Фізика аеродисперсних систем. – 2024. – № 62. – С.168-175

УДК 530.313

Khetselius O.Y., Ignatenko A.V.

Odessa National Polytechnic University, Odessa
E-mail: ignatenkoav13@gmail.com

Chaos-geometric, neural networks and system analysis and modelling of chaotic pollution dynamics of the complex hydroecological systems

An advanced combined neural networks and chaos-geometric method for analysis, modelling, and forecasting of the chaotic pollution dynamics of complex hydroecological systems is presented. The method is based on the use of advanced methods of the theory of chaos and dynamic systems for the analysis of time series of pollutants concentrations. The general approach includes the Gottwald-Melbourne test, the correlation integral method , fractal and multifractal formalism, average mutual information, false nearest neighbours, surrogate data algorithms, analysis on the basis of the Lyapunov's exponents, Kolmogorov entropy, nonlinear forecast models based on algorithms of optimized predicted trajectories, neural networks modelling. As an illustrative example, a chaotic dynamics of the nitrates concentrations in the Small Carpathians river's watersheds in the Earthen Slovakia during 1969-1996 years is considered. The data of calculations of the dynamical and topological invariants are presented.

***Key words**: complex hydroecological systems, chaotic pollution dynamics, chaos-geometric approach, dynamical and topological invariants*

Introduction. In the modern theory of geo-environmental systems [1-5], the problem of studying a quantitative pollution dynamics is one of the most important and fundamental problems. The most models are currently used to assess the state (and forecast) of environmental pollution at the present time using deterministic models or by simplifying them based on simple statistical regressions. The success of these models, however, is limited by their inability to describe the nonlinear characteristics of the behavior of pollutant concentrations, as well as the lack of understanding of the physical and chemical processes involved [1-5].

Although the use of chaos theory methods imposes certain fundamental limitations on long-term forecasts, however, as has been shown in a number of the works (e.g., [3-11] and Refs. therein), these methods can be successfully applied for short-term or medium-term forecasts. These works proved that nonlinear methods of chaos theory and dynamic systems can be applied with satisfactory accuracy for analysis, modelling and forecasting of the temporal dynamics of atmospheric pollutant concentrations [3-5]). This opens up very attractive prospects for using the same methods in studying the dynamics of pollution of other ecological and hydrological systems.

In this work we present some advanced data of study of the temporal dynamics of changes in the nitratesconcentrations in the watersheds of the Little Carpathians using a generalized chaos-geometric and neural networks approach. A chaotic behavior in the time series of the nitrate concentrations is investigated.

Theoretical method. Our approach to modeling the chaotic dynamics of complex environmental systems is based on the chaos -geometric and neural networks

DOI: 10.18524/0367-1631.2024.62.321234

methods. As the methods have been in details considered in the previous papers (e.g. [3-20]), here we are limited only by the key points.

In general, the chaos-geometric approach includes using a combined set of such non-linear analysis, dynamical systems and a chaos theory methods as the Gottwald-Melbourne test, the correlation integral method, algorithms of average mutual information, false nearest neighbors, surrogate data, methods of analysis based on the Lyapunov's exponents, Kolmogorov entropy, power spectrum, nonlinear prediction models, based on algorithms of optimized predicted trajectories, B-spline approximations, neural network simulation algorithms etc (e.g.[3-12]).

The main stages of a chaos-geometric (combined with neural networks technology) to analysis, processing and forecasting data of the hydroecological system pollutants dynamics are follows:

i. General qualitative analysis (in terms of ordinary differential equations or the Arnold analysis) of the hydroecological system pollutants dynamics; modeling the spatial and temporal structure of the fields of concentrations of impurities in the hydroecological system;
ii. Application of different chaos-geometric tests on the presence of chaotic elements, functions and modes in a system; the Gottwald-Melbourne test etc;
iii. Fractal and quantum geometry of a phase space (choice of time delay, determination of embedding dimension by methods of correlation dimension algorithm and false nearest neighbors algorithm);
iv. Analysis and computing the dynamic and topological invariants of a chaotic system and nonlinear forecasting of a temporal (spatial) evolution of system dynamics.

The key points of the whole approach are reflected in the flowchart in Table 1.

