Role of transient processes for reconstruction of model equations from time series

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We perform a global reconstruction of differential and difference equations, which model an object in a wide domain of a phase space, from a time series. The efficiency of using time realizations of transient processes for this purpose is demonstrated. Time series of transients are shown to have some advantages for the realization of a procedure of model structure optimization.

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I. INTRODUCTION

In the last years, different approaches to the reconstruction of model differential and difference equations from time series (finite sets of values of an observable measured at sequential time instants) have been developed [1–9]. Such models are used for prediction [7,10], control [3], signal classification [11], and information transmission [12]. Depending on the purposes of modeling, the obtained equations purport to describe an object evolution in an entire whole phase space (*global* reconstruction) or in a small neighborhood of a given state (*locally*). In the majority of works we are aware of, global models are constructed from time realizations corresponding to attractors in a phase space. Such an approach seems reasonable when the problem of predicting the future behavior of an object is addressed. This work is devoted to a global modeling of an object dynamics in an entire phase space rather than only that of a certain regime. The purpose of this work is to show, by considering several examples, that, under this point of view, it is more efficient to use time realizations of transient processes (when a phase orbit has not yet settled down onto an attractor). Such global models can be useful when it is necessary to predict an object evolution from an arbitrary initial state. There are other possible applications, e.g., a model constructed from a transient was applied successfully to calculating Lyapunov exponents of a periodic orbit [13].

We compare the capabilities of global models constructed from different parts of a time series—some of them include a transient process and others ignore it. We take the most illustrative exemplary dissipative dynamical systems as objects of modeling (Sec. III), and employ well-known approaches to reconstruction (Sec. II). The quality of reconstruction is assessed by comparing functions entering the right-hand sides of an original dynamical system and a reconstructed dynamical system (an object and a model), and by estimating the model ability of short-term predictions from different initial conditions (Sec. II).

In this work we do the following: (1) We show that the use of a transient process allows for a broadening of the domain in a phase space where equations reconstructed by standard methods describe an object dynamics sufficiently well. (2) We propose a procedure for model structure optimization which employs a time series of a transient to detect superfluous terms (Sec. IV). Generalizations of the obtained results, and limitations to the use of transients for modeling are discussed in Sec. V.

II. TECHNIQUE OF INVESTIGATION

The most often used scheme of global modeling from a time series consists of the following three steps.

(1) One specifies the form of model equations drawing on *a priori* information, substantial models, results of time series analysis (e.g., an estimate of the correlation dimension of a phase orbit reconstructed from the time series), and intuition.

(2) One transforms an original time series according to the specified form. That is, one performs noise reduction, numerical differentiation, integration, or another transformation of a scalar time series v: $\{v_i\}_{i=0}^{N-1}$, $v_i=v(t_i)$, and $t_i=i\Delta t$. Then a series of state vectors $\{\mathbf{x}_i\}$ is formed (using methods of time delays [1,2,6], successive derivatives [5,7], etc).

(3) A training part of an obtained series (*a reconstruction window*) is selected. A model type (a discrete map or a differential equation) and explicit forms of functions entering a model are specified. Thus, a model map relates the states of an object at sequential time instants to each other, and reads

$$\mathbf{x}_{i+1}=\mathbf{f}(\mathbf{x}_i).$$

Components of a vector-valued function $\mathbf{f}$ are often assumed to be polynomials of certain orders [1]. After specifying a model structure, one calculates the values of its coefficients from a training time series. A least-squares routine is usually employed [1,8], that is, the values of coefficients are selected so as to minimize the sum of squared errors:

$$\sum_i [\mathbf{x}_{i+1}-\mathbf{f}(\mathbf{x}_i)]^2=\min.$$

When modeling an object with the use of differential equations, the idea remains the same. The only differences are: a dependency $\dot{\mathbf{x}}=\mathbf{f}(\mathbf{x})$ is approximated instead of $\mathbf{x}_{i+1}=\mathbf{f}(\mathbf{x}_i)$ and a preliminary numerical differentiation of the series $\{\mathbf{x}_i\}$ is necessary [2,5–7]. Finally, the quality of an obtained model is assessed using a different (test) part of the series

$\{v_i\}$ with the aid of a criterion corresponding to the purposes of modeling (several possible criteria are discussed below in this section).

