variation even during the testing. We do not discuss this point in more detail, but

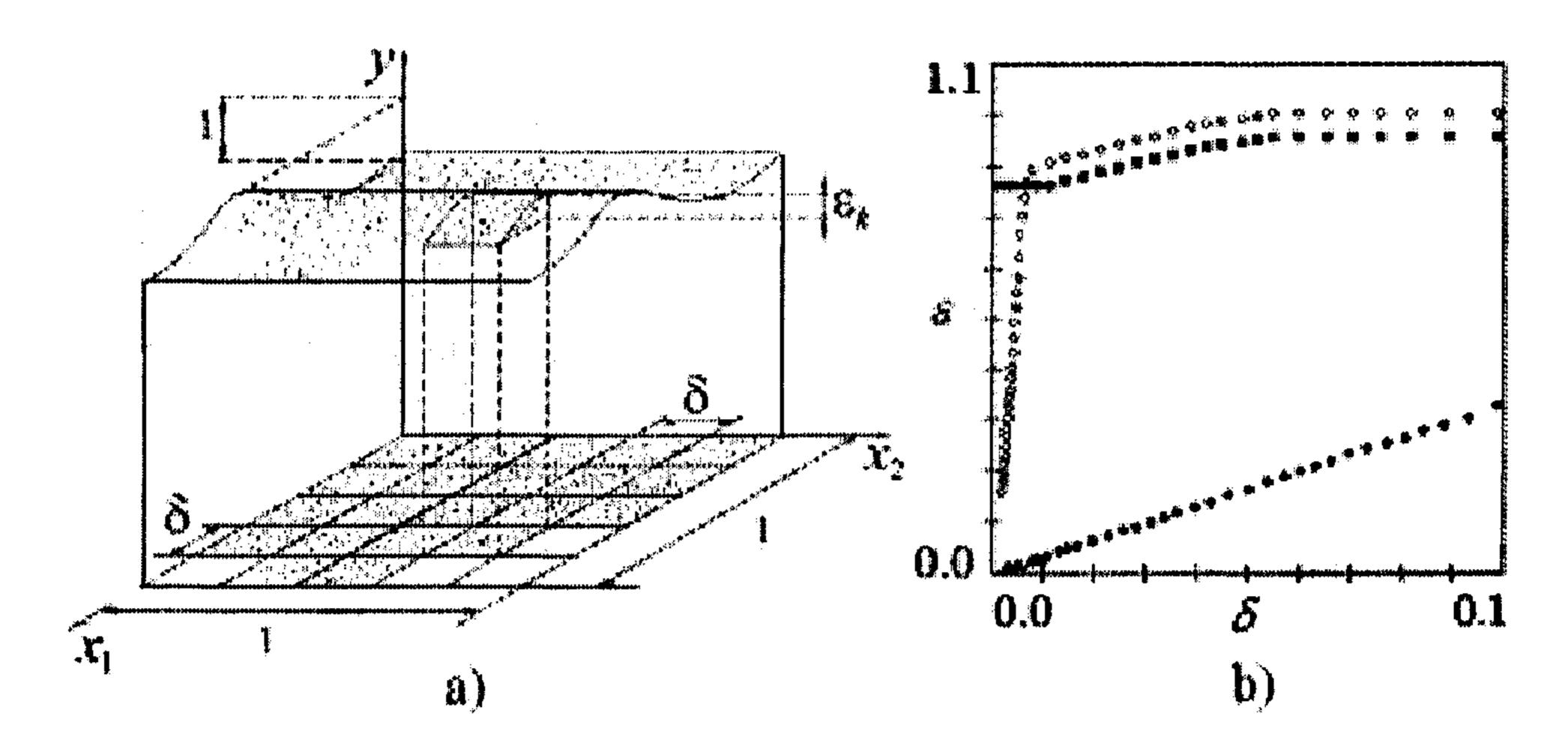


Fig.1. (a) Illustration for a technique of testing a dependency y(x) for single-valuedness and continuity in the case D = 2. (b) Possible appearance of plots \mathcal{E}_{max} (b) for different variants of dynamical variables.

2.2. Experimental Example

The scheme of a nonlinear electric circuit, harmonically driven RLC-circuit with switched capacitors [51,52], is shown in Fig.2,a. The element K is an electronic key that connects and disconnects the capacitor C_2 at a certain threshold value of the capacitor C_1 voltage. As a result, the system in nonlinear and exhibits complex dynamics (in particular, chaotic oscillations) at large driving amplitudes [41,44].

We employ a chaotic time realization of the current I through the resistor R (see Section 3, Fig.6,a) as an observable time series $\{\eta(t_1)\}$. The data are recorded with the aid of a 12-bit ADC, the sampling interval is $\Delta t = 4 \, \mu sec$, the driving period is $T = 84 \Delta t$, the length of the series is $N = 3 \cdot 10^4$. Six examples are considered below, three variants of the model structure for two different observables. The results of the proposed method application (Fig.2,b,c) and of the model construction are presented. The plots in Fig.2 are numbered according to the numbers of the examples.

1. We try a popular model structure

$$dx_{1}/dt = F_{1}(x_{1}, x_{2}, x_{3}),$$

$$dx_{2}/dt = F_{2}(x_{1}, x_{2}, x_{3}),$$

$$dx_{3}/dt = F_{3}(x_{1}, x_{2}, x_{3}),$$
(4)

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. Three dependencies $\frac{dx_j}{dt}(x_1,x_2,x_3)$, j=1,2,3, are analyzed. The value of ε_{\max} does not tend to zero when δ decreases for all j. All plots $\varepsilon_{\max}(\delta)$ look alike; one of them (for j=3) is presented in Fig.2,b with white squares. It indicates impossibility of constructing an efficient global model. The conclusion is confirmed in practice completely.

- 2. We try the standard structure (2) with $x_1(t_i) = \eta(t_i)$. The dependency $\frac{dx_3}{dt}(x_1, x_2, x_3)$ is tested. $\varepsilon_{\text{max}}(\delta)$ decreases for diminishing δ (Fig.2,b, white circles) that points out to possible single-valuedness. The result of modeling is that an efficient model (2),(3) cannot be obtained. Most probably, a polynomial (3) is inappropriate to fit the investigated dependency. Another form of the approximating function F is necessary. Its choice is a separate problem which is not addressed in this section.
- 3. Following the recommendations on nonautonomous systems reconstruction [32,33] (see also Section 3 of this paper), we try a model structure

$$dx_1/dt = x_2,$$

$$dx_2/dt = F(x_1, x_2, \varphi),$$
(5)

where $x_1(t_1) = \eta(t_1)$ and φ is a driving phase. The dependency $\frac{dx_2}{dt}(x_1, x_2, \varphi)$ is tested. The time series of the phase φ is obtained as $\varphi(t_1) = \omega t_1 \pmod{2\pi}$, the angular frequency ω is assumed to be known. The plot $\mathcal{E}_{\max}(\delta)$ (Fig.2,b, filled circles) shows that the dependency is, possibly, single-valued. However, an efficient model (5) with bivariate polynomial and additive harmonic driving (Section 3) cannot be obtained. Again, one needs to select a special form of the function F.

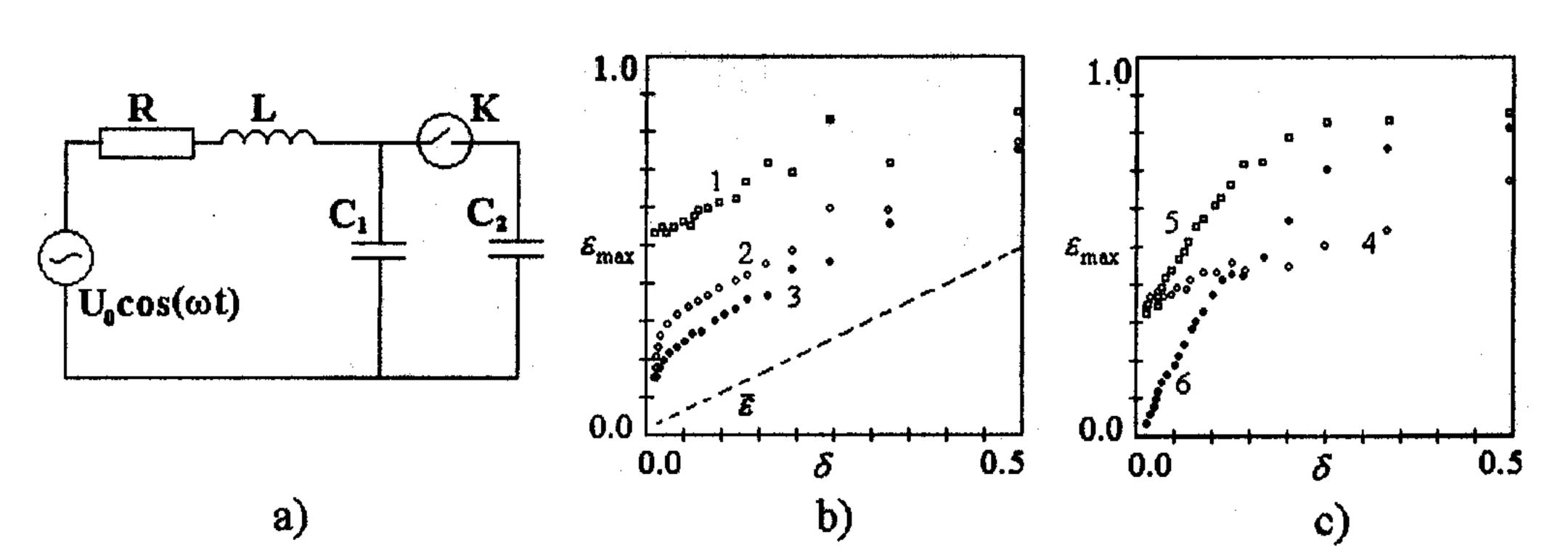
4. We try the standard structure (2) with $x_1(t_1) = \int_{t_1}^{t_2} \eta(t) dt$. This variable makes physical sense, it is the summed charge on the capacitors C_1 and C_2 . The time series $\{x_1(t_1)\}$ is obtained via numerical integration of the measured time series.

