Geometry of Chaos: Advanced approach to treating chaotic atmosphere pollution dynamics

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Abstract It is presented an advanced chaos-geometrical approach to treating of atmospheric pollutants dynamics and its numerical application. It combines together application of the advanced mutual information approach, correlation integral analysis, Lyapunov exponent's analysis etc.

Keywords geometry of chaos, non-linear analysis, chaos theory

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1. Introduction

Earlier [1-10] we have developed a new, chaos-geometrical combined approach to treating of chaotic dynamics of atmospheric pollutants and its forecasting. Here we present the results of its application to studying Odessa atmosphere pollution dynamics. The successful application of new chaos-geometrical approach has been presented for Gdansk and other cities atmosphere systems [10].

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. [1-22]). The outcomes of such studies are very encouraging, as they reported very good predictions using such an approach for different systems.

2. Advanced chaos-geometrical approach to atmospheric pollutants dynamics: Data

2.2.1. Data and methodics

In our study, carbon oxide (CO), nitrogen dioxide (NO_2) and sulphurous anhydride (SO_2) concentration data observed at the above cited Ukrainian industrial cities from 1976 till 2000 years. Let us for definiteness consider the Odessa region. There are eight sites in the region (N8-N20). In our studying we use the multi year hourly concentrations (one year total of 20x8760 data points). The temporal series of concentrations (in mg/m3) of the of the studied pollution substances are presented in [1].

Following to [1-10], further we formally consider scalar measurements $s(n) = s(t_0 + n\Delta t) = s(n)$, where t_0 is a start time, Δt is time step, and n is number of the measurements. In a general case, $s(n)$ is any time series (f.e. atmospheric pollutants concentration). As processes resulting in a chaotic behaviour are fundamentally multivariate, one needs to reconstruct phase space using as well as possible information contained in $s(n)$. Such reconstruction results in set of d-dimensional vectors $\mathbf{y}(n)$ replacing scalar measurements. The main idea is that direct use of lagged variables $s(n + \tau)$, where τ is some integer to be defined, results in a coordinate system where a structure of orbits in phase space can be captured. Using a collection of time lags to create a vector in d dimensions, $\mathbf{y}(n) = [s(n), s(n + \tau), s(n + 2\tau), .., s(n + (d - 1)\tau)]$, the required coordinates are provided. In a nonlinear system, $s(n + j\tau)$ are some unknown nonlinear combination of the actual physical variables. The dimension d is the embedding dimension, d_E.

Let us remind that following to [1,10], the choice of proper time lag is important for the subsequent reconstruction of phase space. If τ is chosen too small, then the coordinates $s(n + j\tau)$, $s(n + (j + 1)\tau)$ are so close to each other in numerical value that they cannot be distinguished from each other. If τ is too large, then $s(n+j\tau)$, $s(n+(j+1)\tau)$ are completely independent of each other in a statistical sense. If τ is too small or too large, then the correlation dimension of attractor can be under-or overestimated. One needs to choose some intermediate position between above cases. First approach is to compute the linear autocorrelation function $C_L(\delta)$ and to look for that time lag where $C_L(\delta)$ first passes through 0. This gives a good hint of choice for τ at that $s(n + j\tau)$ and $s(n + (j + 1)\tau)$ are linearly independent. It's better to use approach with a nonlinear concept of independence, e.g. an average mutual information. The mutual information I of two measurements a_i and b_k is symmetric and non-negative, and equals to 0 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 $I_{AB}(a_i, b_k)$. In ref. [4] it is suggested, as a prescription, that it is necessary to choose that τ where the first minimum of $I(\tau)$ occurs.

In [1,10] it has been stated that an aim 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. 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. The correlation integral analysis is one of the widely used techniques to investigate the signatures of chaos in a time series. If the time series is characterized by an attractor, then correlation integral $C(r)$ is related to a radius r as $d = \lim_{r \to 0, N \to \infty} \frac{\log C(r)}{\log r}$, where d is correlation exponent.

2.2.2 The results for time series

Table 1 summarizes the results for the time lag calculated for first 10^3 values of time series.