Our research concerns only the third step — selecting a location of a reconstruction window inside the original series which provides a model efficient in a wide domain of phase space. Therefore, we use exemplary ordinary differential equations and coupled maps as objects to be modeled, and construct models in agreement with their structure. That is, we reproduce their structure completely and find only unknown values of coefficients, or else we change the types of approximating functions while the number of equations is maintained. Original time series are obtained as numerical solutions. The noise level is insignificant here, since it is determined only by truncation and round-off errors. All this allows one to avoid difficult problems of the first and second steps of the reconstruction procedure, and to concentrate on solving our problem.[1]

In our research, model equations are obtained for different locations of a reconstruction window inside a time series. Hence a reconstruction window contains a larger or smaller part of a transient process. Models are compared to an object using the following criteria of quality.

(1) *A direct comparison* of coefficients entering equations (as in Sec. III A where object and model structures coincide completely).

(2) *An approximation error* ε. Functions entering the right-hand sides of reconstructed and original equations (f_m and f_0, respectively) are compared. This makes sense only when original and model equations have similar structures. That is, in examples of Secs. III B and IV, an object and a model have the forms

$$\dot{x}=y,$$

$$\dot{y}=f(x,y,t), \tag{1}$$

and an approximation error ε is given by

$$\varepsilon=\int\int\int_V (f_m(x,y,t)-f_0(x,y,t))^2 dx\,dy\,dt. \tag{2}$$

V is the domain of integration containing a reconstructed phase orbit, which is significantly wider than the domain of an attractor. The less the value of ε, the better the model.

(3) *A prediction time* τ is a time interval at which a root-mean-squared prediction error $\sigma(t)$ achieves a certain preset threshold value $\sigma(\tau)=\sigma_{thr}$ (we use the value $\sigma_{thr}=0.05$). The greater the value of τ, the better the model. To estimate $\sigma(t)$, one should calculate a squared difference between observed and predicted values of the variable v at a time instant t: $[v_{obs}(t)-v_{pred}(t)]^2$ [when object and model initial conditions coincide, i.e., $\mathbf{x}_{object}(0)=\mathbf{x}_{model}(0)$]. The squared difference is averaged over the set of different initial conditions whose boundaries are situated far beyond the domain of an attractor. The dependency $\sigma(t)$ is derived as $\sigma(t)=\sqrt{\langle[v_{obs}(t)-v_{pred}(t)]^2\rangle_{\mathbf{x}(0)}}$.

The procedure of our investigation is as follows. A certain length of a reconstruction window (M points) is specified. A reconstruction window can be denoted as $\{v_i\}_{i=m}^{m+M-1}$, where m is the number of initial point. The initial point of the original time series corresponds to 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. The part of a time series which provides the most efficient model is detected by considering graphs of the above-mentioned criteria of quality versus m.

III. NUMERICAL EXAMPLES

A. Reconstruction of a discrete dynamical system

A typical situation in nonlinear dissipative systems is that an attractor is contained in a subspace whose dimension is less than the dimension of the entire phase space. Perturbations transversal to this subspace are vanishing, while the dynamical regime is being settled. As a result, some information (potentially useful for modeling) is lost. For example, when a synchronous (uniform) regime in a system of coupled pendulums is settled, each element moves in the same way (as if there were no other elements). That is, a time series contains no information about the complexity of the system. However, time series of transients may contain some information about nonuniform motions and increase possibilities of modeling. Let us demonstrate this by using a system of dissipatively coupled quadratic maps

$$\begin{aligned} x_{n+1}&=\lambda-x_n^2+k(x_n^2-y_n^2),\\ y_{n+1}&=\lambda-y_n^2+k(y_n^2-x_n^2), \end{aligned} \tag{3}$$

