ABOUT POSSIBILITY-THEORETICAL METHOD OF PIECEWISE-LINEAR APPROXIMATION OF FUNCTIONAL DEPENDENCIES IN PROBLEM OF ODOURS' RECOGNITION

Veda Kasyanyuk, Iryna Volchyna

***Abstract**: This paper considers the problem of recognizing and classifying the odorants to preset classes of volatile matters. It is assumed that the data registered by sensory elements and been liable to processing has been distorted by errors – fuzzy values. The possibility-theoretical method of piecewise-linear approximation of functional dependencies is proposed to solve the problem.*

***Keywords**: possibility-theoretical method, odorants, fuzzy errors.*

***ACM Classification Keywords**: I.6 Simulation and Modeling.*

Introduction

The problem of determining the composition of volatile matter and the quantitative characteristics of its elements, as well as the problem of classifying the tested odorants to preset classes of volatile matters are the important tasks arising under the problem of recognizing the odors. Very often the task of clarifying the composition of the volatile matter should be regarded as a sub-task of modeling the olfactory system.

One can choose several ways to create a "good" gas-analysis sensory system: optimization of gas-dynamic characteristics, the use of layers with better selective properties, the improvement of mathematical tools for processing the experiment data. Among the traditional methods used for detecting the gas mixtures, we should like to mention the method of principal component analysis (PCA), the discriminant analysis (DA) and the neural networks [Zieger, 1998, Jurs, 2000]. Unfortunately, these methods either do not provide sufficiently reliable identification or require the significant computing power. Furthermore, under the real conditions the data at the output of olfactory receptors are distorted by noise, and to analyze this data it is necessary to minimize their impact as much as possible. In authors' opinion, the best way out of this situation is to build a gas-analysis system within the concept of "device + PC = new possibilities", according to which the desired effect should be achieved by mathematical processing of received experimental data. The use of such processing algorithms provides a whole number of advantages: these algorithms are robust to errors in the data, they provide more accurate results, and it is quite easily to implement them by usual personal computers, i.e. there is no need to invest the substantial funds in creating a new device with improved characteristics. Furthermore, such algorithms do not require a large number of computations, i.e. it is possible to process the results of the measurements under real time.

Method of piecewise-linear approximation of functional dependencies by fuzzy data

The mathematical formulation of the problem is the following. We assume that the odor is represented by the vector of the concentrations of elementary odorants. The result of the device (gas-analyzer) measurement of some volatile compound is a certain number of numerical sequences which reflects the changes in time of sensors' responses on the tested matter; the number of sequences is equal to the number of sensors. The

problem is the following: it is necessary to find the vector of elementary odorants, i.e. the odor by sequences of sensors' responses on this matter. The method proposed in this paper requires a stage of training when known compounds (they may or may not be the same as those which later are submitted at the input for recognizing) are associated with corresponding sensors' response on it.

To solve such problem of recognizing the odors we should use the method of recovering the functional dependencies proposed in [Pitiev, 2000]. It will be about the problem of approximating the function $y(\cdot): T \to Y$ belonging to the known class of functions (linear in this case) by the results of observing the values of its argument $(t_1,...,t_N)$ and corresponding values of the function $y_1,...,y_N$, and the data of observation isn't precisely known.

We should assume that the number of sensors of the gas analyzer (the basic odorants) is equal to *l*, and concentration of the odorant fixed by sensors of the gas analyzer is a linear function of time. Then, at the output of the device which measures the concentration of some volatile compound we observe *l* vectors: $y_n^{(s)}$, $s = \overline{1,l}$ at moments of time t_n, $n = \overline{1,N}$.

