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Identification of chaotic systems with hidden variables (modified Bock's algorithm)

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Abstract

We address the problem of estimating parameters of chaotic dynamical systems from a time series in a situation when some of state variables are not observed and/or the data are very noisy. Using specially developed quantitative criteria, we compare performance of the original multiple shooting approach (Bock's algorithm) and its modified version. The latter is shown to be significantly superior for long chaotic time series. In particular, it allows to obtain accurate estimates for much worse starting guesses for the estimated parameters.

1. Introduction

The problem of mathematical modeling of complex systems from experimental observables is well-known in different fields of science and practice and has multiple names such as "reconstruction of dynamical systems" in nonlinear science [1] and "system identification" in statistics and control theory [2]. It has different aspects and can be formulated in different ways. Here, we consider the case when the structure of model equations is known a priori from "the first principles". It reads

$$d\mathbf{y}/dt = \mathbf{f}(\mathbf{y}, \mathbf{c}), \tag{1}$$

where $\mathbf{y}$ is D-dimensional state vector, $\mathbf{c}$ is P-dimensional parameter vector. The task is *to estimate the unknown parameters* $c_1, \ldots, c_P$ from a time series—discrete sequence of values observed at subsequent time instants $\{\eta_1, \ldots, \eta_N\}$, where an observable η is assumed to be a function of state vector $\mathbf{y}$ (possibly corrupted with measurement noise), N is a time series length. Let us consider the case when η is a scalar, which is quite typical and the most complicated. Such a formulation has been considered in a number of works not only for differential equations [3–6], but also for maps [7–15]. In practice, it is encountered in chemical kinetics (rate constants estimation) [16], laser physics (rates of transition between energy levels) [17], electric engineering (ferroelectric and semiconductor nonlinearities) [18,19], cell biology (description of signaling pathways [20], neuron modelling [21]), etc.

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Construction of the so-called standard models [22] demands the time series of state vectors $\mathbf{y}$ to be at hand, i.e., one must reconstruct all D components from a scalar time series $\{\eta_i\}$. For example, the observable itself can serve as one of model variables, while others may be obtained via differentiation or integration. However, for a model structure specified from the first principles, some of state variables cannot often be measured or reconstructed from observed data. Such variables are usually called "hidden". The presence of hidden variables makes reconstruction a much more complex problem, because deficit of information about hidden variables (which have also to be included into the set of estimated quantities) requires more sophisticated approaches for parameter estimation. Usually, maximal likelihood principle is appealed to, but practically it reduces to a version of the least-squares method. In the case considered here, the problem is formalised as follows. One searches for initial conditions $\mathbf{s}$ and parameters $\mathbf{c}$ which provide the smallest least-squares difference between the appropriate components of a model orbit $\mathbf{y}(t)$ and observed data $\bar{\mathbf{y}}^l$. The sum of errors (2) involves only l non-hidden variables:

$$S(\mathbf{s},\mathbf{c}) = \sum_{i=1}^{N} \left[\mathbf{y}^l(t_i,\mathbf{s},\mathbf{c}) - \bar{\mathbf{y}}_i^l\right]^2 = \min, \tag{2}$$

where $\bar{\mathbf{y}}_i^l$ are observed vectors, $\mathbf{y}^l(t_i,\mathbf{s},\mathbf{c})$ are l-dimensional vectors consisting of the corresponding model state variables. Minimisation of (2) is performed with the aid of iterative algorithms for some "starting guesses" for $\mathbf{s}$ and $\mathbf{c}$.

In the case of a chaotic time series, a model trajectory is very sensitive to initial conditions. Therefore, "relief" of the cost function (2) is very complex for large N and exhibits a lot of local minima. Thus, the "attracting area" of global minimum is very narrow, so that it is unlikely to find it with arbitrary starting guesses. In order to overcome this difficulty, a special method—multiple shooting approach (Bock's algorithm)—was proposed [16,23]. Later, it was noticed [24] that it also encounters significant difficulties and additional efforts are necessary to succeed, although systematic investigation of this problem is still lacking. In this work, we develop special measures to quantify the performance of different parameter estimation techniques. With their aid, we compare different versions of multiple shooting approach (Section 2). By considering noisy time series of exemplary chaotic systems, we demonstrate that a modified Bock's algorithm allowing discontinuity of a model trajectory is the most efficient.