where x and y are dynamical variables, k is a coupling parameter, and $n=0,1,2,\ldots$ is a discrete time. This exemplary system is characterized by an infinite number of regular and chaotic oscillatory regimes (variants of synchronization of subsystems oscillations) and by multistability [14–20]. Let us specify the values of parameters $\lambda=1.8$ and k in the range from 0.4 to 0.5, at which a synchronous chaotic regime (when x and y change in time in a chaotic but the same manner) is stable. A phase orbit corresponding to the parameter value $k=0.4$ and initial conditions $x_0=0.1$ and $y_0=0.4$ is presented in Fig. 1(a). A transient is shown with filled circles, and sequential numbers of iterations are marked by Figs. 1, 2, ... Oscillations of the subsystems are synchronized quickly, i.e., deviations transversal to the diagonal (and to the attractor) vanish quickly. Time realizations of a difference signal x_n-y_n (which is proportional to a transversal deviation) for $k=0.4$ and 0.42 are shown in Fig. 1(b) by filled circles and crosses, respectively. Note that smaller values of k from the specified range correspond to

[1]When modeling real systems, one cannot point out the best form of the equation to be reconstructed. In addition, it is necessary to solve the problem of noise. This can affect the success of modeling dramatically and prevent us from estimating the effect of location of a reconstruction window on the results, which is the purpose of this work.

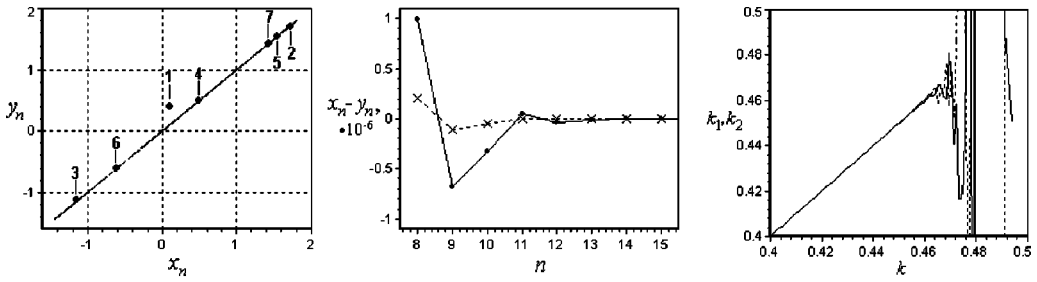

FIG. 1. (a) A phase orbit of the system of coupled quadratic maps [Eq. (3)] at $\lambda=1.8$ and $k=0.4$, starting from the point $x_0=0.1$, $y_0=0.4$. (b) A difference signal x_n-y_n of system (3) at $k=0.4$ (filled circles, the solid line) and at a greater value of k: $k=0.42$ (crosses, the dashed line). (c) The values of coefficients k_1 and k_2 of a model [Eq. (4)] reconstructed from time realizations of system (3) at $\lambda=1.8$ and different k. The length of a reconstruction window is $M=100$, and the number of the initial point is $m=7$.

longer transients. This is explained by the fact that the synchronous regime is stable (at the specified value of λ) only if $k\geqslant 0.361$ [17], and perturbations vanish more slowly near bifurcation values of a parameter. Let us reconstruct model equations from a time series which starts from the point $(x_0=0.1, y_0=0.4)$ lying apart from a synchronous attractor. We consider different variants of a model equations structure, an original time series, and criteria of quality.

1. Reconstruction from a vector time series

Model difference equations are reconstructed in the forms

$$x_{n+1}=\lambda_1-x_n^2+k_1(x_n^2-y_n^2),$$
$$y_{n+1}=\lambda_2-y_n^2+k_2(y_n^2-x_n^2), \tag{4}$$

where λ_1, λ_2, k_1, and k_2 are parameters to be determined from a time series (see the modeling procedure in Sec. II). A vector time series — a sequence of values of x_n and y_n obtained by iterating map (3) — should be used for this purpose. In this case, a simple coincidence of values of the coupling parameters k_1, k_2, and k (and also of λ_1, λ_2, and λ) may serve as a criterion of model quality. Thus in Fig. 1(c), where reconstructed values k_1 and k_2 are ordinates and original values of k are abscissas, the diagonal corresponds to the ''correct'' values. That is, the greater the distances of points from the diagonal, the worse the model.

