Nonuniqueness of global modeling and time scaling

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Starting from an observed single time series, it is shown how to reconstruct a global model in the original phase space by using the ansatz library approach. This model is then compared to the underlying dynamical system that describes the initial time series, and the nonuniqueness of the reconstructed model is discussed. This framework is extended by taking an additional time scaling factor in the reconstructed model class under consideration.

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I. INTRODUCTION

To study an mth order dynamical system, all m physical quantities should be known to have a complete description of the system under investigation. In most experimental situations, only a single quantity can be measured. The embedding theorem of Takens [1] shows us how to get insight into the whole dynamical system from this incomplete set of measurements. Examples of modeling of physical experiments on chaotic systems include chemical reactions [2,3], vibrating strings [4], optical fiber ring resonators [5], and laser and sunspot data [6], among others. There are two main model types: the phenomenological models that need specialized knowledge about the system under study and models that are based on the time series data, which are the subject of this paper. Time series based modeling can yield linear stochastic models (e.g. AutoRegressive Moving Average models) or deterministic models (local or global). There are several different types of global deterministic models, such as neural networks or differential equation models, and the basis functions of these models can be, e.g., polynomials or radial basis functions. A nice data driven introduction to all these techniques can be found in [7], which is based on the freely available software package TISEAN [8]. Another good review of modeling techniques (local and global, linear and nonlinear) can be found in [9]. In this paper, global nonlinear deterministic ordinary differential equations (ODE) models with polynomials will be considered. Global modeling strongly depends on the time series available, and the papers of Letellier and Aguirre [10,11] explain how the choice of observables influences the amount of information we can achieve from such a single time series of a nonlinear dynamical system. Reconstruction of a system of ODEs from a single time series then can be done using differential coordinates [12,13]. The ansatz library [13–15] can then further be used to reconstruct a dynamical system in the original phase space. The problems that have been neglected in these papers are the questions on uniqueness of the reconstructed model and the role of time scaling in the time series under consideration.

In this paper, it is assumed that a time series is available and the following questions are asked: (1) Is it possible to create a model, within a certain class of models, that describes the initial time series? (2) Is the model unique? If not, what is the degree of nonuniqueness within the class of models treated? (3) What is the role of time scaling?

To answer these questions, the ansatz library approach [13] is used where a three-dimensional (3D) system of ODEs is proposed that can be converted to jerk form with polynomial functions. The transformation between the original dynamical system and the jerk or differential model provides a relation between the parameters of these two systems. When a differential model is extracted from a scalar time series, this relation of the parameters can be used to extract the coefficients and model form in the initial model. This idea is illustrated with the example of the Rössler system.

The paper is organized as follows: In Sec. II, the transformation of a dynamical system to its differential model is introduced. This transformation is discussed, and it is shown that there exists a whole class of dynamical systems that share the same differential model. In Sec. III, this is extended to an additional time scaling factor. Section IV is the conclusion.

II. GENERAL DESCRIPTION OF THE PROBLEM

A. Background

The class of models considered here is a 3D system of ODEs with the right-hand sides containing polynomials with up to second order nonlinearities, which can be written in a general form as

$$\begin{aligned}\dot{x}_i &= a_{i,0} + a_{i,1}x_1 + a_{i,2}x_2 + a_{i,3}x_3 + a_{i,4}x_1^2\\ &\quad + a_{i,5}x_1x_2 + a_{i,6}x_1x_3 + a_{i,7}x_2^2 + a_{i,8}x_2x_3\\ &\quad + a_{i,9}x_3^2, \quad i = 1,2,3. \end{aligned} \tag{1}$$

Usually, only a small subset of coefficients $a_{i,*}$ is assumed to be nonzero [13]. This subset defines the class of models under consideration. This class has N_m nonzero parameters $a_{i,*}$.

1. *Rössler-type models*

We ask the following question: Is it possible that the time series corresponds to a function of the variables $\phi(x_i)$? For simplicity, does it correspond to one of the variables x_i?