Chaotic dynamics and deficit of a priori information about system parameter values are typical in practice. Therefore, the task considered here is of significant practical interest. We note also that the methods analysed here give possibility not only to estimate parameters, but also to reconstruct the time courses of hidden variables, which cannot be measured by other means. So, the identification (reconstruction, parameter estimation) procedure acts as a universal indirect "measuring device".

2. Parameter estimation methods for hidden variable case

2.1. Initial value approach

This "naive" method consists in minimisation of (2) directly, where N is the length of the entire original time series. In practice, N should be large enough to allow one to extract necessary information from noisy data. Furthermore, the time series should involve all relevant time scales of the modeled dynamics. But for a chaotic time series, exponential sensitivity of model orbits to initial conditions $\mathbf{s}$ makes the attracting area of the global minimum of (2) very narrow. Therefore, the initial value approach encounters great difficulties. The disadvantages of this approach are clearly shown, e.g., in [27,19], so we do not pay significant attention to it here.

2.2. "Multiple shooting based" approaches

The name takes its origin from an analogy with well-known numerical methods for solution of a boundary-value problem in ordinary differential equations. Since the multiple shooting approach accepts a number of variations, we call all of them "multiple shooting based" approaches while the original one [16] just Bock's algorithm.

2.2.1. Original Bock's algorithm

It is a modification of initial value approach which allows an increase in the time series length N and the use of starting guesses for parameters not so close to their true values. This is possible since the entire time series is divided into L segments (n is the length of a segment, $N = Ln$) and initial conditions for each of them $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_L$ are considered as additional arguments of S (as quantities to be estimated):

$$S(\mathbf{s}_1,\ldots,\mathbf{s}_L,\mathbf{c}) = \sum_{i=1}^{L}\sum_{j=1}^{n}\left[\mathbf{y}^l(t_j,\mathbf{s}_i,\mathbf{c}) - \bar{\mathbf{y}}^l(i-1)n+j\right]^2 = \min, \tag{3}$$

Time moments $\tau_i = t_{(i-1)n+1}$ correspond to $\mathbf{s}_i$. In order to avoid a great number of free estimated quantities, that increases variances of the estimates, one imposes a constraint of model trajectory continuity over the entire observed interval:

$$\mathbf{y}(\tau_{i+1},\mathbf{s}_i,\mathbf{c}) = s_{i+1}, \quad i = 1,\ldots,L-1. \tag{4}$$

Minimisation of (3) under the constraints (4) is the problem of constrained multidimensional optimisation. For arbitrarily chosen starting guesses for parameters and initial conditions, the model trajectory consists of L "disconnected" pieces. However, it becomes "more continuous" gradually, after each iteration of the minimisation procedure. Bock's algorithm coincides with the initial value approach for $L = 1$ and $n = N$.

It was claimed [23] that Bock's algorithm does not require "genuine" starting guesses. Meanwhile, experience shows that *this is not typically the case*. The algorithm extends the modelling capabilities only in part, since the condition (4) is very strong. Therefore, often only local minima of (3) can be found.

2.2.2. Segmentation technique

In order to estimate parameters more accurately from a longer time series (where original Bock's algorithm cannot be applied due to local minima problem), it is divided into l shorter segments and parameters are estimated from each segment independently without any constraints. The estimates obtained are averaged: $\bar{\mathbf{c}} = \frac{1}{l}\sum_{i=1}^{l}\mathbf{c}_i$. Such an approach is called "piecewise" or "segmentation" technique [24]. If Bock's algorithm is used for each segment, it is reasonable to call it "segmentation Bock's algorithm". The disadvantage of this method is that the parameter estimators may be strongly biased (even asymptotically) since an estimate from each short segment may be biased, which is not eliminated via averaging. Therefore, the segmentation technique gives low accuracy of estimates as compared to the original Bock's algorithm if the global minimum can be easily found for both methods.