The value of $\mathcal{E}_{\text{max}}(\mathcal{S})$ for the dependency $\frac{dx_3}{dt}(x_1, x_2, x_3)$ does not decrease

when δ decreases (Fig.2,c, white circles). An efficient model cannot be constructed.

constructed.

- 5. We try the structure (4) with $x_1(t_1) = \int_{t_1}^{t_2} \eta(t) dt$ and delayed coordinates $x_2(t_1) = x_1(t_1 + \tau)$ and $x_3(t_1) = x_1(t_1 + 2\tau)$, where τ is again the first zero of the ACF. The dependencies $\frac{dx_j}{dt}(x_1, x_2, x_3)$, j=1,2,3, are tested. The plots $\mathcal{E}_{\max}(\mathcal{E})$ do not go through the origin in all three cases. One of them is shown in Fig.2,c with white squares (for k=1). An efficient model cannot be
- 6. We try the structure (5) with $x_1(t_1) = \int_{t_1}^{t_2} \eta(t) dt$. The plot $\mathcal{E}_{\text{max}}(\delta)$ shows that the dependency $\frac{dx_2}{dt}(x_1, x_2, \varphi)$ is single-valued and, moreover, varies "gradually" (Fig.2,c, filled circles). A reconstructed model (5) with additive harmonic driving and bivariate polynomial of the 11th order demonstrates a chaotic attractor qualitatively similar to the experimental one (see also section 3, Fig.6) and



provides a forecast 5T ahead with relative error less than 5%.

Fig.2. (a) The scheme for the circuit with switched capacitors. Here, $C_1 = 0.1 \, \mu F$, $C_2 = 4.4 \, \mu F$, $L = 0.03 \, H$, $R = 10 \, \Omega$, $U_{thr} = -0.2 \, V$, $U_0 = 2.344 \, V$, driving frequency is 2.98 kHz, sampling frequency is 250 kHz. (b) The plots $\varepsilon_{\rm max}(\delta)$ for different dynamical variables when the variable $\mathbf{X}_1 = \mathbf{I}$. The typical for all the examples plot $\overline{\varepsilon}(\delta)$ is shown with the dashed line. (c) The plots $\varepsilon_{\rm max}(\delta)$ for different dynamical variables when the variable \mathbf{X}_1 is an integral of the current \mathbf{I} .

It is significant that an optimistic assessment according to the criterion $\mathcal{E}_{\max}(\delta)$ and successful results of the global reconstruction are achieved only in the last (the sixth) case. Yet, plots of the mean local variation $\overline{\mathcal{E}}(\delta)$ are practically identical for all above-mentioned

sets of variables; one of the plots is shown in Fig.2,b with the dashed line. Thus, it follows that the averaged quantity $\overline{\mathcal{E}}$ does not provide all information necessary for global modeling. Therefore, in general $\overline{\mathcal{E}}$ can be used only as an additional characteristic.

2.3. Refinement of Technique and Testing for Nonlinearity

Here, we describe briefly an approach to refinement of the technique and its use for assessment of nonlinearity of a dependence y(x). Besides, we present the application of the refined technique to the analysis of a biological time series. These novel results will be published in more detail elsewhere.

The procedure described in Section 2.1 is a technique with a fixed set of non-overlapping

boxes (independent of the distribution of data points). It has the disadvantage that a vector \mathbf{x} lying near a box boundary is *never* compared to the close vectors from the neighboring boxes, but it *may* be compared to more distant vectors from its own box. It can lead to intensive oscillations in the $\varepsilon_{\max}(\delta)$ for small δ in the presence of noise. (The reason is that at a certain small δ -value a pair of vectors may fall into the same box and at a close, but different, δ -value those two vectors may fall into different boxes.) The non-monotony makes the assessment of the considered dynamical variables more difficult. An example of such a situation is illustrated in Fig.3,c, where the results of noisy time series testing are presented for chaotic regime of the logistic map $x_{n+1} = \lambda - x_n^2$ at $\lambda = 2.0$. The observable is $\eta_n = x_n + \xi_n$ where ξ_n is a sequence of independent identically uniformly distributed random values. We test the dependencies corresponding to the first iteration $\eta_{n+1}(\eta_n)$, to

The disadvantage of the technique may be obviated by using the set of overlapping boxes centered at the vectors of the time series instead of the fixed set of boxes. In other words, for each vector $\mathbf{X}(t_i)$ one should consider all its δ -neighbors, i.e. to calculate local variation of y in the box with the side 2δ centered at $\mathbf{X}(t_i)$. The number of considered boxes is then equal to the number of vectors N_0 . The largest value of local variation obtained in such a way (let us denote it $\mathcal{E}'_{\text{max}}$) monotonically decreases or, at least, does not rise with decrease

in δ . This advantage of the modified procedure is shown in Fig.3,c,d for the above mentioned

the second one $\eta_{n+2}(\eta_n)$, and to the third one $\eta_{n+3}(\eta_n)$ from the time series containing

1000 data points.

case of the logistic map.

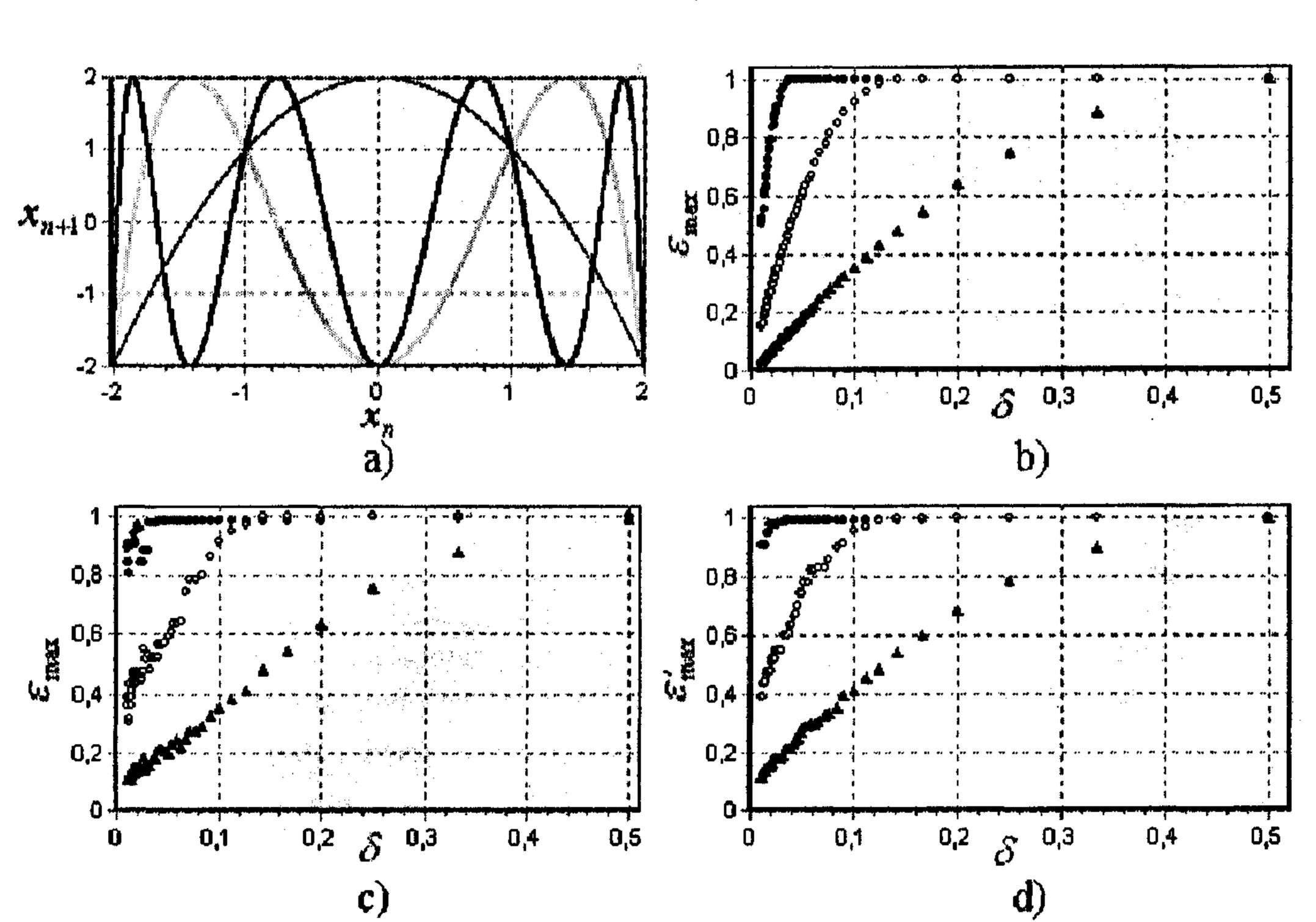


Fig.3. Comparison of testing techniques in a numerical experiment. (a) The first, the second, and the third iterations of the chaotic logistic map. (b),(c) Results of testing with the fixed-set-of-boxes technique from noise-free and noisy data, respectively. (d) Results of testing with the modified technique from noisy data.