To answer these questions, the x_2 variable of the Rössler system [16]

$$\begin{aligned}\dot{x}_1 &= a_{1,2}\,x_2 + a_{1,3}\,x_3,\\ \dot{x}_2 &= a_{2,1}\,x_1 + a_{2,2}\,x_2,\\ \dot{x}_3 &= a_{3,0} + a_{3,3}\,x_3 + a_{3,6}\,x_1\,x_3\end{aligned} \tag{2}$$

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is assumed to be the observed scalar signal. For this class of models, $N_m = 7$.

B. Transformation

The Rössler system is rewritten as differential model starting from $X = x_2$ as

$$\dot{X} = Y, \quad \dot{Y} = Z, \quad \dot{Z} = F(X,Y,Z), \tag{3}$$

where the successive derivatives of $X = x_2$ define the new state space variables Y and Z. The function $F(X,Y,Z)$ is explicitly

$$F(X,Y,Z) = \alpha_1 + X\alpha_2 + X^2\alpha_3 + Y\alpha_4 + XY\alpha_5 + Y^2\alpha_6 + Z\alpha_7 + XZ\alpha_8 + YZ\alpha_9, \tag{4}$$

where the coordinates α_r of the differential embedding are related to the coordinates $a_{i,*}$ of the Rössler model by

$$\begin{aligned} &\alpha_1 = a_{1,3}\,a_{2,1}\,a_{3,0}, \quad \alpha_2 = -a_{1,2}\,a_{2,1}\,a_{3,3}, \\ &\alpha_3 = a_{1,2}\,a_{2,2}\,a_{3,6}, \quad \alpha_4 = a_{1,2}\,a_{2,1} - a_{2,2}\,a_{3,3}, \\ &\alpha_5 = \frac{a_{2,2}^2\,a_{3,6}}{a_{2,1}} - a_{1,2}\,a_{3,6}, \quad \alpha_6 = -\frac{a_{2,2}\,a_{3,6}}{a_{2,1}}, \\ &\alpha_7 = a_{2,2} + a_{3,3}, \quad \alpha_8 = -\frac{a_{2,2}\,a_{3,6}}{a_{2,1}}, \quad \alpha_9 = \frac{a_{3,6}}{a_{2,1}}. \end{aligned} \tag{5}$$

The differential model has $N_d = 9$ nonzero parameters α_r.

C. Jacobian rank

The nine parameters α_1 through α_9 of the differential model are explicit functions of the seven parameters $a_{i,*}$ of the initial class of models Eq. (2) of Rössler type. It would therefore seem that it is not possible to solve for the seven parameters $a_{i,*}$ once the nine parameters α_r have been determined.

There are, however, some subtleties that must be taken into consideration, and that allow inversion of Eq. (5). To be specific, $\alpha_6 = \alpha_8$. In addition, $a_{2,2} = -\alpha_6/\alpha_9$ and $a_{3,3} = \alpha_7 + \alpha_6/\alpha_9$. In short, there are nontransparent relations among the parameters α_r that allow inversion of Eq. (5).

The number of relations is determined by computing the rank of the Jacobian

$$\frac{\partial \alpha_r}{\partial a_{i,*}}. \tag{6}$$

This matrix has rank $5 \leqslant N_m = 7 < N_d = 9$. This means that there are 4 (=9 − 5) relations among the parameters α_r. This also means that an inverse solution to Eq. (5) is not only possible, but there is a 2 (=7 − 5)-parameter family of solutions $a_{i,*}$ to these equations. In retrospect, this result should not be surprising. In attempting to construct a class of models, the x_2 dependence of which matches the initial data set, there is a degree of "floppiness" or lack of rigidity, and this degree is measured by the co-rank $2 = 7 - 5$ of the Jacobian of the transformation.