We divide the received data into *k* groups by intervals Δ_p, $p = \overline{1,k}$ and there are m_p, $p = \overline{1,k}$ observations in each interval. We denote them as $y_{p,i}^{(s)}, i = \overline{1,m_p}$. For each interval we choose the following linear model of relationship between *y* and *t*:

$$y_p^{(s)}(t) = a_{p,1}^{(s)} t + a_{p,2}^{(s)}, \quad p = \overline{1,k}, \; s = \overline{1,l}$$

and assume that the values of the argument $t_{p,i}^{(s)}$, $i = \overline{1,m_p}$ are precisely known, and corresponding values $y_{p,i}^{(s)} = y_p^{(s)}(t_{p,i}^{(s)})$, $i = \overline{1,m_p}$ are modeled as the values of coordinates of the fuzzy vector:

$$\eta_{p,i}^{(s)} = a_{p,1}^{(s)} t_{p,i}^{(s)} + a_{p,2}^{(s)} + \nu_{p,i}^{(s)}, \quad i = \overline{1,m_p}, \; p = \overline{1,k}, \; s = \overline{1,l},$$

where $\eta_p^{(s)} = (\eta_{p,1}^{(s)},...,\eta_{p,m_p}^{(s)})$ - the fuzzy output vector ($y_{p,i}^{(s)}$ - its observed values), $\nu_{p,i}^{(s)}$ - the values of the fuzzy vector of errors $\bar{\nu}_p^{(s)} = (\nu_{p,1}^{(s)},...\nu_{p,m_p}^{(s)})$, which distribution is defined in the following way:

$$\pi^{\bar{\nu}}(\bar{z}) = \rho\left(\max_{1 \le j \le N} \frac{|z_i|}{\varepsilon_i}\right), \quad \varepsilon_j > 0, \; j = \overline{1,N},$$

$\rho: \Re^+ \to [0,1]$ is the continuous function strictly monotonically decreasing on $[0,1]$, which is equal to zero on $[1,\infty]$, $\rho(0) = 1$.

The values ε_i determine how much the error deviates from zero at $j-$th measurement. According to the possibility-theoretical method developed in [Pitiev, 2000] we should find such $a_{p,1}^{(s)}$ and $a_{p,2}^{(s)}$ which deliver a maximum of distribution

$$\pi^{\bar{\eta}_p^{(s)}}(\bar{y}_p^{(s)}, a_{p,1}^{(s)}, a_{p,2}^{(s)}) = \pi^{\bar{\nu}_p^{(s)}}(\bar{y}_p^{(s)} - a_{p,1}^{(s)}, \bar{t}_p^{(s)} - a_{p,2}^{(s)})$$

for each interval of the partition.

Since the input data can be considered as the values of the continuous function, we should require so that the approximating function satisfies the continuity condition:

$$a_{p-1,1}^{(s)} t_{p-1,m_{p-1}}^{(s)} + a_{p-1,2}^{(s)} = a_{p,1}^{(s)} t_{p,m_p}^{(s)} + a_{p,2}^{(s)}, \quad p = \overline{2,k}, \; s = \overline{1,l}.$$

So, to find the estimates $\hat{a}_{p,1}^{(s)}$ and $\hat{a}_{p,2}^{(s)}$ of maximum possibility [Pitiev, 2000] for each $s = \overline{1,l}$ at each interval of the partition Δ_p, $p = \overline{1,k}$ we have the following problem

$$\rho\left(\max_{\substack{1 \le i \le m_p \\ 1 \le p \le k}} \frac{| y_{p,i}^{(s)} - a_{p,1}^{(s)} t_{p,i}^{(s)} - a_{p,2}^{(s)} |}{\varepsilon_{p,i}^{(s)}} \right) \to \max_{a_{p,1}^{(s)}, a_{p,2}^{(s)}, p=\overline{1,k}}$$

$$\left\{ a_{p-1,1}^{(s)} t_{p-1,m_{p-1}}^{(s)} + a_{p-1,2}^{(s)} = a_{p,1}^{(s)} t_{p,m_p}^{(s)} + a_{p,2}^{(s)}, \quad p = \overline{2,k}, \right.$$