Due to this advantage, the plot $\mathcal{E}'_{\max}(\delta)$ is more reliable and informative. In particular, the slope of the straight line passing through the origin and a point $(\delta_0, \mathcal{E}'_{\max}(\delta_0))$ is the estimate of the maximal "effective slope" of the investigated dependence for the chosen scale δ_0 . In the limit $\delta_0 \to 0$, this slope equals to the maximum of the norm of the gradient of $y(\mathbf{x})$ over the investigated domain. Even more important, the plot $\mathcal{E}'_{\max}(\delta)$ is a straight line if the system under investigation is linear. So, the plot $\mathcal{E}'_{\max}(\delta)$ can serve as a test for linearity. Its concavity indicates nonlinearity of the system under investigation. Thus, the above results for different iterations of the logistic map show that nonlinearity is more pronounced for the third iteration.

As an example of the proposed techniques application to a complex real-world system, let us briefly consider testing an acoustic time series. The time series is a digitized recording of the human voice (in fact, air pressure variations), which was done when a man was pronouncing the sound [a:]. Sampling frequency was equal to 44.1 kHz. The recording length was 10^4 data points. A dependence $\eta_{i+2}(\eta_i, \eta_{i-2}, \eta_{i-4})$ was tested. We present the plot $\varepsilon_{\text{max}}(\delta)$ in Fig.4,a; it does not indicate single-valuedness. Other conclusions can hardly be drawn from the figure because of the above-mentioned disadvantages of the fixed-set-of-

boxes technique. The modified technique leads to the monotone plot $\mathcal{E}'_{\max}(\delta)$ (Fig.4,b). It is easily seen that the dependence $\mathcal{E}'_{\max}(\delta)$ is significantly concave that allow drawing a conclusion about nonlinearity of the system under investigation. We do not go further into details here.

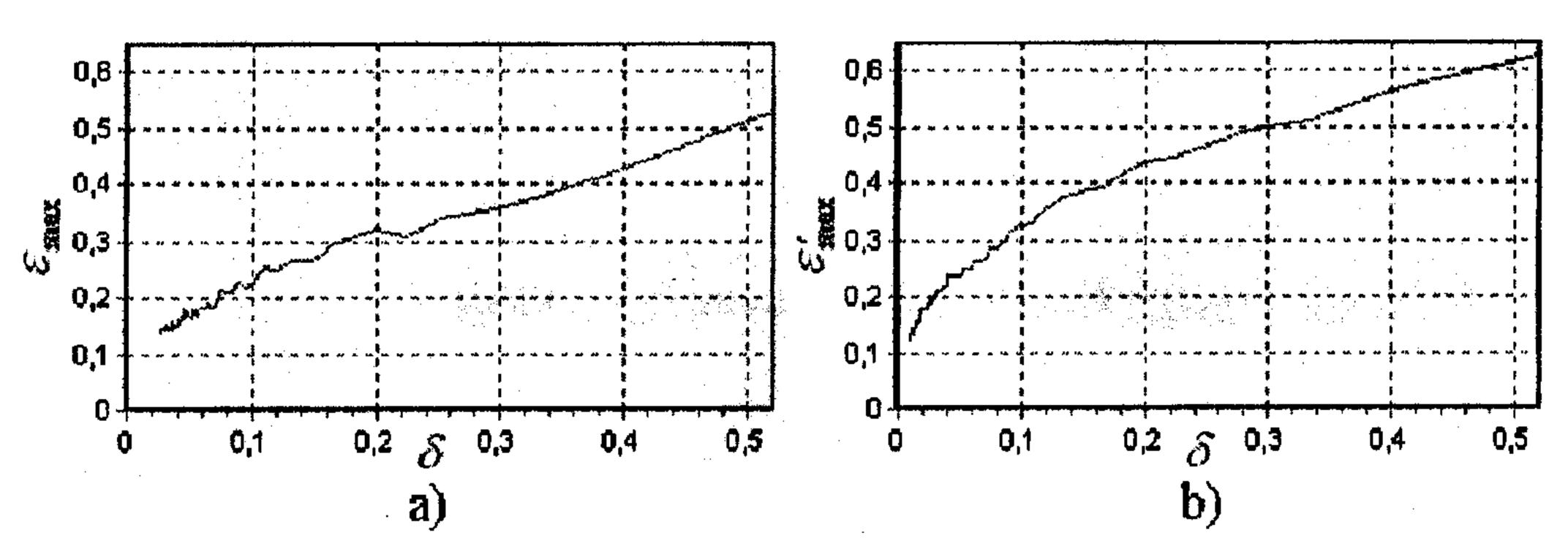


Fig.4. Testing vocal time series described in the Section 2.3. (a) The fixed-set-of-boxes technique indicates many-valuedness. (b) The modified techniques indicates also nonlinearity.

3. Structure Selection (Modeling Nonautonomous Systems)

As it was already mentioned in the Introduction, standard models (2),(3) often prove cumbersome and have divergent trajectories. This is practically inevitable payment for the generality of basic conception, for the saving of time and efforts on the choice of the most suitable mathematical construction. Probability to guess an adequate model form without using a priori information or special preliminary investigation of the object is, in general, very low. The technique described in the previous section provides a possibility to decide between different sets of dynamical variables. But they do not guarantee the success of modeling because one needs also to select an adequate form of functions entering model equations.

Here, we show the expediency of selection of functions based on the use of a priori information with the example of nonautonomous systems being under arbitrary regular (periodic or quasiperiodic) driving. The main idea is that *explicit* functions of time are incorporated into the model equations to describe an external driving efficiently.

3.1. Additive Harmonic Driving

A modification of the standard structure in application to nonautonomous systems was proposed in [32,33] for the simplest case of harmonic additive driving. Even though systems of this kind are widely spread in practice, it is more important for the current consideration that they represent an example illustrating possibility of efficient modification of the standard structure via incorporating certain specific features of the object into the model. We

reproduce briefly the main points of the approach by following [33]. It is suggested to construct a model in the form

$$dx_1/dt = x_2,$$

$$dx_2/dt = x_3,$$
...
$$dx_D/dt = G(x_1, x_2, ..., x_D, t),$$
(6)

$$G(x_1, x_2, ..., x_D, t) = F(x_1, x_2, ..., x_D) + a\cos\left(\frac{2\pi}{T}t\right) + b\sin\left(\frac{2\pi}{T}t\right), \tag{7}$$

One should have certain prerequisites to build a model in the form (6),(7). A priori

where F is an algebraic polynomial. For D = 2, these are general equations of harmonically driven oscillator.

information or a discrete peak in the power spectrum of an observed time series may be such prerequisites. Location of the peak may be viewed also as a rough estimate of the driving period. Given the value of T, parameters a and b and polynomial coefficients are estimated via the linear least-squares routine. To estimate T is not so simple since it enters the equation (7) nonlinearly. An error in its estimation $\Delta T = T - T_0$ (where T_0 is an unknown "true" value) inevitably leads to a significant "phase shift" between the true driving and the corresponding model terms if the training time series is quite long. It is shown in [32,33] that the relative error of driving approximation \mathcal{E}_T depends only on the ratios $\Delta T/T_0$ and T_N/T_0 via

$$\varepsilon_T \sim \frac{\Delta T}{T_0} \frac{T_N}{T_0},\tag{8}$$

where T_N is the duration of the training time series. It follows that the driving period should be estimated more accurately for longer training time series, otherwise incorporation of explicit time dependence is useless. From this point of view, a too long time realization becomes an obstacle for constructing a model (6),(7).

To estimate accurately the driving period T, two preliminary steps are included into the reconstruction procedure. Firstly, a good starting guess for the period should be made. A peak value T^* of the power spectrum can be taken as such a guess since power spectrum with the shape shown in Fig.5,a is often exhibited by periodically driven systems. Secondly, model dimension D and reasonably large value of K are fixed and trial value of T is varied in the vicinity of the starting guess T^* . Equations (6),(7) are fitted to time series data for each trial T. The presence of a profound minimum on the plot ε versus T is a sign of adequacy of the

structure (6),(7). The minimum point of this plot coincides with true period value to a great accuracy (typical form of the plot $\lg \varepsilon(T)$ is shown in Fig.5, b).

