

DEVELOPMENT OF A SELF-ADJUSTING METHOD FOR CALCULATING RECURRENT DIAGRAMS IN A SPACE WITH A SCALAR PRODUCT

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Abstract

A self-adjusting method for calculating recurrence diagrams has been developed. The proposed method is aimed at overcoming the metric-threshold uncertainty inherent in the known methods for calculating recurrence diagrams. The method provides invariance to the nature of the measured data, and also allows to display the recurrence of states, adequate to real systems of various fields. A new scientific result consists in the theoretical justification of the method for calculating recurrence diagrams, which is capable of overcoming the existing metric-threshold uncertainty of known methods on the basis of self-adjusting by measurements by improving the topology of the metric space. The topology is improved due to the additional introduction of the scalar product of state vectors into the operation space. This allowed to develop a self-adjusting method for calculating recurrence diagrams with increased accuracy and adequacy of the display of recurrence states of real systems. Moreover, the method has a relatively low computational complexity, providing invariance with respect to the nature of the irregularity of measurements.

Verification of the proposed method was carried out on the basis of experimental measurements of concentrations of gas pollutants of atmospheric air for a typical industrial city. The main gas pollutants of the atmosphere are formaldehyde, ammonia and nitrogen dioxide, caused by stationary and mobile sources of urban pollution. The obtained experimental verification results confirm the increased accuracy and adequacy of the display of the recurrence of atmospheric pollution states, as well as the invariance of the method with respect to the nature of the irregularity of measurements. It has been established that the accuracy of the method is influenced by the a priori boundary angular dimensions of the recurrence cone. It was shown that with a decrease in the boundary angular dimensions of the recurrence cone, the accuracy of the recurrence mapping of the real states of dynamical systems in the calculated diagrams increases. It was experimentally established that the accuracy and adequacy of the mapping

of the recurrence states of real dynamical systems acceptable for applications is provided for a boundary angular size of the recurrence cone of 10° or less.

Keywords: metric-threshold uncertainty, recurrence diagram, self-adjusting method, metric, metric space, scalar product of vectors.

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1. Introduction

The methods for calculating recurrence diagrams (RP) and quantitative assessment of recurrence diagrams (RQA) allow to analyze the behavior of complex dynamic systems of various fields [1]. Modern RQA methods are used to quickly identify hazardous conditions in urban air pollution [1]. The development of well-known methods for computing RP in spaces of improved topology is considered in [3]. At the same time, the capabilities of existing RQA methods are substantially limited by the quality of the calculated RP, which depends on the method used to calculate the RP and the reliability of the measurement information. Known methods for calculating RP are characterized by uncertainty due to the parameters of the methods themselves, as well as the conditions for their use. In this regard, the problem of overcoming the indicated uncertainty of the methods for calculating RP becomes especially urgent.

An important feature of RP methods, in contrast to the methods of correlation dimension [4], is the ability to map multidimensional state trajectories of complex dynamic systems into 2-dimensional space. Moreover, the recurrence of the states of systems at different instants of time means that arbitrary points of the trajectory of states turn out to be close in some sense [5]. The displayed RPs take into account the structure and characteristics of the dynamics of the state of the systems, as well as the distortion of the measuring channels. Following the embedding dimension theorem, one can judge the dynamics of the states of the system as a whole by calculating RP only for one of the coordinates of the measured state vector [6]. In this case, the dimension of the attachment does not have a clear definition and can change during the measurement process. Therefore, due to the unknown a priori dimension of the investment, the general uncertainty of the known methods of computing RP increases. In [7], it was proposed to eliminate the uncertainty of the embedding dimension by calculating the RP for one coordinate of the state vector. In this case, the uncertainty of the method is partially overcome by choosing the distance metric in the space of real numbers. Overcoming threshold uncertainty and using other metrics is not considered. The features of computing RP for localization of transition states under conditions of uncertainty are considered in [8]. It is noted that the norm used in calculating RP can be determined by various metrics [9]. However, each metric is characterized by different computational complexity and features of determining close states. Therefore, under conditions of uncertainty in spaces with different metrics, the result of calculating RP will be different. The method for calculating the RP concentration of carbon monoxide in rooms with the aim of detecting early fires is considered in [10]. Research is limited to considering a one-dimensional phase space with an ordinary and power metric. Self-adjusting methods under conditions of uncertainty caused by factors of ignition in a one-dimensional phase space are considered in [11]. It is noted that the choice of an appropriate threshold is important [12].