$$s = \overline{1,l}$$

Using the definition of the function $\rho(\cdot)$, we have

$$r = \max_{\substack{1 \le i \le m_p \\ 1 \le p \le k}} \frac{| y_{p,i}^{(s)} - a_{p,1}^{(s)} t_{p,i}^{(s)} - a_{p,2}^{(s)} |}{\varepsilon_{p,i}^{(s)}} \to \min_{a_{p,1}^{(s)}, a_{p,2}^{(s)}, p=\overline{1,k}}$$

$$\left\{ a_{p-1,1}^{(s)} t_{p-1,m_{p-1}}^{(s)} + a_{p-1,2}^{(s)} = a_{p,1}^{(s)} t_{p,m_p}^{(s)} + a_{p,2}^{(s)}, \quad p = \overline{2,k} \right.$$

$$s = \overline{1,l}$$

Let us transform the resulting problem to a standard linear programming problem:

$$r \to \min_{a_{p,1}^{(s)}, a_{p,2}^{(s)}, p=\overline{1,k}}$$

$$\begin{cases} a_{p-1,1}^{(s)} t_{p-1,m_{p-1}}^{(s)} + a_{p-1,2}^{(s)} = a_{p,1}^{(s)} t_{p,m_p}^{(s)} + a_{p,2}^{(s)}; p = \overline{2,k} \\ \dfrac{| y_{p,i}^{(s)} - a_{p,1}^{(s)} t_{p,i}^{(s)} - a_{p,2}^{(s)} |}{\varepsilon_{p,i}^{(s)}} \le r; p = \overline{1,k}, p = \overline{1,m_p} \end{cases}$$

$$s = \overline{1,l},$$

and to solve it we can use the simplex-method (or one of its modifications). The following vector is the solution of this problem:

$$\overline{a}^{(s)} = (a_{1,1}^{(s)}, a_{1,2}^{(s)}, \ldots, a_{k,1}^{(s)}, a_{k,2}^{(s)}), \quad s = \overline{1,l}$$

of the dimension $2 \cdot k$.

Constructing the solutions for linear programming problems for all $s = \overline{1,l}$ we obtain the vector:

$$\overline{a} = (a_{1,1}^{(1)}, a_{1,2}^{(1)}, \ldots, a_{k,1}^{(1)}, a_{k,2}^{(1)}, \ldots, a_{1,1}^{(l)}, a_{1,2}^{(l)}, \ldots, a_{k,1}^{(l)}, a_{k,2}^{(l)})$$

of the dimension $l \cdot 2 \cdot k$ which can be considered as a characteristic (characteristic vector) of the tested matter.

Computational experiment

Let us present one example of using the method of piece-linear approximation for recognizing the volatile matters by their odors. As mentioned above, at the beginning we have input the known matters and mixtures into the gas-analysys system. For each of them we should find the above-mentioned characteristic vector and enter it into the database. For the characteristic vectors we introduce the metric $\rho(A,B) = sqrt([A-B, A-B])$, where $[.,.]$ - scalar product, and then we choose the threshold of closeness δ which is constrained in the following way: if A and B are the characteristics of the known matters then $\rho(A,B) > 2\delta$.

Then, we input the unknown matter into the gas-analysis system and calculate its characteristic A . Among all characteristics from the database we should find such characteristic B that $\rho(A,B) < \delta$. If B exists then we conclude that the tested matter coincides with the matter which corresponds to B , otherwise, we assume that the composition of the tested matter differs very much from all matters from the database.

Let us consider the application of this method giving the example of recognizing the odor of the matter chlorine. During performing the computational experiment we used the data obtained by the gas-analysis sensory system developed at the Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine [Shirshov, 2002, Kalchenko, 2002]. According to the experiment, the air under pressure with a high concentration of chlorine was input into gas-analysis system. Measurements were made using eight sensors at the time $t \in [0,72]$ as shown in Fig.1.