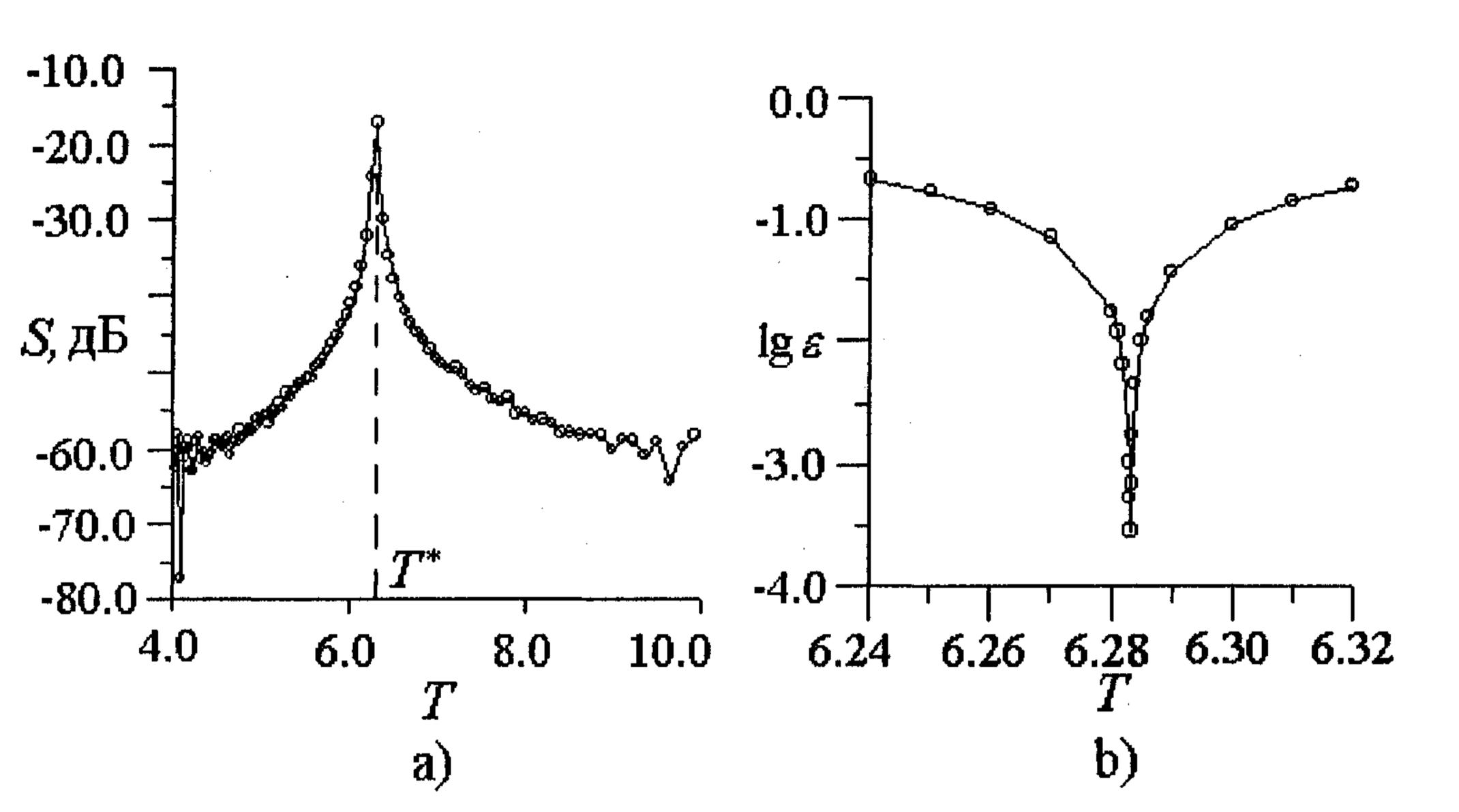


Fig. 5. (a) Typical appearance of the power spectrum for harmonically driven chaotic systems. There is a pronounced peak. (b) $\lg \varepsilon$ versus a trial value of driving period T for a model (6),(7).

This approach is shown to be efficient, in particular, for modeling nonlinear radiophysical systems. Some of the results of its application⁸ are presented in Fig.6. This is the example of modeling driven RLC-circuit with switched capacitors (see the scheme in Fig.2,a) from the integrated chaotic time series of current I, that is for the dynamical variables selected as the best ones in Section 2. An obtained model (6),(7) with D = 2 and K = 9 behaves like the original system and provides a forecast with relative error less than 5 % quite far ahead (namely, on the interval 5T that is big for the considered chaotic regime).

Note that the main cause of efficiency of the structure (6),(7) is that it allows obtaining a model of *lower dimensionality* than it would be necessary under the standard approach. Modeling harmonically driven oscillators with the aid of the standard structure (2),(3) was considered in [47]. In particular, in the absence of noise an adequate 4-dimensional model was obtained for a 3-dimensional original system that required numerical estimation of the time derivatives up to the fourth order. Seemingly, the standard approach could hardly be efficient already for low noise levels since sufficiently accurate calculation of high-order derivatives would be impossible. Besides, it is more probable for the standard polynomial approximation to be efficient when a model phase space is low-dimensional.

Various approaches have been developed to validate empiric models. They include comparison of invariant measures, topological indices, etc, see the section "Model validation" in the review by G.Gouesbet et al in this book. We use only two simple techniques: prediction time and visual inspections of phase orbits

projections. They are sufficient for the purposes of illustration of the approaches developed here.

Exclusion of spurious terms from the model structure was also performed with the aid of a procedure similar to the one described in Section 4.

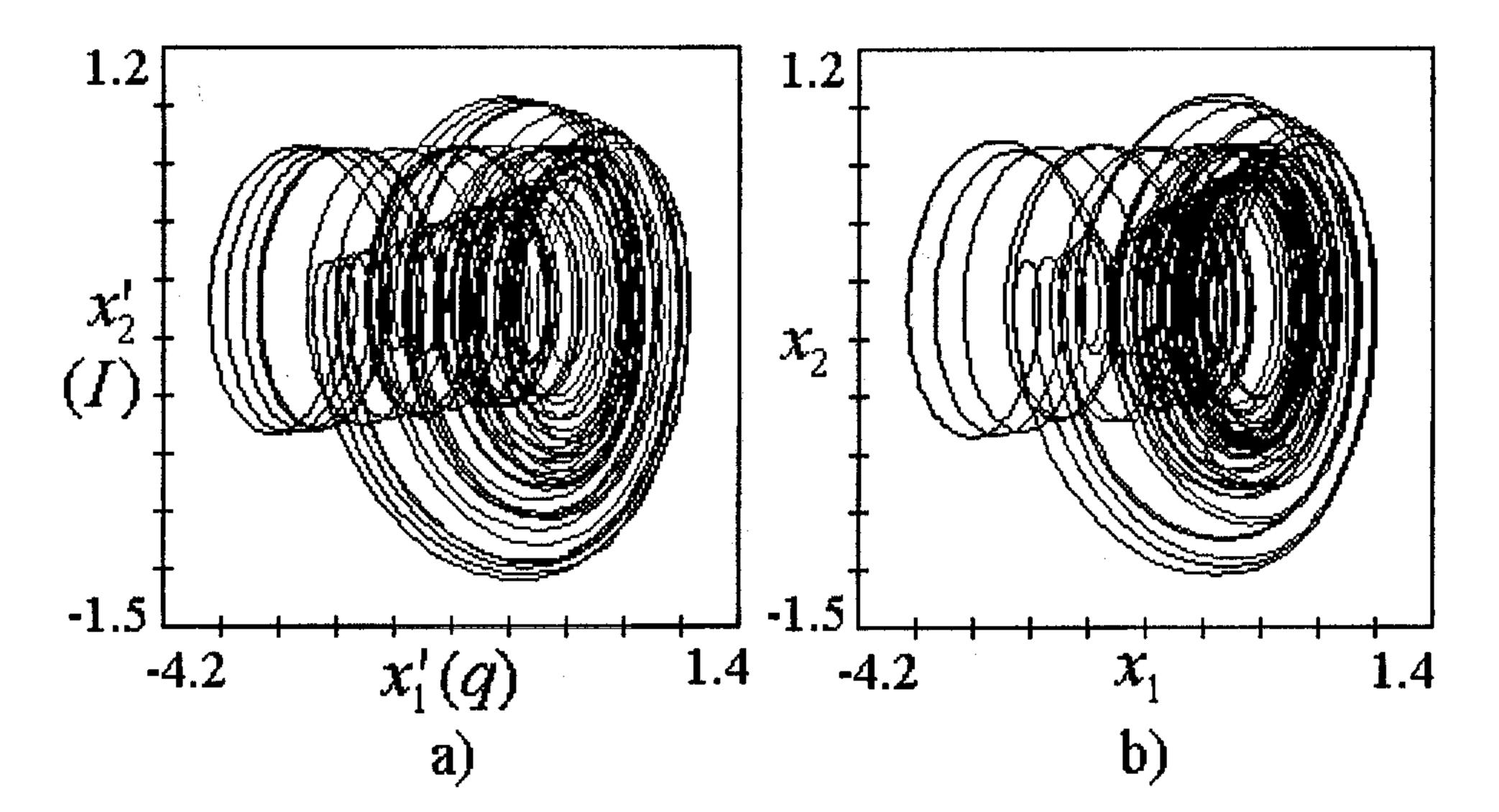


Fig.6. (a) A projection of an experimental orbit for the circuit with switched capacitors onto the plane charge – current. (b) A corresponding projection for the best reconstructed model (6),(7) with D = 2 and K = 9.