2.2.3. Modified Bock's algorithm

It is known from statistical theory, e.g., [28], that the use of the entire time series in maximum likelihood estimation is preferable for obtaining unbiased estimators than segmentation approach. So, we suggest to pay attention to a modification of Bock's algorithm that has been already applied in [17,25,26] for non-chaotic signals consisting of a number of independent shot realisations as a technique for "multiple experiment approach" problem solution. It was also briefly mentioned in [24]. The idea is to refuse the constraints (4) for several $(v-1)$ time instants holding the same parameter values $\mathbf{c}$ for the entire time series. So, the initial conditions for the v time instants, including the first one, become independent quantities to be estimated. We choose these instants equidistantly within the time series. Such an approach involves two adjustable parameters: the number of segments v and the number of subsegments within each segment L $(N = vLn)$. Subsegments are required to apply Bock's algorithm within each of the v segments.

The modified approach is not widely applied so far, even though it should have a number of advantages. The fact that a final model trajectory is discontinuous is not an indication that the model is "bad" but weakening of the constraints (4) may help to find global minimum and reasonable model when "strict" Bock's algorithm is not feasible.

3. Comparative study in numerical experiment

3.1. Comparison technique

We compare the methods using gray-scale "convergence diagrams" on the planes of starting guesses for parameters c_{i_1}, c_{i_2} (Fig. 1). White points denote starting guesses for which the global minimum is achieved, i.e., quite accurate estimates are obtained. Gray colour means starting guesses from which minimisation procedure converges to a number of local minima, darker colour corresponds to stopping at local minima situated further from the true values. We normalise starting guesses so that the centre of a diagram corresponds to genuine guesses, i.e., to the true values of parameters c_i^0. The normalised starting guesses are denoted $b_i = (c_i - c_i^0)/c_i^0$. The size of white area on the diagrams quantifies the estimation method's performance. The broader this area, the better the method. Such areas typically have a very complex structure (e.g., Fig. 1a), therefore we suggest an integral measure which is relative number μ of white points within a circle of radius r. The larger μ (for a given r), the better the method. We denote r_μ the maximum value of the circle radius corresponding to the relative ratio of white points equal to μ. Here, we use mainly the value of r_{100}, which is the radius of "100% convergence" to global minimum.

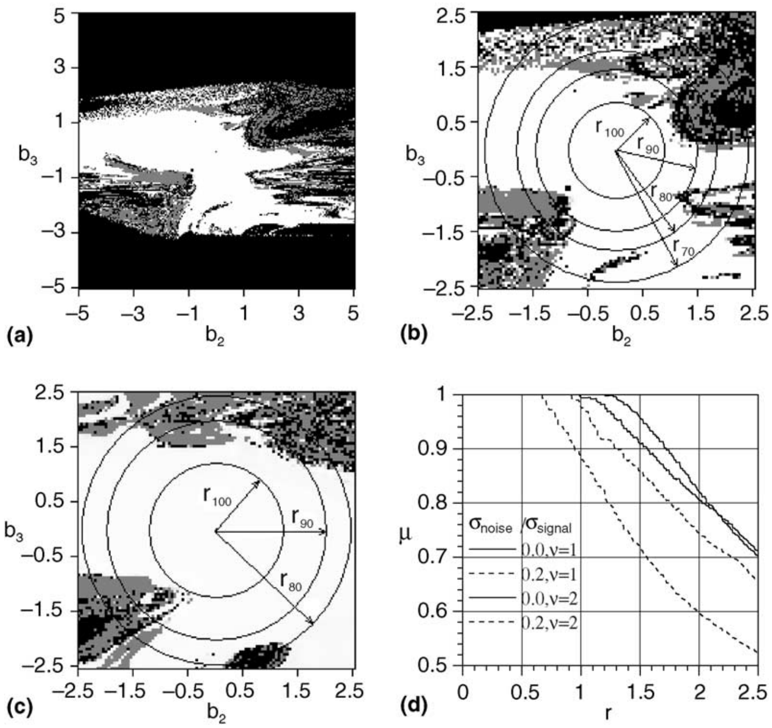

Fig. 1. The plane of normalised starting guesses for parameters of the Lorenz system (section with the plane $b_1 = 0$). (a) Bock's algorithm with $L = 30$, $n = 35$; (b) is a magnification of (a); (c) the modified method with $L = 15$, $n = 35$, $\nu = 2$; (d) the dependence $\mu(r)$ for Bock's algorithm (black) and the modified method (gray) at different noise levels.