Thus, the well-known methods for calculating RP are based on linear normed spaces of finite dimension with various types of metrics. The main ones are uniform, Euclidean and maximum metrics. Moreover, all known methods are characterized by metric-threshold uncertainty due to the set of selectable possible metrics and corresponding thresholds. It should be noted that the metric determines its own topology of space, and the threshold defines the region of recurrence in this space. Therefore, RPs for the same system, but calculated in spaces with different metrics and thresholds, will not be the same. In [13, 14], it is noted that the problem of the correct choice of the threshold in RP calculation methods is crucial in obtaining adequate mappings of the structure of recurrent states for real systems. In [15, 16], threshold uncertainty is proposed to be overcome based on heuristics. However, well-known heuristics are of a private nature, limited to well-known metrics and have significant implementation difficulties and shortcomings. In this regard, an important and unresolved part of the problem is the development of a method for calculating RP

aimed at overcoming metric-threshold uncertainty in order to obtain adequate mappings of recurrent states of real systems.

The aim of research is in development of a self-adjusting measurement method for calculating RP in the space of an improved structure based on the scalar product of vectors to overcome metric-threshold uncertainties.

To achieve the aim, the following objectives are set:

- to carry out a theoretical justification for the method of calculating RP in a space with a scalar product, which allows to overcome metric-threshold uncertainty due to the improvement of the metric space and self-adjusting threshold;
- to check the proposed method for calculating RP on the example of the real dynamics of the state of the main gas pollution of the urban atmosphere.

2. The theoretical basis of the proposed method for calculating recurrence diagrams

Known methods for RP calculation ($R_{i,j}^m$) for an arbitrary m-dimensional vector Z_i of states of the studied dynamic system measured at discrete time moments i can be represented in a generalized form

$$R_{i,j}^{m,\varepsilon} = F(\|Z_i - Z_j\|, \varepsilon), \quad Z_i \in \Omega^m, \quad Z_j \in \Omega^m, \quad i, j = 1, 2, \dots, N_s, \quad (1)$$

where $F(*)$ is the given characteristic function of its arguments; ε is a certain threshold defining an admissible neighborhood of recurrence of the vector Z_i ; $\|*\|$ is a certain functional defining a norm in the space Ω^m , that induces the metric $\|Z_i - Z_j\|$; N_s is the maximum number of measurements of the vector Z_i of system states. The characteristic function in (1) is defined as

$$F(\|*\|, \varepsilon) = \begin{cases} 1 & \text{if } \|*\| < \varepsilon, \\ 0 & \text{if } \|*\| \geq \varepsilon. \end{cases} \quad (2)$$

The ambiguity of the functional of the norm inducing the metric and the threshold in (1) determine the essence of the metric-threshold uncertainty of the known methods for calculating RP. This means that, for metric-threshold uncertainty, the trajectories of the vector Z_i of states of the system under study in the m-dimensional normed space will be mapped onto a two-dimensional matrix for arbitrary functionals of norms generating metrics in space Ω^m and threshold ε . Moreover, each matrix element equal to unity for different times i and j will characterize the recurrence (repeatability) of the state vector of the system under study taking into account metric-threshold uncertainty. The coordinate axes of the graphical representation of RP will be the time axes corresponding to the discrete time instants of the state vector measurement.

To overcome the metric-threshold uncertainty in the calculation of RPs, they are usually given a specific form of the norm functional that uniquely induces a metric in the space under consideration. Let two state vectors $X^T = (x_1, x_2, \dots, x_m)$ and $Y^T = (y_1, y_2, \dots, y_m)$ be given in an m-dimensional normed linear space. Then, for the norm functionals most often used in the RP calculation methods in (1), the induced metrics can be represented following [3] in the form:

$$\|X - Y\|_1 = \sum_{i=1}^m |x_i - y_i|, \quad (3)$$

$$\|X - Y\|_2 = \left[\sum_{i=1}^m |x_i - y_i|^2 \right]^{1/2}, \quad (4)$$

$$\|X - Y\|_3 = \max\{|x_i - y_i|; i = 1, 2, \dots, m\}. \quad (5)$$

For the octahedral, spherical, and cubic norms, the induced metrics (3)–(5) are usually called uniform, Euclidean, and maximal. It can be seen from (3)–(5) that the indicated metrics for the same vectors will be different in magnitude. Moreover, only the Euclidean metric (4) for vectors

of a linear normed space will determine the distance in the generally accepted geometric sense. Other metrics (3), (5) have a different geometric meaning. The main advantages and limitations of these norms and metrics in the calculations of RP are outlined in [1]. Therefore, by choosing a specific type of functional of the norm and the generated metric (3)–(5), it is possible to overcome only part of the metric-threshold uncertainty associated with the metric. Another part of the metric threshold uncertainty due to the threshold needs to be overcome. To overcome this part of the uncertainty, various heuristic approaches and methods for choosing a threshold are known, which are of a private nature [17, 18].

