Geometry of Chaos I: Theoretical foundations of a consistent combined approach

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Abstract Problem of a chaos manifestation in dynamical systems is treated from the geometrical point of view. We present the theoretical foundations of a consistent chaos-geometrical approach to treating of chaotic dynamical systems. It combines together the non-linear analysis methods to dynamics, such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov exponent's analysis, surrogate data method etc.

Keywords geometry of chaos, dynamical systems, non-linear analysis and chaos theory techniques

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1. Introduction

Predicting a future state of dynamical system under consideration is one of fundamental purpose of every science (e.g.[1-34]). In fact, the main fundamental problem of science can be defined as: "Is it possible to predict a future behaviour of process using its past states?". Conventional approach applied to resolve this problem consists in building an explanatory model using an initial data and parameterizing sources and interactions between process properties. Unfortunately, that kind of approach is realized with difficulties, and its outcomes are insufficiently correct; moreover, sources and/or interactions of process cannot always be exactly defined. In our opinion [10,11,27-34], the geometrical approaches in a chaos theory can be a good fundamental basis for solution of the cited key evolutionary problem for stochastic dynamical systems. According to modern theory of prediction, time series can be considered as random realization, when the randomness is caused by a complicated motion with many independent degrees of freedom. Chaos is alternative of randomness and occurs in very simple deterministic systems. Although chaos theory places fundamental limitations for long-rage prediction, it can be used for short-range prediction since ex facte random data can contain simple deterministic relationships with only a few degrees of freedom.

The systematic study of chaos is of recent date, originating in the 1960s. One important reason for this is that linear techniques, so long dominant within applied mathematics and the natural sciences, are inadequate when considering chaotic phenomena since the amazingly irregular behaviour of some non-linear deterministic systems was not appreciated and when such behaviour was manifest in observations, it was typically explained as stochastic. It is well known the meteorological example of the chaos problem. Namely, starting from the meteorologist E.Lorenz, who observed extreme sensitivity to changes to initial conditions of a simple non-linear model simulating atmospheric convection, the experimental approach relies heavily on the computational study of chaotic systems and includes methods for investigating potential chaotic behaviour in observational time series [1-12]. During the last two decades, many studies in various fields of science have appeared, in which chaos theory was applied to a great number of dynamical systems, including those are originated from nature (e.g. [1-18]). As the illustrative examples, one could cite the corresponding papers in a field of mathematical statistics and economics, financial analysis, geophysics, hydrometeorology and climatology, theoretical and experimental physics and chemistry, evolutionary biology etc [1-34]. The above-mentioned studies concerning the key dynamical characteristics of different systems allow concluding that methodology from chaos theory can be applied and the short-range forecast by the non-linear prediction method can be satisfactory. The outcomes of such studies are very encouraging, as they not only revealed that the dynamics of the apparently irregular phenomena could be understood from a chaotic deterministic point of view but also reported very good predictions using such an approach for different systems. Chaos theory establishes that apparently complex irregular behaviour could be the outcome of a simple deterministic system with a few dominant nonlinear interdependent variables. At the same time the methods applied to the different chaotic dynamical systems in the above cited papers are characterized as sufficiently correct, but one-sized and limited ones. In the series of papers (e.g. [10,11,24-34]) it has been proposed an idea to combine different non-linear analysis and chaos theory methods and schemes (such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov exponent's analysis, memory matrix formalism, Green's function constructive method, evolutionary differential equations approach, surrogate data method etc) into the uniform, universal consistent approach to any chaotic dynamical systems and applied in the partial problems of environmental science and physics of systems and elements. Using these papers here we present the chaos–geometrical theoretical foundations of an advanced version of such a combined method. In the following papers the illustrative numerical examples concerning different chaotic dynamical systems will be presented.