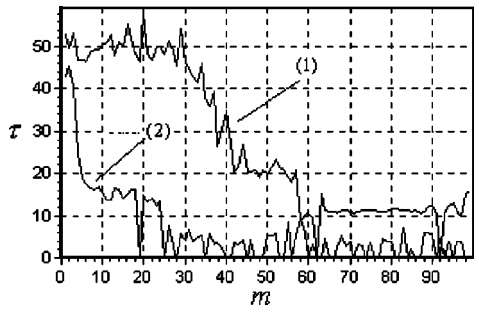

FIG. 2. Prediction time τ of a model [Eq. (5)] with a polynomial of the fourth order vs the number m of an initial point of a reconstruction window for $k=0.2$ (curve 1) and for $k=0.3$ (curve 2). The length of a reconstruction window is $M=100$.

Calculations show that the larger the part of a reconstruction window occupied by a transient, the better the results of reconstruction. That is, a range of successful reconstruction for $m=7$ is an interval of small k [Fig. 1(c)] which corresponds to less stability of a synchronous regime and to longer transients. In the region of large values of k where the synchronous motion is more stable and transients are shorter, the results of reconstruction are bad (see the right-hand side of the figure). In addition, the dependencies of model coefficients on k began to oscillate intensively. This means that model coefficients are sensitive to insignificant peculiarities of an original time series. On decreasing m to 0, when the relative length of a transient is the longest, equations are reconstructed successfully in the whole specified range of k. On increasing m, points of a transient are, conversely, no longer used for reconstruction, and the domain of bad results is almost the whole specified range of k.

2. Reconstruction from a scalar time series

Let us complicate the problem of reconstruction by considering a scalar original time series. Models are reconstructed from a time series $\{x_n\}$ of the same object in the form

$$x_{n+1}=P(x_n,x_{n-1}), \tag{5}$$

where $P(x_n,x_{n-1})$ is a standard algebraic polynomial whose optimal order is selected during a modeling process (see the modeling procedure in Sec. II). In this case it appears to be equal to 4. We use a prediction time τ as a criterion of model quality (see the third criterion of quality in Sec. II): the greater the value of τ, the better the model.

Dependencies of τ on the number of an initial point m for model (5) are shown in Fig. 2. It can be seen from the graphs that using a transient (decreasing m) leads to an increase of model quality. The same conclusion can be made noting that the interval of m providing a good model prediction becomes smaller when the relative length of a transient decreases. Curve 2 corresponds to a larger value of the coupling coefficient k in original equations (3) when a transient is significantly shorter than for the curve 1.

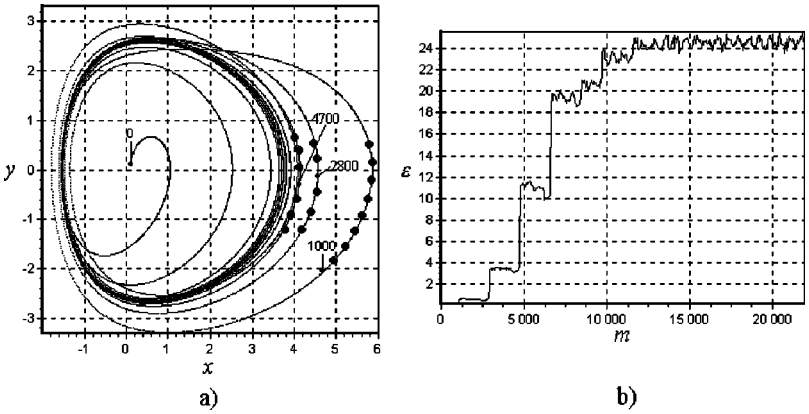

FIG. 3. (a) A projection of a phase orbit of a system [Eq. (6)] starting from the point $x(0)=y(0)=0.1$. This orbit corresponds to an original time series. (b) An approximation error ε vs the number m of an initial point of a reconstruction window.

B. Reconstruction of a continuous-time system

Consider an example of reconstructing differential equations — a nonautonomous Toda oscillator:

$$\dot{x}=y,$$
$$\dot{y}=-0.1y-1+e^{-x}+\cos t. \tag{6}$$

This system is a representative of a wide class of nonlinear dynamical systems. It comprises exponential nonlinearity and an explicit time dependence. A scalar time series of values of the x coordinate is obtained by integrating Eqs. (6) numerically using the standard fourth-order Runge-Kutta routine with a step 0.01. Initial conditions are chosen outside of an attractor which is a limit cycle at the chosen values of the parameters. A projection of a phase orbit underlying an original series is shown in Fig. 3(a), where the numbers of some points are presented by figures (an initial point has the number 0). An attractor is situated where the points of the orbit are more dense. As can be seen from the figure, motions near the attractor occupy rather a small part of the area bounded by the orbit.