Below, we consider the case of three unknown parameters. So, three-dimensional diagrams for all three starting guesses for parameters would contain complete information about the method's performance. Nevertheless, we use two-dimensional projections for simplicity of illustration taking into account that they lead to the same qualitative conclusions about the methods' inferiority/superiority.

3.2. Identification of the Lorenz system

As the first test system for investigation of the performance of different parameter estimation techniques in case of long chaotic time series and different starting guesses, we choose the Lorenz system

$$\dot{y}_1 = c_1(y_2 - y_1), \qquad \dot{y}_2 = -y_2 + y_1(c_3 - y_3), \qquad \dot{y}_3 = -c_2 y_3 + y_1 y_2, \tag{5}$$

with parameters $c_1 = 10$, $c_2 = 8/3$, $c_3 = 46$ corresponding to a chaotic regime, and initial conditions $y_1 = -7.60$, $y_2 = -12.37$, $y_3 = 38.66$ chosen arbitrarily on the chaotic attractor. The largest Lyapunov exponent is equal here to $\lambda_1 = 1.23$ [23]. The equations are integrated with the fourth-order Runge–Kutta technique with stepsize 0.001 and sampling interval 0.002 to generate a time series. An observed scalar time series is a realisation of the variable y_1 corrupted with additive Gaussian white noise: $\eta = y_1 + \xi$. The variables y_2 and y_3 are regarded hidden.

Since the choice of genuine starting guesses for the values of y_2 and y_3 is unrealistic, we use the observable values as starting guesses for all state variables $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_L, \ldots, \mathbf{s}_{\nu L}$. Even though such a choice is not the best possible, it is simple and sometimes efficient [23]. To minimise the function (3) the generalised Gauss–Newton method is used [23].

Convergence of the original Bock's algorithm and the modified method to global minimum is illustrated in Fig. 1a and b. These results correspond to the time series length for which the Bock's approach exhibits the best performance (the broadest convergence region). Only the section of starting guesses space with the plane $b_1 = 0$ is shown since unlucky choice of b_1 is not so crucial as the choice of b_2, b_3. It can be seen that the area of 100% convergence of Bock's algorithm is broad and the radius r_{100} is greater than 1.0, so relative deviations of starting guesses from true values (let us call them errors in starting guesses) may exceed 100%. There is also a wide area which is very distant from global minimum but allows to find global minimum (Fig. 1a). However, the modified method allows larger errors in starting guesses as it can be seen from comparison of Fig. 1b and c. The values of r_{100}, r_{90}, and r_{80} are greater for the modified method and the white area is wider.

The value of $\mu(r)$ for different noise levels is shown in Fig. 1d. The performance of both methods remains almost unchanged for moderate noise. The horizontal line of 100% convergence ($\mu = 1$) becomes shorter but not significantly: in a noise-free setting its length is 1.2 for the modified approach and 1.1 for Bock's method, while for 20% noise-to-signal ratio (ratio of rms amplitudes) it is 0.9 and 0.7, respectively. Similar conclusions can be drawn from Fig. 3c, where the dependencies $r_{100}(N)$ (for $v = 1$ and $v = 4$) are shown with black for noise-free setting and with gray for noisy case.

The dependence $r_{100}(L, n)$ shown in Fig. 2 also demonstrates the advantage of the modified method. Darker colour corresponds to smaller values of r_{100} (they are indicated on the contour lines) at given starting guesses. For the modified method, not only the area with $r_{100} \geqslant 1$ is larger, but also there is an area where $r_{100} \geqslant 1.2$ inside of it. This advantage takes place for longer times series that is revealed by white hyperboles $N = \text{constant}$ which are the lines of constant time series length.