Thus, for commonly defined norm functionals and generated metrics (3)–(5), it is not generally possible to overcome the threshold uncertainty of methods for computing RP in the general case. This is explained by the fact that well-known approaches to overcoming the considered metric-threshold uncertainty of methods are based on the traditional paradigm of independence of metric and threshold uncertainty [3]. To develop methods for calculating RP, invariant or partially invariant, the metric-threshold uncertainty under consideration requires a change in the traditional paradigm. The developed paradigm consists in representing the metric-threshold uncertainty as a whole in the form of dependent metric and threshold components. Following this paradigm, overcoming the existing metric-threshold uncertainty of known methods for calculating RP (1) by choosing the functionals of norms that induce metrics and thresholds must be carried out from a unified position.

Within the framework of the development of the developed paradigm, it is advisable to move from considering the norms and generating metrics that define the corresponding spaces traditional for the methods of computing RP functionals to the corresponding improved space [2, 3]. Such an improvement in [3] is proposed to be implemented by introducing an additional geometric characteristic in the form of a scalar product of two vectors. The scalar product is the mapping of ordered pairs of linear space vectors onto the real axis. If denote this map by (Z_i, Z_j) , then the scalar product $Z_i^T Z_j = (Z_i, Z_j)$ of two arbitrary state vectors of the system can be interpreted as some angle θ between the corresponding vectors

$$\cos \theta = \frac{(Z_i, Z_j)}{\sqrt{(Z_i, Z_i)} \sqrt{(Z_j, Z_j)}}. \quad (6)$$

An important known property of a scalar product is

$$(Z_i, Z_i)^{0.5} = \|Z_i\| = (Z_i^T Z_i)^{0.5}. \quad (7)$$

Relation (7) indicates that in the proposed improved space the scalar product generates the norm. This norm, in turn, induces a corresponding metric defined by a relation of the form

$$\|Z_i - Z_j\| = \sqrt{(Z_i - Z_j)^T (Z_i - Z_j)}. \quad (8)$$

From relation (8) it can be seen that this metric in the proposed improved space determines the usual distance between two arbitrary vectors Z_i and Z_j of the system under study. For convenience, let's introduce the notation for the state vectors Z_i and Z_j and their differences: $Z_i = A$, $Z_j = B$ and $Z_i - Z_j = C$, respectively. Then, following the cosine theorem, in the improved space (8), the representation

$$C^T C = A^T A + B^T B - 2\sqrt{A^T A} \sqrt{B^T B} \cos \theta. \quad (9)$$

Since the threshold ε in expressions (1) and (2) defines the boundary value of the metric (8) for the corresponding vectors, then, taking into account the introduced notation, the representation similar to (9) holds for the threshold

$$\varepsilon^T \varepsilon = A^T A + B^T B - 2\sqrt{A^T A} \sqrt{B^T B} \cos(\theta_\varepsilon \pi / 180), \quad (10)$$

where θ_ε is the maximum angle (in degrees) between the vectors at which state vectors are still considered recurrent in the sense of the selected threshold value ε . In this case, the characteristic function (2) in the improved space can be represented as

$$F(\|\cdot\|, \varepsilon) = \begin{cases} 1 & \text{if } \|\cdot\| < \varepsilon \\ 0 & \text{if } \|\cdot\| \geq \varepsilon \end{cases} \rightarrow F(A, B, \theta_\varepsilon) = \begin{cases} 1 & \text{if } A^T B > \sqrt{A^T A} \sqrt{B^T B} \cos(\theta_\varepsilon \pi / 180), \\ 0 & \text{if } A^T B \leq \sqrt{A^T A} \sqrt{B^T B} \cos(\theta_\varepsilon \pi / 180). \end{cases} \quad (11)$$

Passing from the notation in (11) to the corresponding state vectors of the system under study, the characteristic function (2) takes the following form

$$F(Z_i, Z_j, \theta_\varepsilon) = \begin{cases} 1 & \text{if } Z_i^T Z_j > \sqrt{Z_i^T Z_i} \sqrt{Z_j^T Z_j} \cos(\theta_\varepsilon \pi / 180), \\ 0 & \text{if } Z_i^T Z_j \leq \sqrt{Z_i^T Z_i} \sqrt{Z_j^T Z_j} \cos(\theta_\varepsilon \pi / 180). \end{cases} \quad (12)$$