The structure of model equations is that of Eq. (1), with the function f in the form

$$f(x,y,t)=P_n(x)+\gamma y+A\cos\omega t+B\sin\omega t, \tag{7}$$

where $P_n(x)$ is a standard polynomial of the fifth order. We use a reconstruction technique which draws upon the scheme of Sec. II, and is modified for nonautonomous systems [21–24]. The values of the parameters γ, A, B, and ω and of the polynomial coefficients are calculated from the time series (via a least-squares routine; see Sec. II).

The dependence of an approximation error ε on m is shown in Fig. 3(b). The length of a reconstruction window is $M=2000$, and a basic period of oscillations contains about 600 points. The best models are obtained at small values of m when a transient is taken into account. The graph $\varepsilon(m)$ has a specific ''steplike'' form that illustrates the worth of one part or another of the series for the purpose of reconstruction. Thus the almost horizontal parts of the graph correspond to ignoring points from the vicinity of the attractor, which indicates their small influence on a model quality. The jumps between flat steps on the graph, where the quality of the model decreases quickly with the increase of m, correspond to excluding the points marked by circles in Fig. 3(a) from a reconstruction window. These points belong to a transient, and are the most distant from the attractor.

IV. USING A TRANSIENT PROCESS FOR MODEL STRUCTURE OPTIMIZATION

Increasing the amount of information about an object is not a unique reason for the use of transients for reconstruction of model equations. The second, not less important, cause for employing nonstationary data is the possibility of their efficient use for model structure optimization (namely, for exclusion of superfluous terms from a polynomial in our case). Let us illustrate this with an example of reconstructing a model of a van der Pol–Toda oscillator,

$$\dot{x}=y, \tag{8}$$

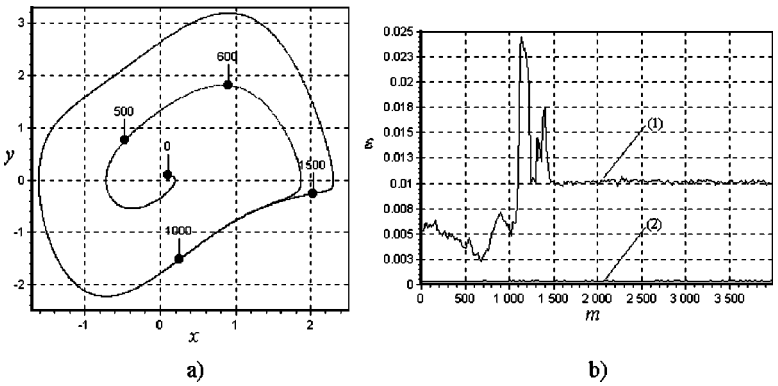

FIG. 4. (a) A projection of a phase orbit of a system [Eq. (8)] which corresponds to an original time series. (b) An approximation error ε vs m for models (1) and (9) with a standard polynomial of the seventh order (curve 1) and for the models (1) and (10) (curve 2).