This conclusion is confirmed by Fig. 3a where the 100% convergence radius is shown versus time series length N for different number of segments v. The number of subsegments L has been selected to make r_{100} as large as possible by the use of hyperboles (Fig. 2) and choice of points from lighter areas. Hill-like shape of plots $r_{100}(N)$ is determined by two factors. For small N, the amount of data is insufficient to "average out" the noise influence, while for large N, the exponential sensitivity to initial conditions takes place (small initial perturbations reaches the magnitude comparable to the size of the attractor during time interval $\tau_\Lambda = 1/\lambda_1$) that leads to complication of the cost function "relief". The curves for larger v attain larger values of r_{100}, i.e., the modified method is more efficient than the original Bock's algorithm. Those curves correspond also to larger values of N, therefore they are located closer to the right-hand side of the panel. Furthermore, the range of time lengths within which the modified method is "100% convergent" increases with the number of discontinuity points v, so the curves for greater v are "wider".

The investigation reveals (Fig. 3b) that the optimal value of segment length Ln is connected with Lyapunov time τ_Λ. Optimal time series lengths correspond to 1–2 Lyapunov times, see the upper horizontal axis in Fig. 3b. It is explained as follows. The success of estimation depends on the segment length Ln (over which small initial perturbations of the model orbit should not increase too strongly, so Ln should not be very large) and also on the number $P + vD$ of free parameters to be estimated (this number should not be very large since in very high-dimensional space relief of the cost function may become very complicated also, i.e., Ln should not be very small). As a consequence, there exists some intermediate optimal value of Ln related via a certain proportionality constant to the characteristic time scale τ_Λ of the divergence of nearby model trajectories.

Fig. 3d shows the dependence of r_{100} on L, given a certain Ln. At that, there is also an optimal value of L as usually for Bock's algorithm within each segment. The greatest r_{100} is achieved here for $v = 2$ since greater v correspond just to longer time series.

Similar results have been obtained from time series generated at different initial conditions, from time series of the variable y_2, and from time series of y_1 generated at a different set of "true" parameter values $c_1 = 10$, $c_2 = 8/3$, $c_3 = 28$ that is known as a "classical" chaotical set for the Lorenz system.

We also had studied the jumps allowed by modified approach in points of discontinuity and we showed that these jumps are small in comparison with attractor size: they are about 10^{-3} from signal standard deviation even if 1% noise

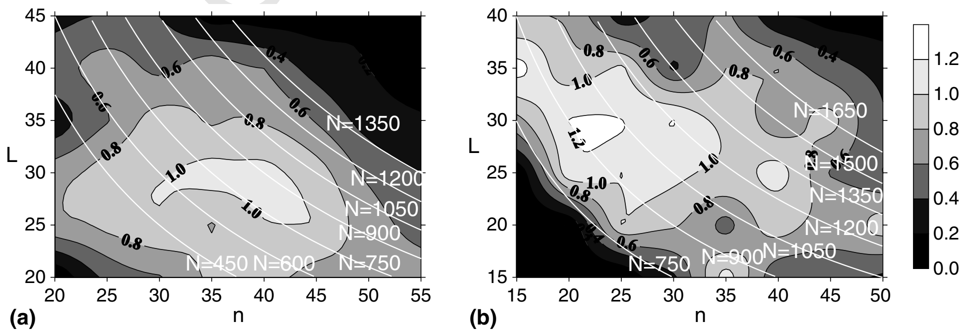

Fig. 2. The dependence $r_{100}(L, n)$: (a) for Bock's algorithm, (b) for the modified method with $v = 2$. Darker areas correspond to less radius r_{100}. The values of r_{100} are shown on the border lines. The white hyperboles are the lines of constant time series length $N = \text{constant}$.