The fundamental ideas of the combined chaos-geometric (plus differential equations one and the Armold analysis) approach to modelling, processing and prediction of chaotic dynamics are ideologically reduced to reproduction (and reconstruction) of a phase space of the geosystems, prediction of the temporal evolution of the main parameters of a system. From the viewpoint of mathematical modelling it is a question of consideration of unambiguous representations of a kind:

$$\boldsymbol{F}_{i+1} = \mathbf{G}(F_i), \tag{1}$$

where $F \in \mathbf{R}^D$ – is the state vector, $D$is the dimension, i – discrete time, $\mathbf{G}$ is the D-dimensional mapping. To implement the ideology of simulation of a compact geometric attractor and the use of chaos-cybernetic algorithm of predicted phase trajectories of the system to restore the phase space of the system, it is possible to use several concepts, first, the concept of average mutual information, and secondly, the concept of using the properties of the corresponding linear autocorrelation function (see Table 1).

The master task of mathematical modeling is to determine the corresponding embedding dimension and to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity [12, 14, 18, 29]. 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.$d_E > d_A$.

Table 1. Flowchart of the combined chaos-geometric and neural networks (plus differential equations one and the Armold analysis) approach to modelling, processing and prediction of chaotic dynamics of the hydroecological systems

I. General qualitative analysis (in terms of ordinary differential equations or the Arnold analysis) of the hydroecological system pollutants dynamics ;general dynamics differential equations analysis)

⇓

II. Application of the different chaos-geometric and neural networks tests on a presence of chaotic (stochastic) elements, functions and modes in the geosystem;

1. Gotwald-Melbournetest; Chirikov test; Naïve model tests;

⇓

2. Energy and spectral methods and algorithms: energy and power spectra, energy level statistics, random matrix analysis; characteristic distributions of the Wigner-Dyson type

⇓

III. Multifractal and quantum geometry of a phase space and dynamics of resonances

3. Computing the fractal parameters, multifractal spectra; wavelet analysis; cepstrum analysis

⇓

4. The Packard-Takens algorithm; the advanced autocorrelation function or average initial information algorithms; The Green's function method

⇓

5. Reconstruction of a phase space; Computing embedding dimension, correlation dimensions; using the methods of the correlation integral by Grassberger-Procaccia OR the false nearest neighbor points formalism

⇓

IV. Forecasting chaotic dynamics of the complex geosystems

6. Computing the invariants; The global Lyapunov's dimension analysis;Kolmogorov entropy analysis; The Kaplan-York dimension analysis; Method of nearestneighboring points

⇓

7. New methods and algorithms of nonlinear forecasting chaotic dynamics of the geosystems and ecosystems ("minmax" algorithms, methodsofthe stochastic propagators;

Neural networks modelling algorithms with application of the polynomial or B-spline models, wavelets etc …

In order to reconstruct the corresponding attractor dimension (e.g., [3,5-8]) one could use two main standard approaches. The first approach is the well-known correlation integral analysis (e.g. [9]), which is one of the widely used techniques to investigate the signatures of chaos in a time series. The method introduces the correlation integral, $C(r)$, to distinguish between chaotic and stochastic systems. To compute the correlation integral, the standard algorithm by Grassberger-Procaccia [9] is usually used. The problem is reduced to computing the next quantity:

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

where H is the Heaviside step function with $H(u) = 1$ for $u > 0$ and $H(u) = 0$ for u δ 0, r is the radius of sphere centered on $\mathbf{y}_i$ or $\mathbf{y}_j$, and N is the number of data measurements.

One of the principally important points of the whole approach to modeling and forecasting chaotic dynamics of the geosystems is computing the topological and dynamical invariants [3-12]. The latter include, in particular, local and global Lyapunov's dimensions or Lyapunov's exponents. It is worth to remind the classical definition of the Lyapunov's exponents through e logarithms of absolute values of eigenvalues of linearized dynamics focused on the attractor, more precisely:

$$\lambda = \lim_{\substack{t\to\infty \\ d(0)\to 0}} \left(\frac{1}{t}\right) \log_2 \left[\frac{d(t)}{d(0)}\right], \quad d(t) = \left[\sum_{i=1}^{n} \delta F_i^2(t)\right]^{1/2} \tag{3}$$

Here, the norm determines the degree of divergence of two adjacent trajectories, that is, the master trajectory and the adjacent trajectory with initial conditions $S(0)+\delta S(0)$ ($S = F$). It is important to note that the negative dimensions indicate the local average compression rate and the positive ones indicate the expansion one. The Lyapunov's exponents are independent of the initial conditions, and do comprise an invariant measure of attractor. Usually, the computing of the Lyapunov's exponents allows quickly determine whether the system is chaotic or not.