Harmonic force represents an important but sufficiently narrow class of possible ways of driving. Here, we present extensions of the approach to more complex and realistic situations. Besides, we somewhat modify the technique for driving period estimation to make it more efficient. We will treat in turn two cases:

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

3.2. Arbitrary Additive Regular Driving

In this case we propose to use the model structure (6) with explicit time dependence but not necessarily harmonic. That is, we employ

$$G(x_1, x_2, ..., x_D, t) = F(x_1, x_2, ..., x_D) + g(t)$$
(9)

where F is an algebraic polynomial, and function g(t) describes the driving and also involves 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 variant is much more general and can be used in the absence of detailed knowledge of the driving form. It consists in exploiting trigonometric polynomials

$$g(t) = a_0 + \sum_{l=1}^{m} \sum_{j=1}^{k_l} \left[a_{l,j} \cos\left(\frac{2\pi jt}{T_l}\right) + b_{l,j} \cos\left(\frac{2\pi jt}{T_l}\right) \right],$$

where m=1 for a periodic case, and quasiperiodic driving is described by the sum of m>1 trigonometric polynomials with different periods T_l and orders k_l . The technique for parameter estimation of the model (6),(9) relies on the least-squares routine (LSR). But, since several free parameters can enter *nonlinearly* the expression for g (this is, at least, the driving period in the case of periodic driving), it is reasonable to use one of iterative techniques to solve a nonlinear least-squares problem. We have used the modified Levenberg — Marquardt routine implemented in the IMSL library.

Note, that considering the driving period as a free parameter for nonlinear least-squares problem alters the above conclusion (Section 2.1) that a long time series is an obstacle for modeling driven systems. That conclusion is true only under the condition that the driving period is preliminary determined and is not adjusted any more with LSR. But if it is estimated along with all the model parameters via LSR, then the accuracy of its estimation just depends on the time series length. This is again because the "phase shift" between the true driving and model terms is large for inaccurate determination of the period. So, long time series allow, and even force, *more accurate* determination of the period value. But a good starting guess for the driving period is still important to apply nonlinear LSR and power spectrum analysis remains useful for that (Fig.5,a). If power spectrum gives a bad starting guess that may occur in special cases, then the approach of [32,33] (Fig.5,b) can help, but a trial value of T should be varied over a wide range rather than near a good starting guess.

We examine efficiency of the approach in numerical experiments by reconstruction of equations from chaotic time series of the x-coordinate of Toda oscillator

$$d^{2}x/dt^{2} + r dx/dt + 1 - e^{-x} = \varphi(t)$$

for different forms of driving $\varphi(t)$. Namely, for impulse periodic, periodic with subharmonics, and quasiperiodic driving. Here, we present just one of the examples when $\varphi(t)$ is a sequence of Gaussian impulses of alternating polarity (Fig.7):

$$\varphi(t) = A \left(\exp \left(-\left(\frac{\tau(t)}{\sigma}\right)^2 \right) - \exp \left(-\left(\frac{\tau(t+T/2)}{\sigma}\right)^2 \right) \right); \ \tau = (t-t_0) \bmod T - \frac{T}{2},$$

where T is a driving period, A is a driving "amplitude", t_0 is an initial phase, σ is an impulse width. Time series is obtained here (and in all numerical examples below) by numerical integration of the original equations with the Runge-Kutta routine (step size and sampling interval are equal to 0.01, the time series length is 5000).

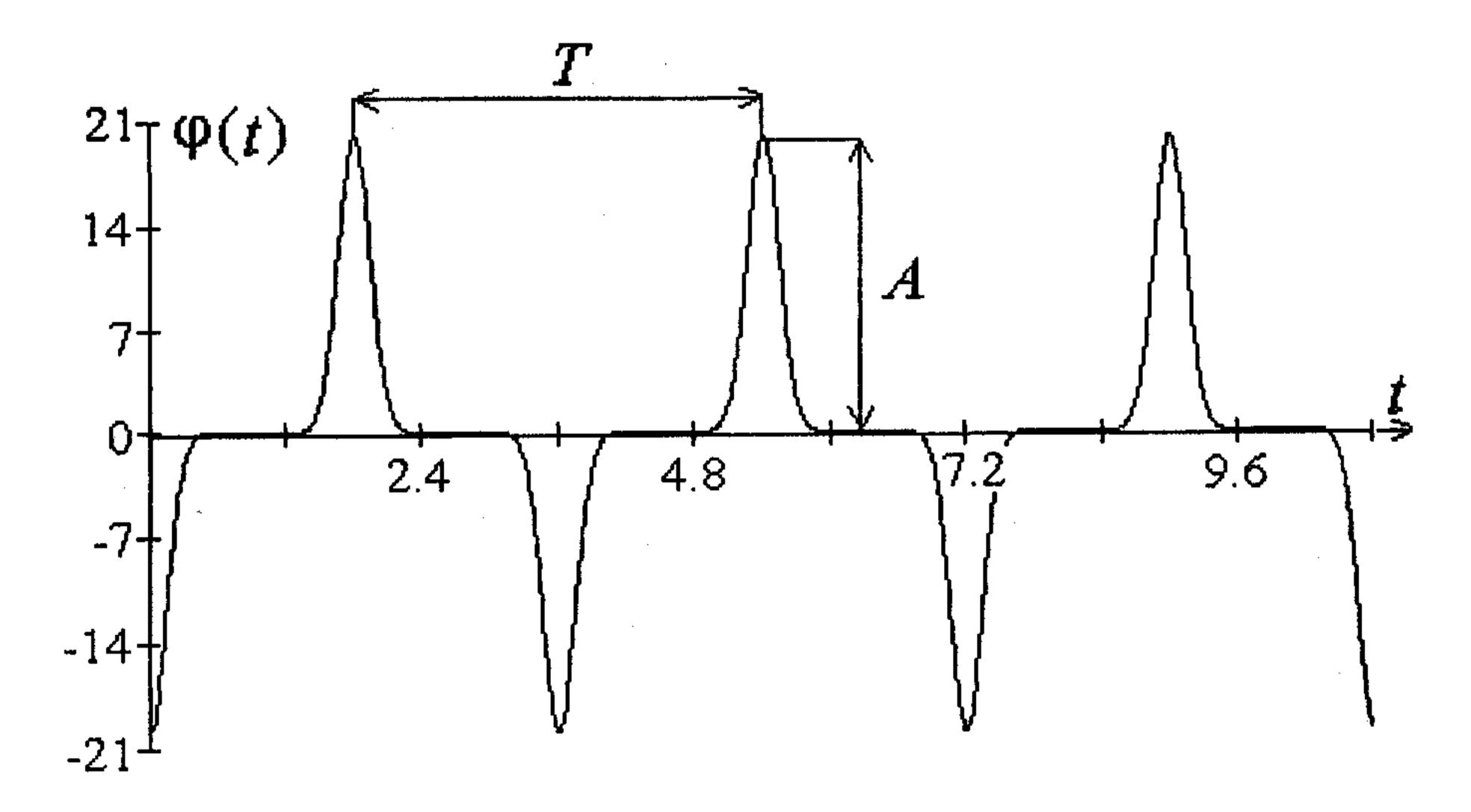


Fig.7. Periodic sequence of Gaussian pulses (12), T=3.6, A=20, $\xi_0=0$, $\sigma=0.2$.

We compared different approaches to structure selection that include standard structure (2),(3), nonautonomous models (6),(9) with a special formula, and nonautonomous models with trigonometric polynomials (6),(9),(10). The results of their application are illustrated in Fig.8 where model and original phase orbits are shown. The standard approach gives bad results: for the best model an approximation error is large $\varepsilon = 86.9\%$, prediction time is small $\tau_{pred} = 0.08T$, and phase orbit does not resemble the original one, see Fig.8,b. As it is expected, a model (6),(9) with D = 2, K = 8 and special formula (12) for description of driving (in effect, only the parameters T, A, t_0 , σ are estimated from time series) demonstrates practically ideal coincidence with the object: $\varepsilon = 0.003\%$, $\tau_{pred} = 21T$ and chaotic attractor is indistinguishable from the original one. Results for models (6),(9),(10) with D = 2, K = 8, m = 1 depend on the number of harmonics k_1 . Qualitative similarity of model and original phase orbits is achieved already at $k_1 = 8$, but quantitative characteristics are not yet the best: $\varepsilon = 4.3\%$, $\tau_{pred} = 2.26T$. Model quality rises with the number of harmonics, see Fig.9. The best results are obtained at $k_1 = 15$: $\varepsilon \approx 0.1\%$, prediction time is quite big¹⁰ $\tau_{pred} = 19.24T$, the attractor is shown in Fig.8c.

The horizon of predictability for the given largest Lyapunov exponent and noise level (truncation and round-off errors) is $\tau_{hor} \approx 60T$. Prediction time τ_{pred} is of the same order of magnitude as τ_{hor} . Their distinction is explained by the imperfection of the model class: an algebraic polynomial is used to approximate an exponential function.