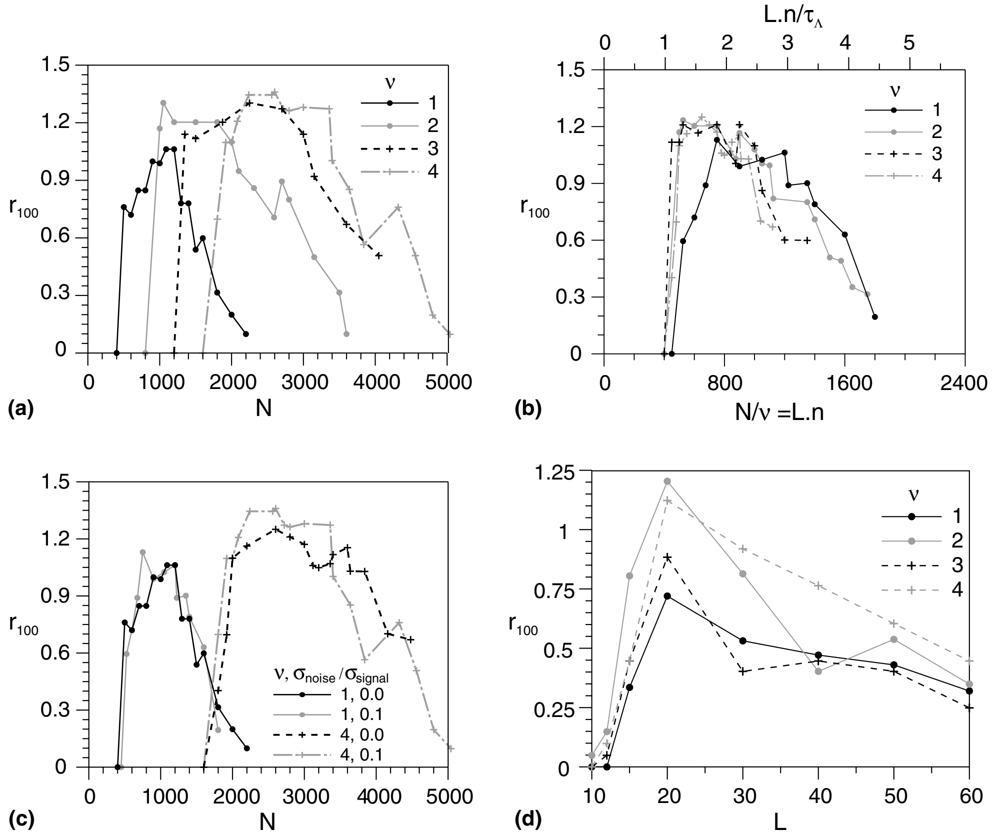

Fig. 3. The dependence of 100% convergence radius r_{100} on different factors: (a) on the entire time series length N for different numbers of discontinuity points allowed; (b) on the continuity segment length Ln; (c) on the entire time series length N for different noise levels. (d) The dependence $r_{100}(L)$ for different ν and fixed continuity segment length $Ln = 600$.

is added to the observable. Though the jumps due to original Bock's approach are greatly smaller: 10^{-10}–10^{-12} from signal standard deviation. It also has to be noticed that these "original" jumps decrease than discontinuity is allowed so it can be said that the model imperfection is concentrated from the whole set of nodes to the nodes between the segments.

3.3. Identification of Rössler system

In order to check whether our results hold for other systems, we perform the same investigation for the Rössler's system.

$$\dot{y}_1 = -y_2 - y_3, \qquad \dot{y}_2 = y_1 + c_1 y_2, \qquad \dot{y}_3 = c_2 + y_3(y_1 - c_3), \tag{6}$$

with parameters $c_1 = 0.2$, $c_2 = 0.15$, $c_3 = 10$, that corresponds to a chaotic regime and initial conditions $y_1 = 0.21$, $y_2 = 6.5$, $y_3 = 0.022$. The basic "period" of oscillations is 6.0, the largest Lyapunov exponent is $\lambda_1 = 0.1$. The equations (6) are integrated with fourth-order Runge–Kutta technique with stepsize 0.0002 and sampling interval 0.01. The variable y_1 is used as an observable both in a noise free setting and corrupted with additive Gaussian white noise.

We have chosen this system as an object since the "shape" of its attractor differs from the Lorenz one. The Lorenz system oscillates near one of the two unstable fixed points in turn with irregular switchings between them. The simultaneous values of its y_1 and y_2 variables are relatively close to each other. Their "shift by a quarter of rotation period" is a relatively small effect in absolute value as compared to the switchings between the two wings. The dynamics on the Rössler attractor is a rotation about a single unstable fixed point (in projection onto the plane $y_3 = 0$). So that the variables y_1 and y_2 are shifted in time by a quarter of the rotation period which is the main time scale here.