Taking into account (12), the method of calculating RP in the improved space proposed on the basis of (1) is determined by the relation

$$R_{i,j}^{m,\theta_\varepsilon} = F(Z_i, Z_j, \theta_\varepsilon), \quad Z_i \in \Omega^m, \quad Z_j \in \Omega^m, \quad i, j = 1, 2, \dots, N_s. \quad (13)$$

The proposed self-adjusting method (13) is obtained on the basis of a new paradigm for joint overcoming of the metric-threshold uncertainty components of existing methods for calculating RP (1). Moreover, the improvement of space based on the introduction of a scalar product of vectors, considered in [3], made it possible to carry out a joint choice of the norm functional inducing the corresponding metric and the recurrence threshold. In contrast to the known methods, in the proposed method for calculating RP, the norm and threshold turn out to be self-adjusting by measurements. In this case, the threshold is self-adjusting to the changing length of the measured state vectors of the system, and the threshold angle θ_ε of the angle between the vectors is chosen so that the state vectors of the system are assumed to be recurrent in a given sense. In the general case, the value θ_ε of the pore angle will determine the recurrence for nonzero state vectors. If the state vectors turn out to be zero, then the threshold $\sqrt{Z_i^T Z_i} \sqrt{Z_j^T Z_j} \cos(\theta_\varepsilon \pi / 180)$ will be equal to zero for any quantity θ_ε . In this case, the self-adjusting method of computing RP (13) gives a zero value – the absence of recurrence of system states. Moreover, the existing methods for calculating RP (1) at a fixed threshold in this case will display a unit value corresponding to the recurrence of states. Therefore, the self-adjusting method for calculating RP (13) is invariant to the length of the measured state vectors. It should be noted that the scalar product of vectors in the space under consideration gives rise to a new type of conical neighborhood of recurrence instead of the traditional spherical neighborhood generated by the Euclidean metric. When using a conical neighborhood of state recurrence, the concept of classical recurrence loses its original meaning. Therefore, the proposed self-adjusting method for calculating RP in an improved space will actually reflect the dynamics of generalized recurrence (conical recurrence).

3. Experimental verification of the method for calculating recurrence diagrams by the example of the dynamics of atmospheric pollution

During the experimental verification, it was assumed that the main sources of urban air pollution are motor vehicles [19], fires [20, 21] and accidents at critical infrastructure facilities [22]. The well-known connection of global atmospheric pollution with the greenhouse effect, the appearance of acid rain [23], as well as the pollution of various aquifers [24] was also taken into account. In this regard, the concentrations of formaldehyde, ammonia, and nitrogen dioxide were chosen as the measured components of the state vector of atmospheric pollution. The technique of measurements and experimental studies of atmospheric pollution is described in detail in [3]. When testing the method, the results of measurements of the concentrations of these atmospheric pollutants during May 2018 were considered, starting from 480 counts and ending with 604 counts. However, in order to compare the results of [2], the same interval was chosen as a test interval for testing, starting from 13:00 on May 3, 2018 ($i=490$) to 01:00 on May 11, 2018 ($i=520$). During this interval,

the results of measuring the excess of the maximum permissible concentrations (MPC) were analyzed.

As an illustration in **Fig. 1** shows RPs calculated in accordance with the known method in the case of the Euclidean metric for various fixed threshold ε , as well as in accordance with the proposed self-adjusting method with $\theta=1^\circ$ for the pore angle.

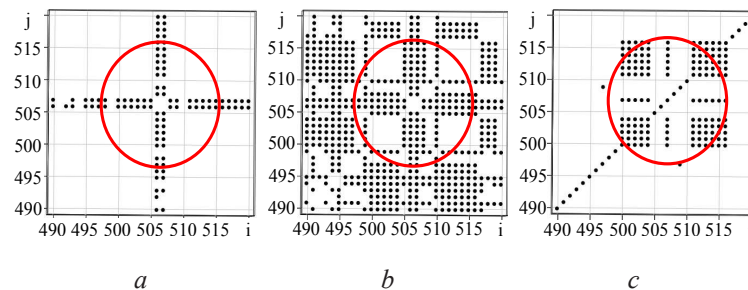


Fig. 1. RP for the vector of states of atmospheric pollution in the test interval: *a* – a well-known method, Euclidean metric, threshold $\varepsilon=8$; *b* – a well-known method, Euclidean metric, threshold $\varepsilon=2$; *c* – self-adjusting method, pore angle $\theta_\varepsilon=1^\circ$

Hereinafter, by a well-known method, one should understand the method of calculating RP described by relations (1) and (2) in Section 2 for the Euclidean metric. In **Fig. 1**, the RP region corresponding to the dangerous states of atmospheric pollution in the interval between 504 and 511 samples is marked in red. Throughout the test interval, the values of the measured concentrations of pollutants exceeded their MPC. Moreover, in the areas marked in red in **Fig. 1** RP structure is different.