D. Determining the differential model

There are two possible ways to fit the differential model to the initial time series data. The more rigorous but more difficult way is to determine the four constraints satisfied by the nine parameters α_r and then carry out a fit subject to these constraints. A second procedure is to allow each of the nine parameters α_r to vary independently, carry out a fit, then check to see that the constraints are satisfied. A variation of this latter procedure has been followed.

As a first step, the nine parameters α_r have been fitted to the data using a least squares method. These nine values have been used as inputs to a genetic algorithm (GA) that has been used repeatedly to estimate the values of the seven parameters $a_{i,*}$. These values have, in turn, been substituted into Eq. (5) to verify that the indicated functions of the $a_{i,*}$ do in fact reproduce the estimated values of the α_r. It can be found, for example, that the fitted values of α_6 and α_8 are always within a standard deviation.

The genetic algorithm has been run many times to estimate sets of values of the parameters $a_{i,*}$ because of the lack of uniqueness of the inverse transformation. Numerically, certain parameters, such as $a_{2,2}$ and $a_{3,3}$, have the same value each time the genetic algorithm has been run. These correspond to the values identified above ($a_{2,2} = -\alpha_6/\alpha_9$ and $a_{3,3} = \alpha_7 + \alpha_6/\alpha_9$). Other parameters $a_{i,*}$ have values that vary from one run to another. This variation is indicative of the lack of rigidity in the model formulation (i.e., the co-rank 2 of the Jacobian).

E. Scaling

We simplify the general arguments by introducing a scaling transformation. It is typical that, if some set of parameters $a_{i,*}$ satisfies the inverse transformation Eq. (5), then a new set of parameters $\tilde{a}_{i,*}$ also satisfies the inverse transformation. The new parameters are related to the original set by a scaling transformation

$$\tilde{a}_{i,*} = \lambda^{p(i,*)} a_{i,*}. \tag{7}$$

The simplest way to determine these scaling relations, specifically, the set of exponents $p(i,*)$, is to note that each coefficient α_r is a sum of products of powers of the original model parameters $a_{i,*}$. Take the logarithms of these nonlinear product functions, construct the appropriate coefficient matrix, and look for the null space.

This is illustrated with an example. The scaled version of the inverse transformation Eq. (5) with $a_{i,*} \to \lambda_{i,*} a_{i,*}$ is

$$\begin{aligned} \alpha_1 &= (a_{1,3}a_{2,1}a_{3,0})\,(\lambda_{1,3}\lambda_{2,1}\lambda_{3,0}), \\ \alpha_2 &= (-a_{1,2}a_{2,1}a_{3,3})\,(\lambda_{1,2}\lambda_{2,1}\lambda_{3,3}), \\ \alpha_3 &= (a_{1,2}a_{2,2}a_{3,6})\,(\lambda_{1,2}\lambda_{2,2}\lambda_{3,6}), \\ \alpha_4 &= (a_{1,2}a_{2,1})\,(\lambda_{1,2}\lambda_{2,1}) - (a_{2,2}a_{3,3})\,(\lambda_{2,2}\lambda_{3,3}), \\ \alpha_5 &= \frac{a_{2,2}^2 a_{3,6}}{b_1}\,\frac{\lambda_{2,2}^2\lambda_{3,6}}{\lambda_{2,1}} - (a_{1,2}a_{3,6})\,(\lambda_{1,2}\lambda_{3,6}), \\ \alpha_6 &= -\frac{a_{2,2}a_{3,6}}{a_{2,1}}\,\frac{\lambda_{2,2}\lambda_{3,6}}{\lambda_{2,1}}, \\ \alpha_7 &= a_{2,2}\lambda_{2,2} + a_{3,3}\lambda_{3,3}, \\ \alpha_8 &= -\frac{a_{2,2}a_{3,6}}{a_{2,1}}\,\frac{\lambda_{2,2}\lambda_{3,6}}{\lambda_{2,1}}, \quad \alpha_9 = \frac{a_{3,6}}{a_{2,1}}\,\frac{\lambda_{3,6}}{\lambda_{2,1}}. \end{aligned} \tag{8}$$