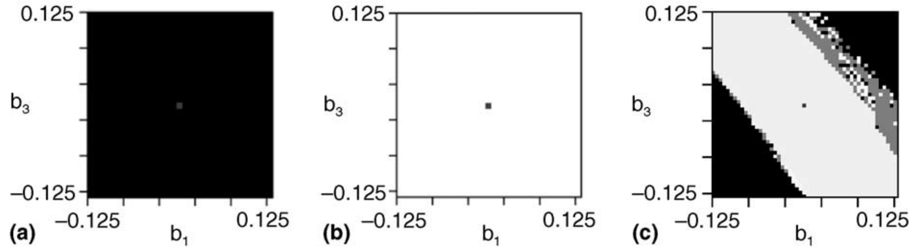

Fig. 4. The plane of normalised starting guesses for parameters of the Rössler system (section with the plane $b_2 = 0$) illustrating convergence of the original Bock's algorithm: (a) all starting guesses for the hidden variables are equal to simultaneous observable values; (b) genuine starting guesses; (c) starting guesses are obtained via the time shift of the observed time series by a quarter of basic period.

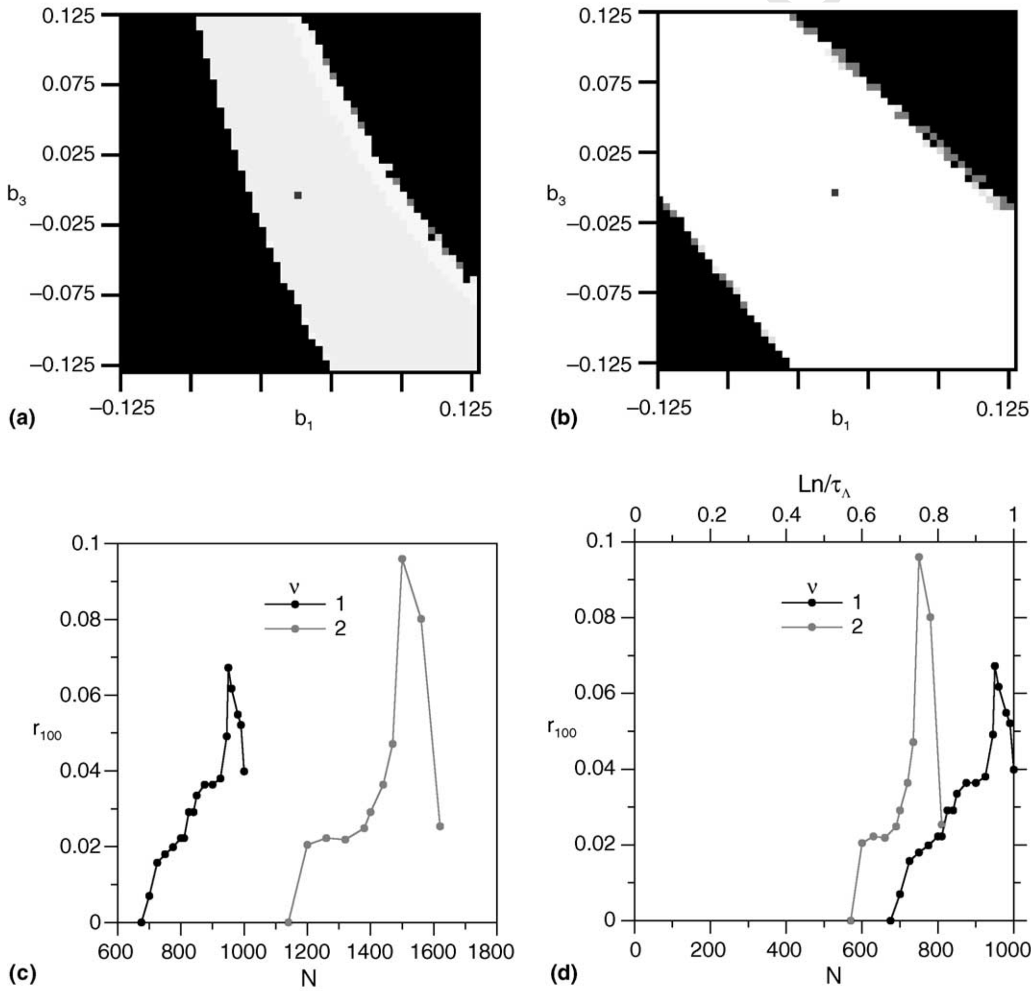

Fig. 5. The plane of normalised starting guesses for parameters of the Rössler system (section with the plane $b_2 = 0$): (a) Bock's algorithm; (b) the modified method. (c) The dependance of r_{100} on the entire time series length N for the best choice of L. (d) The dependance of r_{100} on the segment length Ln for the best choice of L.

Due to such relationships between the state variables, the choice of starting guesses for the hidden variables equal to the simultaneous observable value is more or less appropriate for the Lorenz system (as we have shown above) but leads to unsuccessful results of parameter estimation in the Rössler system using any of the estimation techniques considered. In Fig. 4a it is shown that $r_{100} = 0$, i.e., one cannot find the global minimum for such a choice of starting guesses for the hidden variables at all. Quite good results are achieved if one uses genuine starting guesses for the hidden variables (Fig. 4b). To develop "good" and realistic starting guesses is also possible if one takes into account the knowledge about character of the original dynamics which can be gained by studying model dynamics. Namely, for the Rössler system it is relevant to take the observed time series shifted by a quarter of basic period as a starting guess for the variable y_2 and zero as a starting guess for y_3 because due to attractor features this variable is close to zero most of the time (Fig. 4c).

For starting guesses we proposed, the results of investigation are similar to that presented above for the Lorenz system and are shown in Fig. 5. They indicate that the modified method is successful in finding global minimum given starting guesses for parameters very far from the true values (Fig. 5b) while the original Bock's algorithm demands more lucky starting guesses (Fig. 5a). Fig. 5c shows the dependence on the time series length N analogously to Figs. 3a and 5d shows the dependence on the segment length Ln analogously to Fig. 3b. The curves corresponding to larger v are "wider" and shifted to the right, i.e., the range of time series length allowing accurate estimation is greater for them. This advantage is observed for relatively long series that is similar to the results obtained for the Lorenz system.