As an illustration of an important feature of the proposed method for calculating RP surfaces are presented in **Fig. 2** that describe the dynamics of a self-adjusting threshold when setting the value of the limiting angle $\theta_\varepsilon=5^\circ$ for four test intervals with different levels of excess concentrations of the contaminants under consideration.

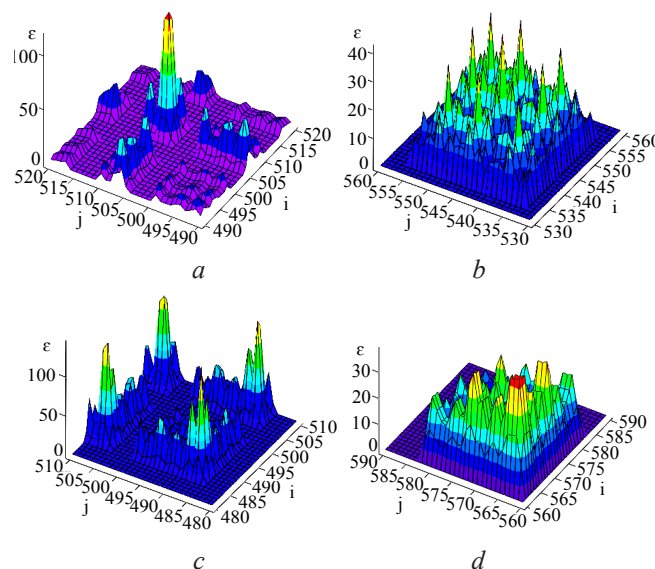


Fig. 2. The surface dynamics of the threshold in the proposed method at different sampling intervals: *a* – 490–520; *b* – 530–560; *c* – 480–510; *d* – 560–590

Examples calculated by RP in accordance with the proposed self-adjusting method for atmospheric pollution state vectors measured in the test interval for various threshold angles θ_ε equal to 10° and 20° are presented in **Fig. 3**.

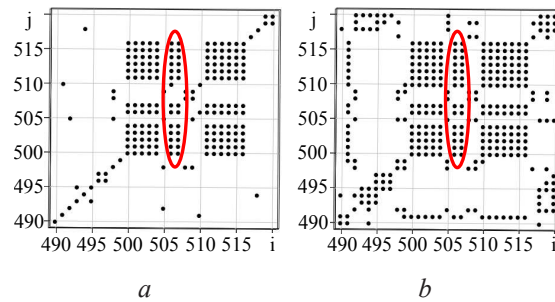


Fig. 3. RP of the state vector of atmospheric pollution in the test interval, calculated on the basis of the self-adjusting method for various values of the pore angle: $a - 10^\circ$; $b - 20^\circ$

The oval in **Fig. 3** marks the region of recurrence of hazardous states of a polluted atmosphere, corresponding to a 10-fold excess in MPC for formaldehyde, 1–2 times for ammonia, and 1–4 times for nitrogen dioxide.

4. Discussion of the results of experimental verification of the proposed self-adjusting method

Illustration of RP in **Fig. 1, a, b**, calculated on the basis of the well-known method for the Euclidean metric for various values of the fixed threshold ε , indicates insufficient accuracy and adequacy of the obtained RPs for a real atmospheric pollution system. Therefore, it is problematic to identify the dangerous state of atmospheric pollution by such RPs. It can be seen that the RP structure for the Euclidean metric depends on the threshold value. Following the RP in **Fig. 1, a, b**, for adequate display with the Euclidean metric under certain conditions it will be necessary to select the best threshold. However, when conditions change, the selection of the corresponding threshold will be required. The application of the proposed method for calculating RP, in contrast to the known method (1) (as well as methods with various metrics), allows for reliable display and identification of dangerous states of atmospheric pollution, regardless of conditions. From an analysis of the nature of the surfaces describing the dynamics of the threshold in the case $\theta_\varepsilon = 5^\circ$ for various intervals shown in **Fig. 2**, it follows that in the self-adjusting method, the calculation of RP is performed at a threshold that is automatically adjusted by measurements, tracking their dynamics. This fact is illustrated by the different dynamics of the threshold at all intervals for measuring pollution. It should also be noted that the improvement of space based on the introduction of the scalar product operation of vectors allows for self-adjusting of the measurement method. Moreover, the traditional concept of recurrence of states in a ball extends to the recurrence of states in a cone, which is valid for arbitrary values of state vectors, including zero vectors. This is the essence of self-adjusting and the novelty of the proposed method.