2. Combined chaos-geometrical approach to dynamical systems: Theoretical foundations

2.1. Introducing remarks

For definiteness, we consider some chaotic dynamical system and suppose that the typical dynamics time series for key characteristics are known (from experiment or bymeans numerical modelling). It is clear that a visual inspection of the (irregular) amplitude level series does not provide any clues regarding its dynamical behaviour, whether chaotic or stochastic. To detect some regularity (or irregularity) in the time series, the Fourier power spectrum is often analyzed, however it often fails too. Chaotic signals may also have sharp spectral lines but even in the absence of noise there will be continuous part (broadband) of the spectrum. The broad power spectrum falling as a power of frequency is a first indication of chaotic behaviour, though it alone does not characterize chaos [2-4,10]. From this point of view, the corresponding series analyzed in this study is presumably chaotic. However, more well-defined conclusion on the dynamics of the time series can be made after the data will be treated by non-linear analysis methods.

Let us consider scalar measurements $s(n) = s(t_0 + n\Delta t) = s(n)$, where t_0 is the start time, Δt is the time step, and is n the number of the measurements. In a general case, $s(n)$ is any time series, particularly the amplitude level. Since processes resulting in the chaotic behaviour are fundamentally multivariate, it is necessary to reconstruct phase space using as well as possible information contained in the $s(n)$. Such a reconstruction results in a certain set of d-dimensional vectors $\mathbf{y}(n)$ replacing the scalar measurements. Packard et al. [14] introduced the method of using time-delay coordinates to reconstruct the phase space of an observed dynamical system. The direct use of the lagged variables $s(n + \tau)$, where τ is some integer to be determined, results in a coordinate system in which the structure of orbits in phase space can be captured. Then using a collection of time lags to create a vector in d dimensions,

$$\mathbf{y}(n) = s(n), s(n + \tau), s(n + 2\tau), \ldots, s(n + (d-1)\tau), \tag{1}$$

the required coordinates are provided. In a nonlinear system, the $s(n + j\tau)$ are some unknown nonlinear combination of the actual physical variables that comprise the source of the measurements. The dimension d is called the embedding dimension, d_E. Example of the Lorenz attractor given by Abarbanel et al. [12,13] is a good choice to illustrate the efficiency of the method.

2.2. Choosing time lag.

According to Takens [19] and Mane [20] any time lag will be acceptable is not terribly useful for extracting physics from data. If τ is chosen too small, then the coordinates s(n + jτ) and s(n + (j + 1)τ) are so close to each other in numerical value that they cannot be distinguished from each other. Similarly, if τ is too large, then s(n + jτ) and s(n + (j + 1)τ) are completely independent of each other in a statistical sense. Also, if τ is too small or too large, then the correlation dimension of attractor can be under- or overestimated respectively. It is therefore necessary to choose some intermediate (and more appropriate) position between above cases. First approach is to compute the linear autocorrelation function

$$C_L(\delta) = \frac{\frac{1}{N}\sum_{m=1}^{N}[s(m+\delta) - \bar{s}][s(m) - \bar{s}]}{\frac{1}{N}\sum_{m=1}^{N}[s(m) - \bar{s}]^2}, \tag{2}$$

where $\bar{s} = \frac{1}{N}\sum_{m=1}^{N} s(m)$,

and to look for that time lag where $C_L(\delta)$ first passes through zero. This gives a good hint of choice for τ at that $s(n + j\tau)$ and $s(n + (j + 1)\tau)$ are linearly independent. However, a linear independence of two variables does not mean that these variables are nonlinearly independent since a nonlinear relationship can differs from linear one. It is therefore preferably to utilize approach with a nonlinear concept of independence, e.g. the average mutual information. Briefly, the concept of mutual information can be described as follows (e.g.[10,16]). Let there are two systems, A and B, with measurements a_i and b_k. The amount one learns in bits about a measurement of a_i from a measurement of b_k is given by the arguments of information theory as