Table 1. Time lags (hours) subject to different values of C_L, and first minima of average mutual information,I_{min1}, for the time series of NO_2 , SO_2 (Odessa; 1976-1978)

	Fontan		Peresyp	
	NO_2	SO_2	NO_2	SO_2
C_L=*0.1*	148	252	62	165
C_L=*0.5*	9	17	7	32
I_{min1}	13	24	10	22

The autocorrelation function crosses 0 only for the NO_2 time series at the Peresyp, whereas this statistic for other time series remains positive. The values, where the autocorrelation function first crosses 0.1, can be chosen as τ, but in [6,9] it's showed that an attractor cannot be adequately reconstructed for very large values of τ. So, before making up final decision we calculate the dimension of attractor for all values in Table 1. The large values of τ result in impossibility to determine both the correlation exponents and attractor dimensions using Grassberger-Procaccia method [1,16]. As in a case of the chaos-geometric Gdansk region pollution dynamics [10], here the outcome is explained not only inappropriate values of τ but also shortcomings of correlation dimension method. If algorithm [14] is used, then a percentages of false nearest neighbours are comparatively large in a case of large τ. If time lags determined by average mutual information are used, then algorithm of false nearest neighbours provides $d_E = 6$ for all air pollutants.

2.2.3. Nonlinear prediction model

The fundamental problem of theory of any dyanmical system is in predicting the evolutionary dynamics of a chaotic system. Let us remind following to [1-,2,10] that the cited predictability can be estimated by the Kolmogorov entropy, which is proportional to a sum of positive LE. As usually, the spectrum of LE is one of dynamical invariants for non-linear system with chaotic behaviour. The limited predictability of the chaos is quantified by the local and global LE, which can be determined from measurements. The LE are related to the eigenvalues of the linearized dynamics across the attractor. Negative values show stable behaviour while positive values show local unstable behaviour. For chaotic systems, being both stable and unstable, LE indicate the complexity of the dynamics. The largest positive value determines some average prediction limit. Since the LE are defined as asymptotic average rates, they are independent of the initial conditions, and hence the choice of trajectory, and they do comprise an invariant measure of the attractor. An estimate of this measure is a sum of the positive LE. The estimate of the attractor dimension is provided by the conjecture d_L and the LE are taken in descending order. The dimension d_L gives values close to the dimension estimates discussed earlier and is preferable when estimating high dimensions. To compute LE, we use a method with linear fitted map, although the maps with higher order polynomials can be used too. Non-linear model of chaotic processes is based on the concept of compact geometric attractor on which observations evolve. Since an orbit is continually folded back on itself by dissipative forces and the non-linear part of dynamics, some orbit points [1,10] $\mathbf{y}^r(k)$, $r = 1, 2, .., N_B$ can be found in the neighbourhood of any orbit point $\mathbf{y}(k)$, at that the points $\mathbf{y}^r(k)$ arrive in the neighbourhood of $\mathbf{y}(k)$ at quite different times than k. One can then choose some interpolation functions, which account for whole neighbourhoods of phase space and how they evolve from near $\mathbf{y}(k)$ to whole set of points near $\mathbf{y}(k+1)$. The implementation of this concept is to build parameterized non-linear functions $\mathbf{F}(\mathbf{x}, \mathbf{a})$ which take $\mathbf{y}(k)$ into $\mathbf{y}(k+1) = \mathbf{F}(\mathbf{y}(k), \mathbf{a})$ and use various criteria to determine parameters $\mathbf{a}$. Since one has the notion of local neighbourhoods, one can build up one's model of the process neighbourhood by neighbourhood and, by piecing together these local models, produce a global non-linear model that capture much of the structure in an attractor itself. Table 2 shows the global LE.

Table 2. First two LE (λ_1, λ_2), Kaplan-Yorke dimension (d_L), and average limit of predictability ($Pr_{max}, hours$) for time series of NO_2,SO_2 (Odessa; 1976-1978)

	Fontan NO_2	Fontan SO_2	Peresyp NO_2	Peresyp SO_2
λ_1	0.0187	0.0168	0.0192	0.0155
λ_2	0.0068	0.0072	0.0059	0.0058
d_L	4.09	5.04	3.92	4.65
Pr_{max}	42	46	43	52

The presence of the two (from six) positive λ_i suggests the system broadens in the line of two axes and converges along four axes that in the six-dimensional space. The time series of SO_2 at the site Fontan have the highest predictability (more than 3 days), and other time series have the predictabilities slightly less than 3 days.

3. Conclusions

In this paper we considered an advanced chaos-geometrical approach to treating of chaotic systems. The approach combines the non-linear analysis methods to dynamics, such as the correlation integral analysis, the LE analysis, surrogate data method etc. We have investigated a chaotic behaviour in the nitrogen dioxide and sulphurous anhydride concentration time series at the Fontan & Peresyp sites in Odessa city and proved an existence of the low-D chaos. We presented an effective nonlinear prediction model and realized a successful short-range forecast of atmospheric pollutant time series. Earlier the same successful results were received for other cases and systems [1-10]. All considered examples has shown high perspectives of a new approach methods to treating dynamics of very complicated chaotic systems.

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