In fact, if one manages to derive the whole spectrum of the Lyapunov's exponents, other invariants and parameters of the system (i.e. Kolmogorov entropy (K_{ent}) as well as an average predictability) can be calculated. The Kolmogorov entropy K_{ent}, which, according to definition, measures the average rate at which information about the state is lost with time. Numerically, the Kolmogorov entropy can be determined as the sum of the positive Lyapunov's exponents. The estimate of the dimension of the attractor is provided by the Kaplan and York conjecture:

$$d_L = j + \frac{\sum_{\alpha=1}^{j} \lambda_\alpha}{\left|\lambda_{j+1}\right|}, \tag{4}$$

where j is such that $\sum_{\alpha=1}^{j} \lambda_\alpha > 0$ and $\sum_{\alpha=1}^{j} \lambda_\alpha < 0$, and the Lyapunov's exponents λ_a are taken in descending order.It should be noted that there are several algorithms for computing a spectrum of the Lyapunov's exponents, among which the most common

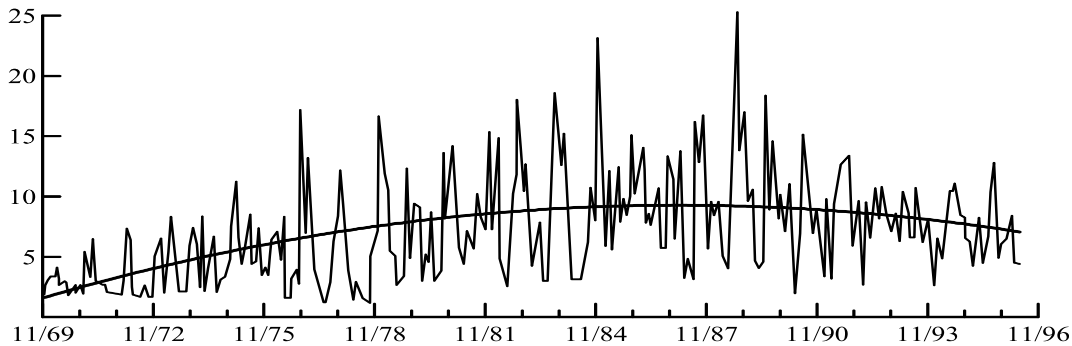

Fig. 1. Monthly average nitrate concentrations (mg l-1) in the Ondava River basin at Stropkov for the hydrological years 1968/69 - 1995/96

is the method based on the Jacobian mapping. The detailed information about the cited characteristics as well as the details of the main computational algorithms to determine the topological and dynamical invariants can be found in Refs. [3-20]). All calculations are performed with using "Geomath", "ScanPoints" PC computational codes [3,5,12].

S**ome results and conclusion.** .The advanced chaos-geometric approach gas been applied to modelling and forecasting of the temporal dynamics of fluctuations of the nitrates concentrations in the Small Carpathians river's watersheds in the Earthen Slovakia during 1969-1996 years. As starting data, the detailed data s of empirical observations have been used for several watersheds in the Small Carpathians region, which were carried out by employees of the Institute of Hydrology of the Slovak Academy of Sciences [1]. Sampling for nitrates at these stations was carried out twice a month during 1991-95. Chemical nitrogen compounds mainly arise from industrial and natural fertilizers, industrial and wastewater and NOx emissions from internal combustion engines and transport. Nitrates are characterized by significant seasonal variability, with their highest values occurring during snowmelt in spring.

As a typical example, Fig. 1 shows the average monthly nitrate concentrations at the Ondava: Stropkov point. According to data [1], until approximately 1988-89 nitrate concentrations increased, reaching a maximum of ~ 25 mg l-1 in the spring of 1989, which was associated with the increasing use of nitrogen fertilizers from year to year, after which agriculture became less intensive, causing a decrease in nitrate concentrations.