4. Conclusions

We compared performance of different methods for estimation of parameters (identification) of dynamical systems from chaotic time series in the case of hidden variables. All the methods rely upon the multiple shooting idea. The comparison is done by using specially developed quantitative measure and considering exemplary chaotic systems. The original Bock's algorithm is shown to be less efficient than its modified version, which allows a model orbit to be discontinuous in several points within an observation interval.

The length of a time series and the number of its segments are shown to have significant influence upon the estimation results, and the choice of starting guesses for the hidden variables is quite important too. The chances for accurate estimation rise with time series length if the number of allowable points of model trajectory discontinuity is also increased. The optimal length of a continuity segment is close to Lyapunov time for long chaotic time series.

The modified method has a number of advantages as compared to the original Bock's algorithm since it is not so demanding with respect to starting guesses for the hidden variables. This is due to weakening the model orbit continuity constraint. Therefore, longer time series can be processed with the modified method that allows to increase accuracy of the estimates. Moreover, the modified method is not so demanding with respect to starting guesses for parameters also, sometimes providing an opportunity to get accurate estimates when the original Bock's algorithm fails.

The effect of measurement noise is shown to be not dramatical for both methods, even if noise-to-signal ratio is as high as 20% in rms amplitude. Note that if the time series length is fixed and the global minimum can be easily found for any estimation method then the accuracy of parameter estimates is the best for the original Bock's algorithm, a bit worse for the modified method, and the worst for the segmentation technique. However, since global minimum can never be equally easily found for any method, the modified method should be considered as the best one from practical point of view. Finally, one should be careful when using the modified method, since specifying too small length of a model orbit continuity segments may lead to the situation where even a model with "incorrect", "alien" structure is successfully fitted to observed data and erroneous conclusion about model adequacy is drawn.

Acknowledgments

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