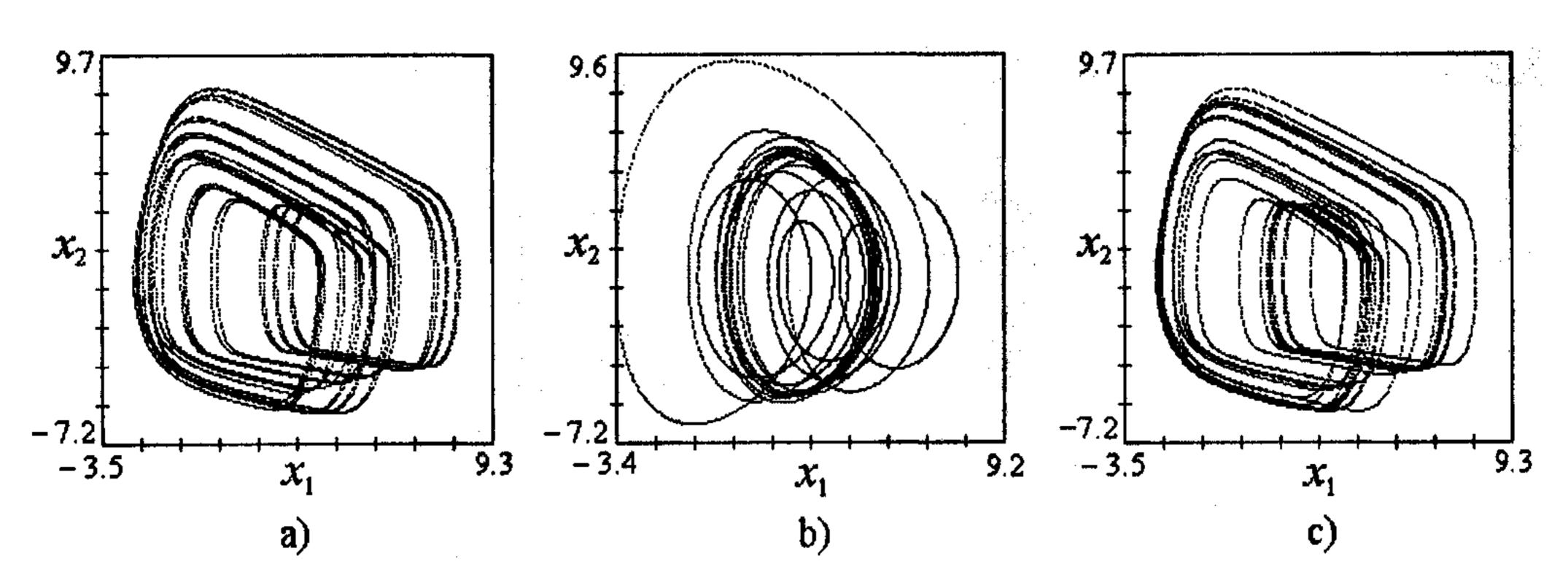


Fig. 8. (a) A projection of phase orbit of an object (11),(12); (b) a projection of phase orbit of the best standard model (2),(3) with D=2, K=9; (c) a projection of phase orbit of the best model (6),(9),(10) with D=2, K=8, m=1, $k_1=15$.

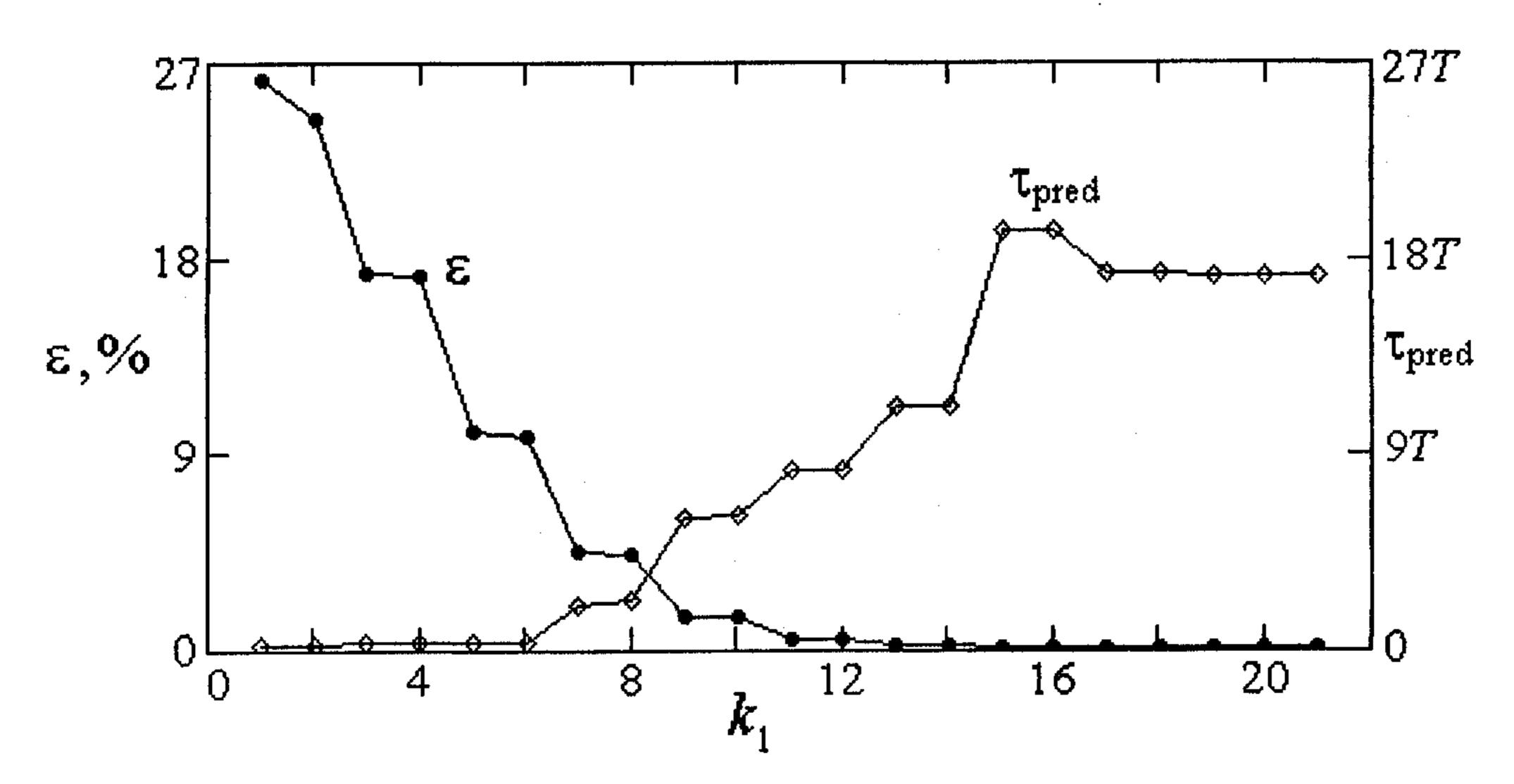


Fig.9. Relative root-mean-squared approximation error and prediction time (in the units of the driving period) versus the number of harmonics for models (6),(9),(10).

Similar results are obtained for regular driving of different kinds and for noisy time series with noise levels up to 1%. They will be reported elsewhere. It is important to note that efficient models (6),(9),(10) can be obtained even with trigonometric polynomials of very high orders, which are necessary to describe non-smooth driving. This is an essential advantage of the approach since instability of models (2),(3) with high-order algebraic polynomials seems the main cause of the standard approach failures. To overcome this difficulty, one should exclude "superfluous" (spurious) terms from the model structure, e.g., the papers [46,23] and section 4 of this paper deal with that problem. Under the use of trigonometric polynomials for driving approximation, the necessity to exclude spurious terms

from them does not arise.

3.3. Arbitrary Way of Regular Driving Entry

Let us consider only the case of harmonic driving here, generalizations to an arbitrary form of periodic and quasiperiodic driving will be straightforward. The degree of generality significantly higher than for a model (6),(7) can be achieved by using the structure (6) and a polynomial with alternating coefficients [41]

$$G(x_1, x_2, ..., x_D, t) = \sum_{l_1, l_2, ..., l_D = 0}^{K} \left(c_{l_1, l_2, ..., l_D} + a_{l_1, l_2, ..., l_D} \cos \omega t + b_{l_1, l_2, ..., l_D} \sin \omega t \right)_{j=1}^{D} x_j^{l_j},$$

$$\sum_{j=1}^{D} l_j \le K.$$

To estimate parameters of the model (6), (13), one can employ the above mentioned LSR. To illustrate efficiency and advantages of the structure (6), (13), we present a numerical example of modeling from a chaotic time series of the U_1 -coordinate of Toda oscillator when driving is not just additive. The original equations read

$$du_1/dt = u_2,$$

$$du_2/dt = -0.45u_2 + (5 + 4\cos t)(e^{-u_1} - 1) + 7\sin t.$$

The best model (6),(13) is achieved at D=2, K=9. It exhibits chaotic attractor practically identical to the original one (Fig.10,a,b). Such results cannot be achieved with models (6),(7) (Fig.10,c). Standard models (2),(3) demonstrate, as a rule, globally unstable orbits (Fig.10d). Prediction times for the best models (6),(13), (6),(7), and (2),(3) are equal to 7T, 1.5T and 0.15T, respectively. See [41] for more details.