$$I_{AB}(a_i, b_k) = \log_2\left(\frac{P_{AB}(a_i, b_k)}{P_A(a_i)P_B(b_k)}\right), \tag{3}$$

where the probability of observing a out of the set of all A is $P_A(a_i)$, and the probability of finding b in a measurement B is $P_B(b_i)$, and the joint probability of the measurement of a and b is $P_{AB}(a_i,\ b_k)$. The mutual information I of two measurements a_i and b_k is symmetric and non-negative, and equals to zero if only the systems are independent. The average mutual information between any value a_i from system A and b_k from B is the average over all possible measurements of $I_{AB}(a_i,\ b_k)$,

$$I_{AB}(\tau) = \sum_{a_i, b_k} P_{AB}(a_i, b_k) I_{AB}(a_i, b_k) \tag{4}$$

.

To place this definition to a context of observations from a certain physical system, let us think of the sets of measurements $s(n)$ as the A and of the measurements a time lag τ later, $s(n+\tau)$, as B set. The average mutual information between observations at n and $n+\tau$ is then

$$I_{AB}(\tau) = \sum_{a_i, b_k} P_{AB}(a_i, b_k) I_{AB}(a_i, b_k) \tag{5}$$

.

Now we have to decide what property of $I(\tau)$ we should select, in order to establish which among the various values of τ we should use in making the data vectors $\mathbf{y}(n)$. In ref. [18] it has been suggested, as a prescription, that it is necessary to choose that τ where the first minimum of $I(\tau)$ occurs. On the other hand, the autocorrelation coefficient failed to achieve zero, i.e. the autocorrelation function analysis not provides us with any value of τ. Such an analysis can be certainly extended to values exceeding 1000, but it is known [18] that an attractor cannot be adequately reconstructed for very large values of τ. The mutual information function usually exhibits an initial rapid decay (up to a lag time of about 10) followed more slow decrease before attaining near-saturation at the first minimum.

One could remind that the autocorrelation function and average mutual information can be considered as analogues of the linear redundancy and general redundancy, respectively, which was applied in the test for nonlinearity. If a time series under consideration have an n-dimensional Gaussian distribution, these statistics are theoretically equivalent. The general redundancies detect all dependences in the time series, while the linear redundancies are sensitive only to linear structures. Further, a possible nonlinear nature of process resulting in the vibrations amplitude level variations can be concluded.

2.3. Choosing embedding dimension. Grassberger and Procaccia algorithm

The goal of the embedding dimension determination is to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity. In accordance with the embedding theorem, the embedding dimension, d_E, must be greater, or at least equal, than a dimension of attractor, d_A, i.e. $d_E > d_A$. In other words, we can choose a fortiori large dimension d_E, e.g. 10 or 15, since the previous analysis provides us prospects that the dynamics of our system is probably chaotic. However, two problems arise with working in dimensions larger than really required by the data and time-delay embedding [10,11,17].

First, many of computations for extracting interesting properties from the data require searches and other operations in R^d whose computational cost rises exponentially with d. Second, but more significant from the physical point of view, in the presence of noise or other high dimensional contamination of the observations, the extra dimensions are not populated by dynamics, already captured by a smaller dimension, but entirely by the contaminating signal. In too large an embedding space one is unnecessarily spending time working around aspects of a bad representation of the observations which are solely filled with noise. It is therefore necessary to determine the dimension d_A.

There are several standard approaches to reconstruct the attractor dimension (see, e.g., [8-20]), but let us consider in this study two methods only. The correlation integral analysis is one of the widely used techniques to investigate the signatures of chaos in a time series. The analysis uses the correlation integral, $C(r)$, to distinguish between chaotic and stochastic systems. To compute the correlation integral, the algorithm of Grassberger and Procaccia [17] is the most commonly used approach. According to this algorithm, the correlation integral is

$$C(r) = \lim_{N\to\infty} \frac{2}{N(n-1)} \sum_{\substack{i,j \\ (1\le i<j\le N)}} H\left(r - ||y_i - y_j||\right) \qquad (6)$$