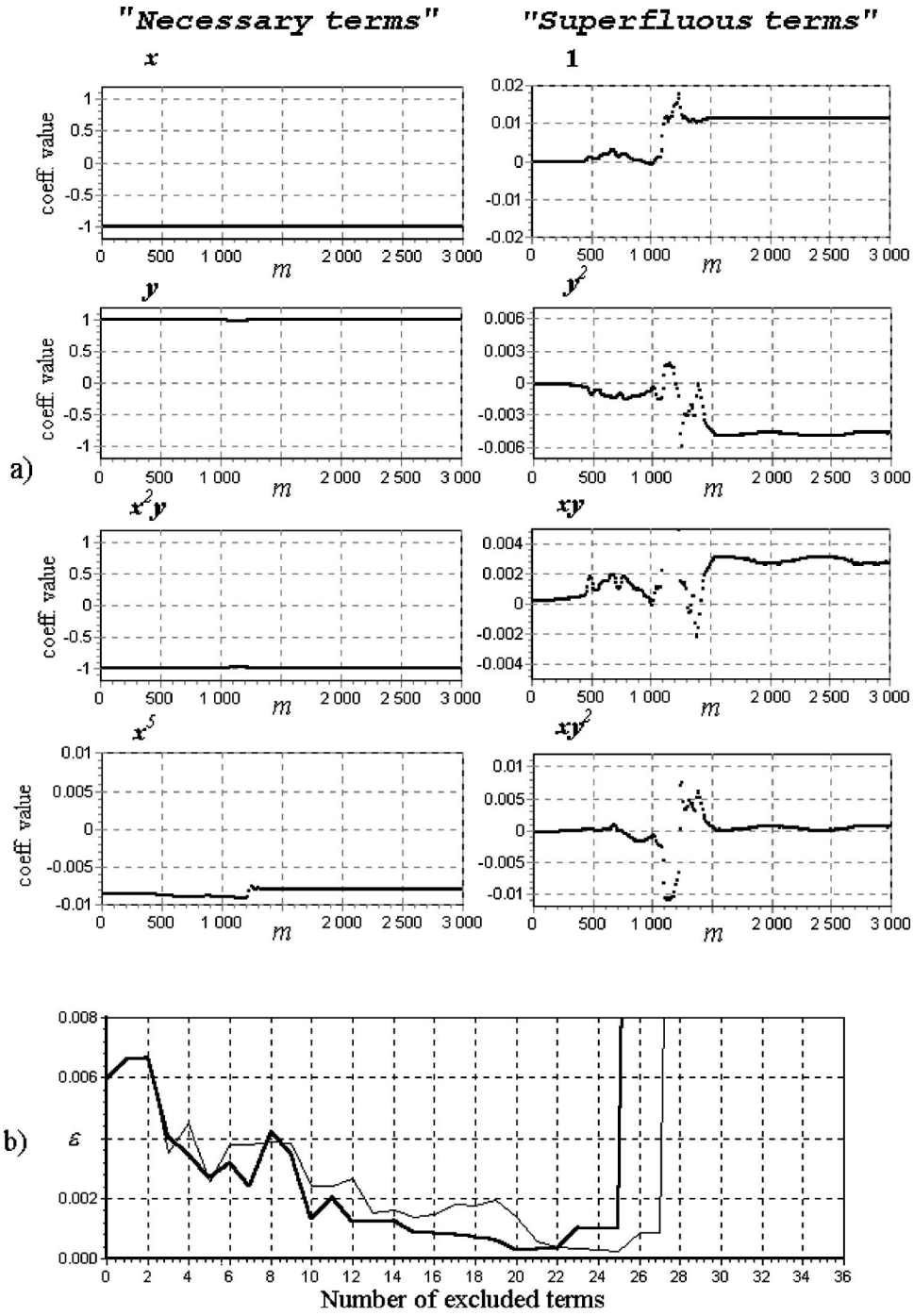

FIG. 5. Results of the reconstruction of system (8) from a scalar series: (a) Reconstructed values of coefficients corresponding to the shown monomial terms of the models (1) and (9) vs m. (b) An approximation error ε vs the number of terms excluded from a model during the process of its structure optimization. The thick line corresponds to using characteristic (11), and the thin line corresponds to using characteristic (12).

$$\dot{y} = (1-x^2)y - 1 + e^{-x},$$

from a scalar time series corresponding to a phase orbit in Fig. 4(a). A model is constructed in the form of Eq. (1) in two variants which differ from each other with the form of a function $f(x,y,t)$ (see the modeling procedure in Sec. II). First, a standard bivariate polynomial is used:

$$f(x,y,t) = P_k(x,y) = \sum_{i,j=0}^{k} a_{ij} x^i y^j, \quad i+j \leqslant k. \tag{9}$$

Second, a function is found in the form

$$f(x,y,t) = (\lambda - x^2)y + P_n(x), \tag{10}$$

where $P_n(x)$ is a standard univariate polynomial which, in fact, approximates an exponential function. The first structure contains many ''superfluous'' terms (e.g., the terms with xy, xy^2, x^2y^2, . . . , and others which do not enter the second equation of the object [Eq. (8)]). Ideally, if the order of a polynomial were infinite, the accuracy infinitely high, and

the time series of an infinite length, then the values of coefficients corresponding to superfluous terms would be equal to zero. In practice, however, their values differ from zero due to truncation and round-off errors, etc. They are fitted so as to minimize an approximation error over the points of a reconstruction window. Outside the window, in a test part of the series, superfluous terms can affect the results essentially, and lead to a significant difference between a model and an object.