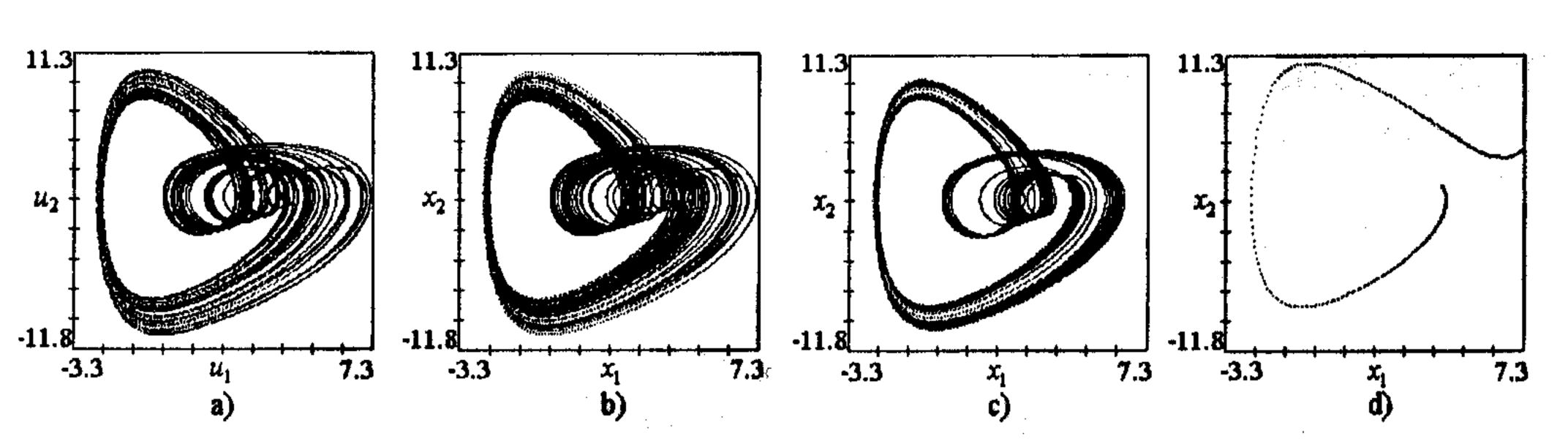


Fig. 10. (a) A projection of attractor of Toda oscillator (14). (b-d) Projections of phase orbits for a model (6),(13) with D = 2, K = 9, a model (6),(7) with D = 2, K = 10, and a standard model (2),(3) with D = 4, K = 6, respectively.

The considered stages (dynamical variables and model structure selection) are the key ones for modeling. However, efficient specialized techniques for model refinement are also useful. Thus, model structures (6),(9),(10) and (6),(13) allow obtaining more parsimonious models since they contain less variables, than it would be needed under the standard approach, due to incorporation of explicit time dependence. Big model size conditioned by a

high-order trigonometric polynomial (10) does not lead to difficulties as it has been shown above. But nonautonomous models involve also algebraic polynomials describing nonlinearity of the object and, hence, a large number of terms in those polynomials can lead to difficulties. Many of their terms can reduce the model quality drastically. So, to construct nonautonomous models involving algebraic polynomials as well as the standard models, it is important to exclude spurious model terms. A feasible special procedure for that is presented in the following section.

4. Model Structure Optimization

Usually, global models are constructed from time realizations of established motions corresponding to attractors in phase space of an object. Such an approach seems reasonable when only the dynamics on the attractor is of interest. However, for modeling object dynamics in a wide domain of the phase space, success is more probable when one uses time realizations of transient processes, i.e. when a phase orbit has not yet settled down onto an attractor. As it was shown in [43], the use of transients can be sometimes useful to refine a model by optimizing its structure. As we hypothesize, this is because they explore a wider domain of the phase space. In this section we briefly describe the main results concerning detection of the time series segment which is optimal for modeling. Then, a model structure optimization procedure will be explained.

To detect a segment optimal for modeling, we compare performance of global models obtained from different segments of the time series, some of them involve a transient while the others do not. For the sake of convenience, it is reasonable to illustrate the idea by using sufficiently simple autonomous system. We choose Van der Pol – Toda oscillator which equations read as

$$dx_1/dt = x_2,$$

 $dx_2/dt = (1 - x_1^2)x_2 - 1 + \exp(-x_1).$

Reconstruction is performed from a scalar time series of the X_1 -coordinate involving a transient. The corresponding phase orbit is shown in Fig.11, a. Models of the form (2) with D = 2 are constructed in two variants differing from each other by the form of the function $F(x_1, x_2)$. In the first case, a standard bivariate algebraic polynomial is employed:

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

In the second case, F is given by

$$F(x_1,x_2) = (\lambda - x_1^2)x_2 + f_K(x_1)$$
,

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

$$\sigma = \iint_{S} (F(x_1, x_2) - F_0(x_1, x_2))^2 dx_1 dx_2 , \qquad (18)$$

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

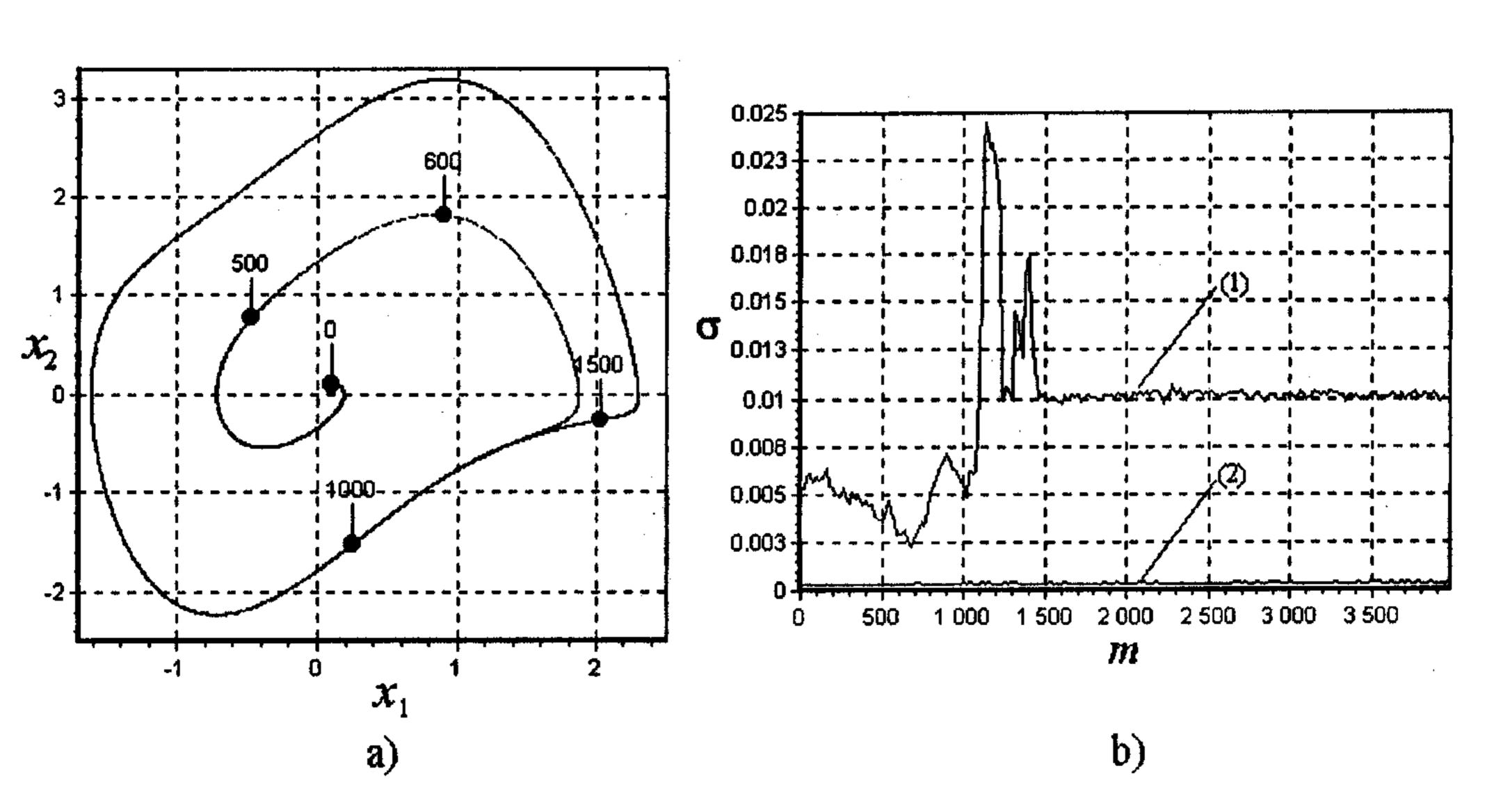


Fig.11. (a) A phase orbit of the system (15). (b) Model error σ versus the location m of a reconstruction window for models (2),(16) (the curve 1) and models (2),(17) (the curve 2) with polynomials of the 7th order.