,

where H is the Heaviside step function with $H(u) = 1$ for $u > 0$ and $H(u) = 0$ for $u \le 0$, r is the radius of sphere centered on $\mathbf{y}_i$ or $\mathbf{y}_j$, and N is the number of data measurements. If the time series is characterized by an attractor, then the integral $C(r)$ is related to the radius r given by

$$d = \lim_{\substack{r \to 0 \\ N \to \infty}} \frac{\log C(r)}{\log r} \tag{7}$$

,

where d is correlation exponent that can be determined as the slop of line in the coordinates

log $C(r)$ versus log r by a least-squares fit of a straight line over a certain range of r, called the scaling region. If the correlation exponent attains saturation with an increase in the embedding dimension, then the system is generally considered to exhibit chaotic dynamics. The saturation value of the correlation exponent is defined as the correlation dimension (d_2) of the attractor. The nearest integer above the saturation value provides the minimum or optimum embedding dimension for reconstructing the phase-space or the number of variables necessary to model the dynamics of the system. On the other hand, if the correlation exponent increases without bound with increase in the embedding dimension, the system under investigation is generally considered stochastic. The correlation exponent value increases with embedding dimension up to a certain value, and then saturates beyond that value. The saturation of the correlation exponent beyond a certain embedding dimension is an indication of the existence of deterministic dynamics. For example, the saturation value of the correlation exponent, i.e. correlation dimension of attractor, for the amplitude level series is about a few units (say, four) and occurs at the embedding dimension value of N_d. The low, non-integer correlation dimension value indicates the existence of low-dimensional chaos in the dynamics of the concrete system. The nearest integer above the correlation dimension value can be considered equal to the minimum dimension of the phase-space essential to embed the attractor. The value of the embedding dimension at which the saturation of the correlation dimension occurs is considered to provide the upper bound on the dimension of the phase-space sufficient to describe the motion of the attractor. Furthermore, the dimension of the embedding phase-space is equal to the number of variables present in the evolution of the system dynamics. The results of such studying can indicate that to model the dynamics of process resulting in the amplitude level variations the minimum number of variables essential is equal to four and the number of variables sufficient is equal to N_d. Therefore, the amplitude level attractor should be embedded at least in a four-dimensional phase-space. The results can indicate also that the upper bound on the dimension of the phase-space sufficient to describe the motion of the attractor, and hence the number of variables sufficient to model the dynamics of process resulting in the level variations is equal to 6. There are certain important limitations in the use of the correlation integral analysis in the search for chaos. For instance, the selection of inappropriate values for the parameters involved in the method may result in an underestimation (or overestimation) of the attractor dimension [17]. Consequently, finite and low correlation dimensions could be observed even for a stochastic process. To verify the results obtained by the correlation integral analysis, one should use the surrogate data method.

2.4. The surrogate data method.

The method of surrogate data [16] is an approach that makes use of the substitute data generated in accordance to the probabilistic structure underlying the original data. This means that the surrogate data possess some of the properties, such as the mean, the standard deviation, the cumulative distribution function, the power spectrum, etc., but are otherwise postulated as random, generated according to a specific null hypothesis. Here, the null hypothesis consists of a candidate linear process, and the goal is to reject the hypothesis that the original data have come from a linear stochastic process. One reasonable statistics suggested by Theiler et al. [23] is obtained as follows.