The influence of different values of the threshold angle θ_ε of the recurrence cone on the structure of the calculated RPs (**Fig. 3**) indicates that with an increase in this angle, the quality of the RP decreases, false black dots appear, and the horizontal and vertical lines of black dots expand with a simultaneous increase in the total number of recurrence points states. The working values of the angle θ_ε should be considered 10° or less. At such threshold angles, the RP structure remains adequate to the recurrent states of the real system. The presence of white dots or clusters of white dots on RP characterizes the absence of recurrence in a given cone for the measured states of atmospheric pollutants. This may be due to both a possible loss of recurrence and a meter failure. The results of the experimental verification, shown in **Fig. 1–3** of the proposed method generally indicate greater information content, accuracy and adequacy of the mapping of recurrence states for real systems in comparison with the known method (1), (2). An important feature of the developed method for calculating RP is the ability to clearly display the presence of dangerous states in dynamic systems in the form of vertical and horizontal lines of black dots. Moreover, the presence of rectangular clusters of black dots on the RP (**Fig. 1, c, Fig. 3**) indicates the presence of recurrent states in the system of atmospheric pollution. In fact, rectangular clusters of black dots turn out to be false for the air pollution system under consideration. Clusters of black dots are caused by the used method of preliminary processing of measurement results, according to which, to identify moments of lack of data, the values were assigned values equal to 10^{-5} . This allowed the RP to display the moments of lack of measurements.

Verification shows that the proposed method for calculating RP has an important applied property related to overcoming the existing metric-threshold uncertainty of the known methods considered (1) together with (2). In addition, the method ensures the invariance of the structure of the calculated RPs to the nature of the measured data, irregularity and the absence of measurements. The recurrent states displayed using the proposed method turn out to be adequate to real systems. These properties significantly expand the field of practical use of the proposed method for calculating RP. This method differs in that it is based on the calculation of a generalized conical neighborhood of recurrence. This means that the traditional concept of recurrence in a ball for a Euclidean metric changes to the concept of recurrence in a cone. In addition, the proposed method makes it possible to ensure the invariance of the calculation of RP with respect to the distance of the considered vector states of the system from the center of space for a given angular size of the recurrence cone. It is established that the angle of the cone of recurrence determines the required accuracy of the proposed method for calculating RP.

5. Conclusions

1. A self-adjusting measurement method for calculating RP has been developed, which allows overcoming the existing metric-threshold uncertainty of known methods. This ensures the invariance of the method to the nature of the measured data and allows to display the recurrence of states on the diagrams, adequate to real dynamic systems. A new scientific result consists in the theoretical justification of the method for calculating RP in the metric space of an improved topology, capable of overcoming the inherent metric-threshold uncertainty inherent in well-known methods of measurements. The topology of space is improved by introducing into it the operation of the scalar product of vectors. It is established that the proposed method has the ability to display properties adequate to real systems. This method has a relatively low computational complexity and is invariant with respect to the type and regularity of measurements.

2. Verification of the proposed self-adjusting method for calculating RP was made on the basis of experimental measurements of gas concentrations of atmospheric air pollutants for a typical area of an industrial city, conducted in May 2018. Formaldehyde, ammonia and nitrogen dioxide were considered as the main gas pollutants of the atmosphere. The obtained results of the verification of the method confirm the increased accuracy and adequacy of the display of the recurrence of atmospheric pollution states, as well as the invariance with respect to the type of measurements and their regularity. It has been established that the accuracy of the method is influenced by the a priori boundary angular dimensions of the recurrence cone. It is shown that with a decrease in the boundary angles, the accuracy of the display of the states of dynamical systems in RP increases due to the elimination of false points. It has been experimentally established that accuracy and adequacy that is acceptable for visual and automatic detection of hazardous conditions in dynamic atmospheric pollution systems is ensured for a boundary angular size of the recurrence cone of 10° or less.

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