Searching for a segment of the time series (a reconstruction window), which is optimal

for modeling, is performed as follows. A certain length of a reconstruction window (M data points) is specified. We denote a reconstruction window as $\{\eta(t_i)\}_{i=m}^{m+M-1}$, where m is the number of its starting point. The initial point of the original time series coincides with the starting point of a reconstruction window for m=1. When m increases, a reconstruction window moves along a time series into the domain of an attractor. Models are constructed for different values of m. Optimal location of the reconstruction window corresponds to a minimum on the plot σ versus m.

Plots o(m) in Fig.11, b show that the best results for a model (2),(16) are obtained with the use of the transient, see the curve 1, small m. For a model (2),(17) the overall results are better by an order of magnitude, see the curve 2, but they are almost independent on the location of the reconstruction window. It can be explained as follows. The structure (2),(16) includes variety of superfluous (spurious) 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 (15). Theoretically, model coefficients corresponding to superfluous terms should vanish. But in practice their estimated values differ from 0 due to round-off and truncation errors and impossibility of accurate approximation of exponential function by an algebraic polynomial. Superfluous terms can become significant outside of a reconstruction window and lead to essential discrepancies between an object and a model. For a model (2),(16) involving spurious terms, σ depends on m essentially (Fig.11,b) that is induced by essential dependence of "spurious coefficients" on m (Fig.12,a). For a model (2),(17), the use of a transient does not have advantages because its good performance is due to the absence of spurious terms rather than the extension of the explored region in the phase space.

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, i.e. in a transient period. Relying on these considerations, we propose a procedure for model structure optimization based on sequential exclusion of the terms corresponding to the less stable coefficients. The stability (reliability) of some coefficient a can be evaluated as the ratio of its mean value to its standard deviation $\langle a \rangle$

Let us look again at Fig. 12, a where the plots for coefficients corresponding to necessary

$$m_1 = \frac{\langle a \rangle}{\sqrt{\langle (a - \langle a \rangle)^2 \rangle}}$$
, 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 the corresponding term is excluded from the model. Reconstruction procedure is repeated for the simplified structure. The next less stable coefficient is detected and the next term is eliminated, and so on until exclusion of a new term leads to model deterioration. In Fig. 12,b we present the error σ versus the number of excluded terms as obtained during reconstruction from the time series of the system (15) starting from the model structure (2),(16). It can be seen that the proposed procedure allows essential reduction of the error (after exclusion of 20 terms) and, hence, enhancement of the model quality.

Despite the above-mentioned successful results, we should make several remarks. Firstly, we cannot guarantee that the use of transients will *generically* help. Secondly, reconstruction from different segments of a realization representing dynamics on an attractor, in principle, can also lead to similar refinement of the model structure. Thus, reconstruction with standard functions from unstable periodic orbits or from laminar phases of an intermittent signal can be successful [54]. But, in our opinion, the use of transients should often be more useful. This is a hypothesis but it relies on an empiric basis. For example, one can see in Fig.12 that coefficients corresponding to spurious terms oscillate quite intensively only in the region of a transient. So, inspection of a transient part of the time series is essentially preferable for their detection in this case.

A similar procedure was considered in [53] where it was called "zeroing and refitting" rather than "model structure optimization". In the current context we prefer the latter term.

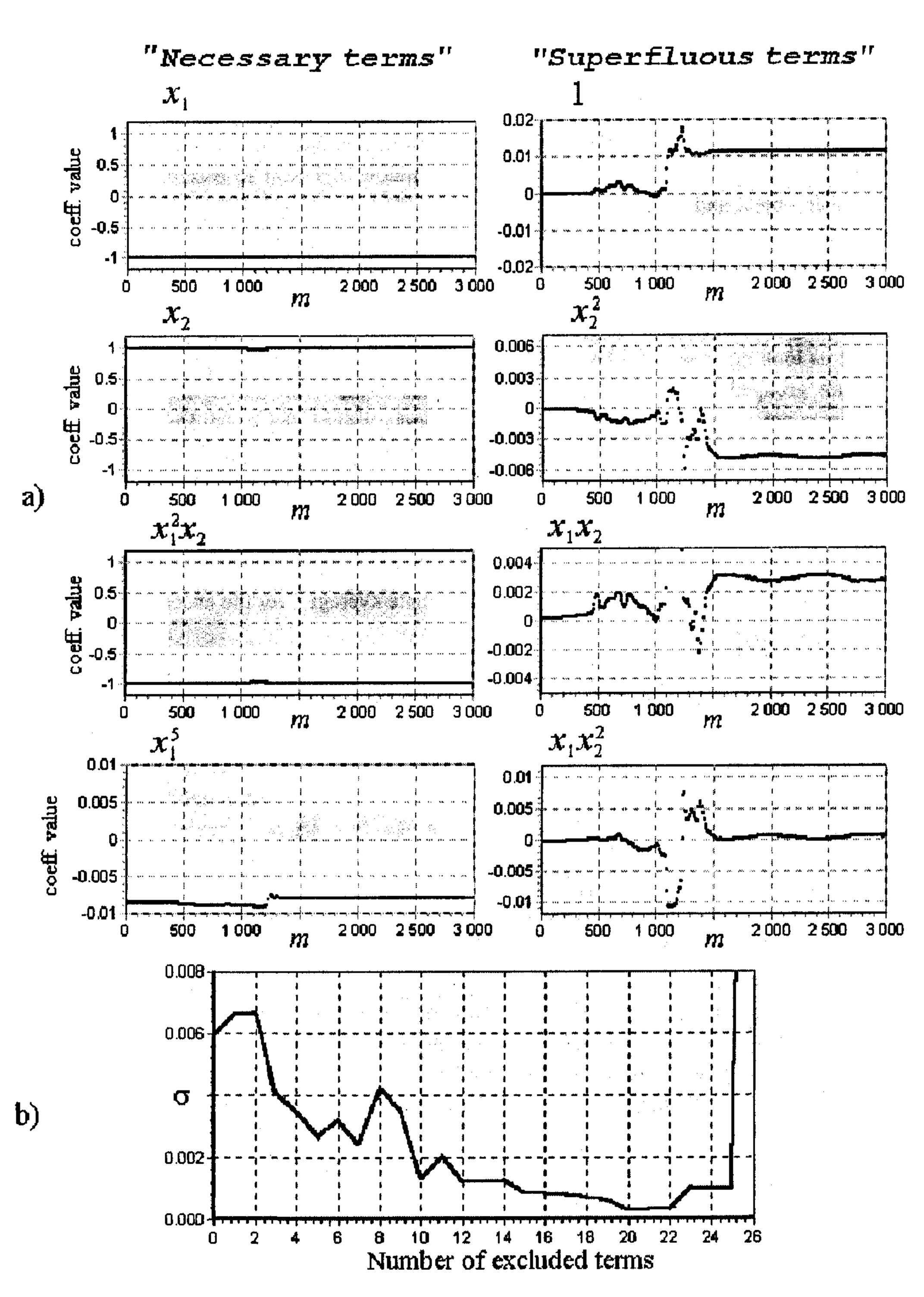


Fig. 12. Results of modeling the system (15) from a scalar time series. (a) Coefficients of a model (2),(16) corresponding to polynomial terms presented near the panels versus the location m of a reconstruction window. (b) The error σ versus the number of excluded terms. Optimization is performed starting from the model structure (2),(16).

5. Conclusions

Analysis of publications shows that to date significant efforts have been made to solve the modeling problems of the kind that we refer to as the highest level of complexity in Section 1.4 (reconstruction of equations in the case of absence of a priori knowledge about an object under investigation). However, examples of successful modeling in such a situation are quite rare and determined by the possibilities of obtaining additional information on the possible model structure.

In the most preferable situation when the model structure is *completely* known, e.g., from the first principles, the results of modeling depend mainly on the amount and precision of experimental data. Estimation of parameters performed in such a situation can, nevertheless, be a very useful tool for many applications. Very interesting researches of this kind are presented in [38,55].

To our best knowledge, there are almost no works addressing the second level of complexity; to a certain extent, the paper [39] can be related to them. However, in our opinion, it is this statement of the problem that is the most promising for obtaining useful results in many fields, since it represents a combination of empiric modeling and modeling from the first principles.

In this paper, we address only the most difficult situation – a reconstruction problem. To advance further in the field of global reconstruction from time series, one needs both the development of novel technical procedures and creation of methods oriented to sufficiently narrow classes of objects. The latter approach is, in a sense, close to the second situation from the systematization given in Section 1.4. And it might be, probably, the most important direction of research. A special preliminary analysis of time series and the use of a priori information are needed for this approach. In our works, prospects and necessity of such a "specialization" are shown and technical procedures are presented. The main results are as follows:

- 1. the proposed technique for preliminary testing of times series of dynamical variables (section 2) provides the variants which are the most suitable for modeling;
- 2. the proposed modifications of the standard model structure (section 3) allow obtaining efficient models of nonautonomous systems for arbitrary periodic and quasiperiodic driving, both for additive and parametric character of driving;
- 3. the proposed procedure of model structure optimization (Section 4) allows elimination of spurious terms from the model structure using properties of transient processes, whereby performance of an empiric model can be significantly refined.

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