If we denote Q_{orig} as the statistic computed for the original time series and Q_{si} for the ith surrogate series generated under the null hypothesis and let μ_s and σ_s denote, respectively, the mean and standard deviation of the distribution of Q_s, then the measure of significance S is given by

$$S = \frac{|Q_{orig} - \mu_s|}{\sigma_s}. \tag{8}$$

An S value of $\sim$2 cannot be considered very significant, whereas an S value of $\sim$10 is highly significant. The details on the null hypothesis and surrogate data generation are described in ref. [10,23]. To detect nonlinearity in the amplitude level data, the one hundred realizations of surrogate data sets were generated according to a null hypothesis in accordance to the probabilistic structure underlying the original data. The correlation integrals and the correlation exponents, for embedding dimension values from 1 to 20, were computed for each of the surrogate data sets using the Grassberger-Procaccia algorithm. The relationship between the correlation exponent values and the embedding dimension values for the original data set and mean values of the surrogate data sets as well as for one surrogate realization gives the necessary foundations for adequate conclusion.
Often, a significant difference in the estimates of the correlation exponents, between the original and surrogate data sets, can be observed. In the case of the

original data, a saturation of the correlation exponent is observed after a certain embedding dimension value (i.e., 6), whereas the correlation exponents computed for the surrogate data sets continue increasing with the increasing embedding dimension. The high significance values of the statistic indicate that the null hypothesis (the data arise from a linear stochastic process) can be rejected and hence the original data might have come from a nonlinear process.

It is worth consider another method for determining d_E that comes from asking the basic question addressed in the embedding theorem: when has one eliminated false crossing of the orbit with itself which arose by virtue of having projected the attractor into a too low dimensional space? By examining this question in dimension one, then dimension two, etc. until there are no incorrect or false neighbours remaining, one should be able to establish, from geometrical consideration alone, a value for the necessary embedding dimension. Such an approach was described by Kennel et al. [13]. In dimension d each vector

$$\mathbf{y}(k) = s(k), s(k + \tau), s(k + 2\tau), \ldots, s(k + (d-1)\tau) \tag{9}$$

has a nearest neighbour $\mathbf{y}^{NN}(k)$ with nearness in the sense of some distance function. The Euclidean distance in dimension d between $\mathbf{y}(k)$ and $\mathbf{y}^{NN}(k)$ we call $R_d(k)$:

$$\begin{aligned} R_d^2(k) &= [s(k) - s^{NN}(k)]^2 + [s(k+\tau) - s^{NN}(k+\tau)]^2 + \\ &+ \ldots + [s(k+\tau(d-1)) - s^{NN}(k+\tau(d-1))]^2. \end{aligned} \tag{10}$$

$R_d(k)$ is presumably small when one has a lot a data, and for a dataset with N measurements, this distance is of order $1/N^{1/d}$. In dimension $d + 1$ this nearest-neighbour distance is changed due to the $(d + 1)st$ coordinates $s(k + d\tau)$ and $s^{NN}(k + d\tau)$ to

$$R_{d+1}^2(k) = R_d^2(k) + [s(k+d\tau) - s^{NN}(k+d\tau)]^2 \tag{11}$$

.

We can define some threshold size R_T to decide when neighbours are false. Then if

$$\frac{|s(k+d\tau) - s^{NN}(k+d\tau)|}{R_d(k)} > R_T \tag{12}$$

,

the nearest neighbours at time point k are declared false. Kennel et al.[13] showed that for values in the range $10 \leq R_T \leq 50$ the number of false neighbours identified by this criterion is constant. In practice, the percentage of false nearest neighbours is determined for each dimension d. A value at which the percentage is almost equal to zero can be considered as the embedding dimension. In refs. [33,34] under studying the chaotic dynamics of the quantum generators was shown that the percentage of false neighbours drops to almost zero at 4 or 5, i.e. a four or five-dimensional phase-space is necessary to represent the dynamics (or unfold the attractor) of the amplitude level series. From the other hand, the mean percentage of false nearest neighbours computed for the surrogate data sets decreases steadily but at 20 is about 35%. Such a result seems to be in close agreement with that was obtained from the correlation integral analysis, providing further support to the observation made earlier regarding the presence of low-dimensional chaotic dynamics in the amplitude level variations.