To leave α_i in Eq. (5) unchanged, the scaling has to be one (e.g., for α_5: $\frac{\lambda_{2,2}^2\lambda_{3,6}}{\lambda_{2,1}} = 1$ and $\lambda_{1,2}\lambda_{3,6} = 1$). Taking the logarithm, they obey a linear relation (e.g., $-\lambda_{2,1} + 2\lambda_{2,2} + \lambda_{3,6} = 0$ and $\lambda_{1,2} + \lambda_{3,6} = 0$). The set of linear relations derived from the

12 term scaling of Eq. (8) is summarized in matrix form

$$\begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 2 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \log(\lambda_{1,2}) \\ \log(\lambda_{1,3}) \\ \log(\lambda_{2,1}) \\ \log(\lambda_{2,2}) \\ \log(\lambda_{3,0}) \\ \log(\lambda_{3,3}) \\ \log(\lambda_{3,6}) \end{pmatrix} = 0. \tag{9}$$

This 12×7 matrix has a two-dimensional null space spanned by the null vectors $(-1,-1,1,0,0,0,1)$, $(0,-1,0,0,1,0,0)$.

This means that, for the Rössler system reconstructed from its x_2 variable, there exists a two-parameter family of solutions

$$\begin{aligned} \dot{x}_1 &= \frac{1}{b} a_{1,2}\, x_2 + \frac{1}{b}\frac{1}{c} a_{1,3}\, x_3, \\ \dot{x}_2 &= b\, a_{2,1}\, x_1 + a_{2,2}\, x_2, \\ \dot{x}_3 &= c\, a_{3,0} + a_{3,3}\, x_3 + b\, a_{3,6}\, x_1\, x_3, \end{aligned} \tag{10}$$

where b and c are real numbers. Any choice of b and c will generate exactly the same time series of $x_2(t)$. Therefore, reconstruction can only be done within the uncertainty of these two parameters b and c.

F. Discussion

The same approach as shown here for the example of the x_2 variable of the Rössler system works for any model function F of the differential model that is composed of monomials

$$F(X,Y,Z) = \sum_l \alpha_l\, X^i Y^j Z^k, \tag{11}$$

where the indices (i,j,k) for the monomials may also be negative, yielding a model with rational monomials. The ansatz library [13] summarizes all 26 general 3D systems Eq. (1) that can be transformed into such a differential model.

It is shown in [13] how the correct structure of the model function F of the differential model can be recovered from a time series without any knowledge of the underlying dynamical system in the case that the original system is covered by the ansatz library. If the correct structure of the differential model has been estimated from the time series, then the ansatz library lists all possible 3D systems Eq. (1) that yield that differential model. Numerically, a GA is then used to select only parameters of the original system that can reproduce the original time series. The example of reconstructing the Rössler system from the time series of the x_3 and x_1 variables is shown in [13].

As pointed out in [13], the differential model of the Rössler system derived from its x_1 variable is not in the form of Eq. (11), but can be brought into such a form by shifting the x_1 variable along the x_1 axis: $x_1 \to x_1 + \frac{a_{2,2}-a_{3,3}}{a_{3,6}}$.

Applying then the same scaling relations as in Sec. II E to each of the three state space variables, the two-parameter family of solutions Eq. (10) is slightly changed to

$$\begin{aligned} \dot{x}_1 &= \frac{1}{b} a_{1,2}\, x_2 + \frac{1}{k}\frac{1}{c} a_{1,3}\, x_3, \\ \dot{x}_2 &= b\, a_{2,1}\, x_1 + a_{2,2}\, x_2, \\ \dot{x}_3 &= c\, a_{3,0} + a_{3,3}\, x_3 + k\, a_{3,6}\, x_1\, x_3. \end{aligned} \tag{12}$$

Note the additional parameter k: There is a slightly different set of parameters b, c, and k depending on the time series used for reconstruction. When reconstructing from the x_1 variable, only b and k are present ($c = 1$); when reconstructing from the x_2 variable, $b = k$ and c are present; and when reconstructing from the x_3 variable, only b and c are present ($k = 1$). This confirms the observation by Letellier and Aguirre [10,11] that the choice of observable is important for global modeling. In the remainder of this paper, only modeling from the x_2 variable will be considered since the above differences in the parameters b, c, and k could be applied one to one to the results of the next section.