Let us compare dependencies $\varepsilon(m)$ for models [Eqs. (1) and (9) and Eqs. (1) and (10)] with polynomials of the seventh order presented in Fig. 4(b). As should be anticipated, the second modeling variant ignoring superfluous terms, gives a result which is better by an order of magnitude. In addition, there is practically no dependence of ε on m for the second variant (see curve 2). Consequently, using a transient does not have any advantages here. This means that an increase of reconstruction quality is achieved in this case due to a decrease in the number of superfluous terms (instead of broadening the domain of a phase space explored by a phase orbit). Conversely, there is an essential dependence of ε on m in the case of using models (1) and (9), which contains many superfluous terms (see curve 1). The dependence is most notable at small values of m, corresponding to a transient where the value of ε oscillates intensively.

The appearance of the graph $\varepsilon(m)$ in the latter case is explained by a sensitive dependence of coefficients corresponding to superfluous terms on m in the region of a transient process. The values of some of the 36 coefficients of the models (1) and (9), with a polynomial of the seventh order [constructed from a time realization of system (8) at different values of m] are presented in Fig. 5(a). Graphs of the coefficients corresponding to ''necessary'' terms are shown on the left-hand side, and graphs for superfluous terms on the right-hand side. It can be observed that ''superfluous'' coefficients are essentially less stable than necessary ones; oscillations appear when m is changed in the region of a transient process.

Drawing on these results, we propose a procedure for the refinement of a model structure which is based on a sequential deletion of terms corresponding to less stable coefficients. One can use the following characteristics as measures of the stability of a coefficient a: the ratio of its mean value to its standard deviation,

$$m_1 = \frac{\langle a \rangle}{\sigma_a}; \tag{11}$$

and the ratio of its mean value to the standard deviation of the first difference is

$$m_2 = \frac{\langle a \rangle}{\sqrt{\langle (a_{m+\delta} - a_m)^2 \rangle}}. \tag{12}$$

Angular brackets denote an average over the ensemble of values of a obtained for different values of m, and δ is a shift between sequential locations of a reconstruction window (we take $\delta = 20$). The first characteristic assesses the intensity of oscillations of the coefficient values, while the second shows how fast these oscillations occur.

The proposed procedure for model structure optimization is illustrated in Fig. 5(b) where the dependence of an approximation error ε on the number of excluded superfluous terms is presented. According to the above characteristics [Eqs. (11) and (12)], the least stable coefficient is selected, and the corresponding term is excluded from a model. The reconstruction process is repeated with a simplified function, the next least stable coefficient is found, the corresponding term is again excluded from the model, etc. The dependencies in Fig. 5(b) are shown for different characteristics of instability. In the considered example the characteristic [Eq. (12)] estimating the variation of the first difference proves more effective. Note that after achieving a minimum, all attempts of further simplification of a model lead to a fast increase of an approximation error, since the procedure can no longer distinct a superfluous term from a necessary one.

V. CONCLUSIONS

By considering examples of the reconstruction of several discrete-time and continuous-time systems from scalar and vector time series with the use of different criteria of model quality, we show that the part of a time series which is the most valuable for the purpose of global modeling of an object dynamics in a wide domain of a phase space corresponds to *a transient process*. It should be stressed, however, that if a model is needed just to predict a settled motion, then a nonstationary part of a time series is harmful for modeling. In addition, transients do not play an important role if the structure of a model is optimal (completely adequate to an object). Using transients is reasonable when one needs to refine a model structure, that is, to detect superfluous terms and exclude them, e.g., when a polynomial representation of functions is employed.

The results presented are obtained by investigating exemplary dynamical systems, but they concern the steps of a reconstruction procedure which is common for both real and artificial objects. Therefore, we assume that these results can appear useful for modeling a wide class of systems.

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