Below we shortly present the data of numerical experiments on the restoration of the embedding dimension (d_E), using the method of correlation integral and the algorithm of false nearest neighboring points. In order to calculate the correlation dimension d_2 it one should calculate the correlation integrals $C(r)$ for different embedding dimensions. The correlation dimension of the attractor (d_A) is defined as the value of the correlation dimension, in which it does not change as the embedding dimension increases.Table 1 summarizes all the results for the recovery of attractors, as well as the calculational data for the K chaotic index (K_{ch}) and different dynamical and topological invariants (time delay τ,correlation dimension *(*d_2), embedding space dimension *(*d_E*),* Lyapunov's exponent (λ_i), Kolmogorov entropy (K_{ent}), Kaplan-York di-

Table 1. Calculational data for the chaotic index (K_{ch}) and different dynamical and topological invariants: time delay τ,correlation dimension *(d_2)*, embedding space dimension *(d_E)*, Lyapunov exponent (λ_i), Kolmogorov entropy (K_{ent}), Kaplan-York dimension *(d_L)*, predictability limit (Pr_{max}) for the for nitrate concentrations in the catchments of the Little Carpathians

Watershed (Point)	τ	d_2	d_E	d_L	Pr_{max}	K
Ondava (Stropkov)	9	5.31	6	4.11	8	0.68
Vydrica (C.Most)	19	5.21	6	5.01	12	0.71
Gidra (Main)	16	5.13	6	5.87	14	0.82
Gidra (Pila)	20	5.82	6	5.17	12	0.75
Ladomirka (Svidnik)	10	3.88	4	3.12	7	0.71
Ondava (Svidnik)	10	3.65	4	3.27	7	0.80
Babie (Olsavka)	8	4.89	5	4.46	8	0.69

mension *(d_L)*, etc for the for nitrate concentrations in the catchments of the Little Carpathians.

In the case considered, the values of the chaos parameter K in all cases exceed 0.68, that is, the considered time series are subject to the influence of chaotic dynamics. The analysis of the dynamical and topological invariants shows that, for example, the resulting Kaplan- York dimension is very close to the correlation dimension. The analysis on the basis of the Lyapunov exponents as well as the other dynamical and topological invariants indicates on a pronouncedchaotic dynamics of the corresponding time series.

To conclude, an advanced version of the chaos-geometric method is adapted for modelling the chaotic dynamics of the nitrates concentrations in the Small Carpathians river's watersheds in the Earthen Slovakia during 1969-1996 years using such chaos theory methods as the Gottwald-Melbourne test, the correlation integral method, the algorithms of average mutual information, false nearest neighbors, surrogate data, methods of analysis based on the Lyapunov's exponents, Kolmogorov entropy, etc.

References

1. *Hastings A.M., Hom C., Ellner S, Turchin P., Godfray Y.* Chaos in ecology: is Mother Nature a strange attractor? // Ann. Rev. Ecol. Syst. – 1993. – Vol.24. – P.1-33.
2. *Pekarova P., Miklanek P., Konicek A., Pekar J.* Water quality in experimental basins. National Report 1999 of the UNESKO. // Project 1.1.-Intern.Water Systems, 1999. – P. 1-98.
3. *Glushkov, A.V.* Methods of a chaos theory. – Astroprint, Odessa, 2012.
4. *Khetselius, O.Yu.:* Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method. In: *Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski J.* (eds.) // Dynamical Systems Applications. – Lodz Univ. Press., Lodz (Poland), 2013. – T.2, – pp. 145–152.
5. *Glushkov A.V., Svinarenko A.A., Khetselius O.Y.,* Modeling an ecological state of environment with accounting radioactive contamination, radionuclides transfer. – Odessa: TES, 2019.
6. *Gottwald G.A., Melbourne I.*, A new test for chaos in deterministic systems// Proc. Roy.