III. TIME SCALING

It is possible to extend the model family by one dimension by introducing a time scaling transformation

$$\tilde{t} = D\, t. \tag{13}$$

With this, the inverse transformation Eq. (5) becomes

$$\begin{aligned} &\alpha_1 = D^3\, a_{1,3}\, a_{2,1}\, a_{3,0}, \quad \alpha_2 = -D^3\, a_{1,2}\, a_{2,1}\, a_{3,3}, \\ &\alpha_3 = D^3\, a_{1,2}\, a_{2,2}\, a_{3,6}, \quad \alpha_4 = D^2\,(a_{1,2}\, a_{2,1} - a_{2,2}\, a_{3,3}), \\ &\alpha_5 = D^2 \left(\frac{a_{2,2}^2\, a_{3,6}}{a_{2,1}} - a_{1,2}\, a_{3,6} \right), \\ &\alpha_6 = -D\, \frac{a_{2,2}\, a_{3,6}}{a_{2,1}}, \quad \alpha_7 = D\,(a_{2,2} + a_{3,3}), \\ &\alpha_8 = -D\, \frac{a_{2,2}\, a_{3,6}}{a_{2,1}}, \quad \alpha_9 = \frac{a_{3,6}}{a_{2,1}}. \end{aligned} \tag{14}$$

To determine the degree of nonuniqueness of the reconstructed solution set in this case, a scaling transformation is introduced in the same way as in Sec. II E with an additional scaling factor $D \to d D$. In this case, the coefficient matrix of

$$\begin{pmatrix} 3 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 3 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 3 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 2 & 0 & 0 & -1 & 2 & 0 & 0 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \log(d) \\ \log(\lambda_{1,2}) \\ \log(\lambda_{1,3}) \\ \log(\lambda_{2,1}) \\ \log(\lambda_{2,2}) \\ \log(\lambda_{3,0}) \\ \log(\lambda_{3,3}) \\ \log(\lambda_{3,6}) \end{pmatrix} = 0 \tag{15}$$

has a three-dimensional null space spanned by the null vectors $(0,-1,-1,1,0,0,0,1)$, $(0,0,-1,0,0,1,0,0)$, and $(-1,2,3,0,1,0,1,0)$.

This means that there is a three-parameter family of solutions

$$\begin{aligned}\dot{x}_1 &= d^2\,\frac{1}{b}\,a_{1,2}\,x_2 + d^3\,\frac{1}{b}\,\frac{1}{c}\,a_{1,3}\,x_3,\\ \dot{x}_2 &= b\,a_{2,1}\,x_1 + d\,a_{2,2}\,x_2,\\ \dot{x}_3 &= c\,a_{3,0} + d\,a_{3,3}\,x_3 + b\,a_{3,6}\,x_1\,x_3,\end{aligned} \tag{16}$$

where the additional parameter d is a time scaling factor for the time series. This parameter can be reconstructed from a single time series. This means, if time series with different time scalings from the same dynamical system is available, this technique can identify those time series as originating from the same dynamical system and reconstruct the time scaling parameter.

IV. SUMMARY AND DISCUSSION

Starting from a single time series, a differential model in a phase space spanned by the successive derivatives of the observed variable can be reconstructed. This differential model is unique and corresponds to a whole class of models. In this paper, it is shown how this class of models in the original phase space can be reconstructed from the differential model and specify the nonuniqueness of these models.

This framework is further extended by taking an additional time scaling factor in the original time series under consideration. This time scaling factor is an additional parameter to be reconstructed, which extends the family of obtained models in the original phase space.

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