2.5. The Lyapunov's exponents.

As it is very well known, the Lyapunov exponents are the dynamical invariants of the nonlinear system (see, e.g. [1,2,8-10,21,22]). In a general case, the orbits of chaotic attractors are unpredictable, but there is the limited predictability of chaotic physical system, which is defined by the global and local Lyapunov exponents. A negative exponent indicates a local average rate of contraction while a positive value indicates a local average rate of expansion. In the chaos theory, the spectrum of Lyapunov exponents is considered a measure of the effect of perturbing the initial conditions of a dynamical system. Note that both positive and negative Lyapunov exponents can coexist in a dissipative system, which is then chaotic.

Since the Lyapunov exponents are defined as asymptotic average rates, they are independent of the initial conditions, and therefore they do comprise an invariant measure of attractor. In fact, if one manages to derive the whole spectrum of Lyapunov exponents, other invariants of the system, i.e. Kolmogorov entropy and attractor's dimension can be found. The Kolmogorov entropy, K, measures the average rate at which information about the state is lost with time. An estimate of this measure is the sum of the positive Lyapunov exponents. The inverse of the Kolmogorov entropy is equal to the average predictability. The estimate of the dimension of the attractor is provided by the Kaplan and Yorke conjecture (see [24]):

$$d_L = j + \frac{\sum_{\alpha=1}^{j} \lambda_\alpha}{|\lambda_{j+1}|} \tag{13}$$

,

where j is such that $\sum_{\alpha=1}^{j} \lambda_\alpha > 0$ and $\sum_{\alpha=1}^{j+1} \lambda_\alpha < 0$, and the Lyapunov exponents λ_α are taken in descending order.

There are several approaches to computing the Lyapunov exponents (see, e.g., [8-10,24,31-34]). One of them is in computing the whole spectrum and based on the Jacobin matrix of the system function. To calculate the spectrum of Lyapunov exponents from the amplitude level data, one could determine the time delay τ and embed the data in the four-dimensional space. In this point it is very important to determine the Kaplan-Yorke dimension and compare it with the correlation dimension, defined by the Grassberger-Procaccia algorithm.

The estimations of the Kolmogorov entropy and average predictability can further show a limit, up to which the amplitude level data can be on average predicted. Surely, the important moment is a check of the statistical significance of results. It is worth to remind that results of state-space reconstruction are highly sensitive to the length of data set (i.e. it must be sufficiently large) as well as to the time lag and embedding dimension determined. Indeed, there are limitations on the applicability of chaos theory for observed (finite) time series arising from the basic assumptions that the time series must be infinite. A finite and small data set may probably results in an underestimation of the actual dimension of the process. The statistical convergence tests, described here, together with surrogate data approach that, was above applied, can provide the satisfactory significance of the investigated data regarding the state-space reconstruction.

3. Conclusions and discussion

Thus, we considered a problem of a chaos manifestation in dynamical systems from the geometrical point of view and presented formally theoretical foundations of a consistent chaos-geometrical approach to treating of chaotic dynamical systems. This approach combines together the non-linear analysis methods to dynamics, such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov's exponent's analysis, surrogate data method etc. Their using allows to study in details an existence of chaotic behaviour in the non-linear dynamical systems on the basis of temporal series. The mutual information approach provided a time lag which is needed to reconstruct phase space. Such an approach allowed concluding the possible nonlinear nature of process resulting in the amplitude level variations. The correlation dimension method provided a low fractal-dimensional attractor thus suggesting a possibility of the existence of chaotic behaviour. The method of surrogate data, for detecting nonlinearity, provided significant differences in the correlation exponents between the original data series and the surrogate data sets. This finding indicates that the null hypothesis (linear stochastic process) can be rejected. The Lyapunov's exponents analysis usually can support the conclusion regarding a chaos existence in a system. In a whole a presented combined approach can provide an alternative approach for characterizing and modelling the dynamics of chaotic processes in the complicated system in relation to the concrete, as a rule, limited physical and mathematical models of these processes.

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