Soc. London. Ser.A: Math.-Phys. Sci. – 2004. – Vol. 460. – P. 603–611
7. *Kennel M., Brown R., Abarbanel H.,* Determining embedding dimension for phase-space reconstruction using a geometrical construction // Phys.Rev.A. – 1992. – Vol. 45. – P.3403-3411.
8. *Packard N.H., Crutchfield J.P., Farmer J.D., Shaw R.S.,* Geometry from a time series// Phys. Rev. Lett. – 1980. – Vol. 45. – P. 712–716.
9. *Grassberger P., Procaccia I.,* Measuring the strangeness of strange attractors// Physica D. – 1983. – Vol. 9. – P. 189–208.
10. *Schreiber T.* Interdisciplinary application of nonlinear time series methods // Phys. Rep. – 1999. – Vol.308. – P. 1 – 64.
11. *Sano M., Sawada Y.,* Measurement of the Lyapunov spectrum from a chaotic time series // Phys. Rev. Lett. – 1985. – Vol. 55. – P. 1082–1085.
12. *Glushkov A.V., Khetselius O.Y., Stepanenko S.M., TernovskyE.V.* Chaos, Bifurcations and Strange Attractors in Environmental Radioactivity Dynamics of Some Geosystems. // In: *Awrejcewicz J.* (ed) Perspectives in Dynamical Systems II: Mathematical and Numerical Approaches. Series: Springer Proceedings in Mathematics &Statistics. – 2021. – Vol. 363. – P.79-88 (Springer, Cham).
13. *Glushkov A., Khetselius O., Brusentseva S., Duborez A.* Modeling chaotic dynamics of complex systems with using chaos theory, geometric attractors, quantum neural networks// Proc Int. Geom. Center. – 2014. – Vol.7(3). – P.87-94.
14. *Glushkov A.V., Khetselius O.Yu., Agayar E.V., Buyadzhi V.V., Romanova A.V., Mansarliysky V.F.* Modelling dynamics of hydroecological system ventilation and industrial city's air pollution analysis / New approach. IOP Conf. Series: Earth and Environm. Sci., 2017. – Vol. 92. – P.012014.
15. *Glushkov A.V., Khetselius O.Yu., Bunyakova Yu.Ya., Prepelitsa G.P., Solyanikova E.P., Serga E.N.* Non-linear prediction method in short-range forecast of atmospheric pollutants: low-dimensional chaos / In: Dynamical Systems. Theory and Applications. – LIF111. Lodz Univ. Press., Lodz (Poland), 2011.
16. *Glushkov A.V., Prepelitsa G.P., Svinarenko A.A., Zaichko P.A.* Studying interaction dynamics of the non-linear vibrational systems within non-linear prediction method (application to quantum autogenerators) / In: *Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski J.* (eds.) Dynamical Systems Theory. – Lodz Univ. Press., Lodz (Poland), 2013. – T.1. – pp. 467–477.
17. Glushkov, A.V., Svinarenko, A.A., Loboda, A.V.: Theory of neural networks on basis of photon echo and its program realization. TEC, Odessa (2003).
18. *Glushkov A.V., Prepelitsa G.P., Svinarenko A.A., Khetselius O.Y.*, Geometry of Chaos 1: Theoretical foundations of a consistent combined approach// Proc. of Intern. Geometry Center.-2013.-Vol.6(1).-P.67-79
19. *Glushkov A.V., Ignatenko A.V., Kuznetsova A.V., et al* Nonlinear Dynamics of Atomic and Molecular Systems in an Electromagnetic Field: Deterministic Chaos and Strange Attractors // In: Perspectives in Dynamical Systems II: Mathematical and Numerical Approaches Series: Springer Proceedings in Mathematics & Statistics, Cham: Springer. – 2021. – Vol.363. – P.111-120;
20. *Ignatenko A., Buyadzhi A., Buyadzhi V., Kuznetsova, A., et al* Nonlinear chaotic dynamics of quantum systems: molecules in an electromagnetic field // Advances in Quant Chem. – 2019. – Vol.78. – P.149-170.

Хецеліус О.Ю., Ігнатенко Г.В.

Хаос-геометричний, нейронно-мережевий та системний аналіз і моделювання хаотичної динаміки забруднення складних гідроекологічних систем

АНОТАЦІЯ

Представлено вдосконалений комбінований хаос-геометричний та нейронно-мережевий підхід до аналізу, моделювання та прогнозування динаміки хаотичного забруднення складних гідроекологічних систем. Метод заснований на використанні оптимізованих методів теорії хаосу та динамічних систем для аналізу часових рядів концентрацій забруднюючих речовин. Зокрема, підхід комбіновано використує критерій Готвальда-Мельбурна, метод кореляційного інтегралу, мультіфрактальний формалізм, алгоритми середньої взаємної інформації, помилкових найближчих сусідів, сурогатних даних, аналіз на основі показників Ляпунова, ентропії Колмогорова, а також нелінійні моделі прогнозу. Як наочний приклад, розглянуто хаотичну динаміку концентрацій нітратів у вододілах річок Малих Карпат (Словаччина) протягом 1969-1996 років та наведені дані обчислень динамічних та топологічних інваріантів.

Ключові слова: *складні гідроекологічні системи, хаотична динаміка процесу забруднення, хаос-геометричний підхід, динамічні та топологічні інваріанти.*