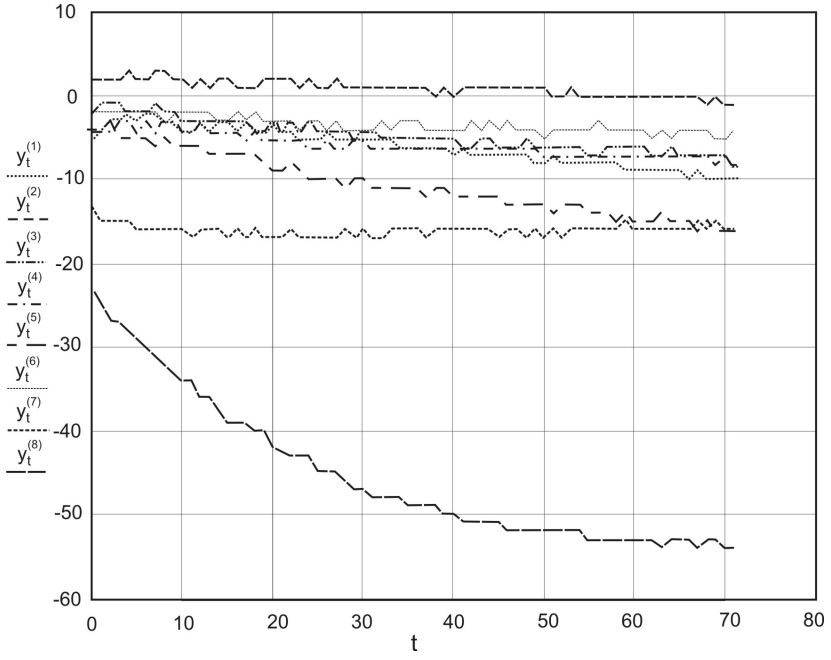

Figure 1. Measurement results for matter chlorine (first measurement)

After portioning the data into intervals, we considered 12 intervals with 12 measurements for each sensor and solved the canonical linear programming problem using the modified simplex-method. The resulting solution $\bar{a}^{CHLOR}$ were considered as a characteristic of the matter chlorine and consisted from 192 elements. Then, the back actions were conducted: the approximant of measurements' results were constructed in accordance with the vector $\bar{a}^{CHLOR}$ (see Fig. 2). Fig. 3-5 represents the results of comparing the real and modeled data $y_t^{(s)}$ for $s = 2,5,8$, i.e. for 2nd, 5th and 8th sensors, respectively.

The Figurers show that modeled data slightly deviates from measured ones.

We can improve the model by reducing the value of group intervals and reducing ε for each sensor, respectively, as well as by removing some of the time intervals at which measurements are questionable. Usually such decisions are made by the decision maker – the person, who knows much about physics of the process and can take into account the various factors and measurement conditions.

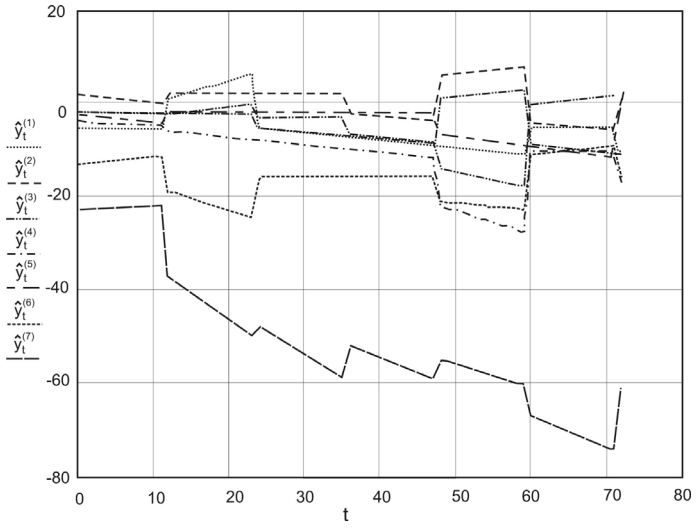

Figure 2. Approximation of measurement of chlorine

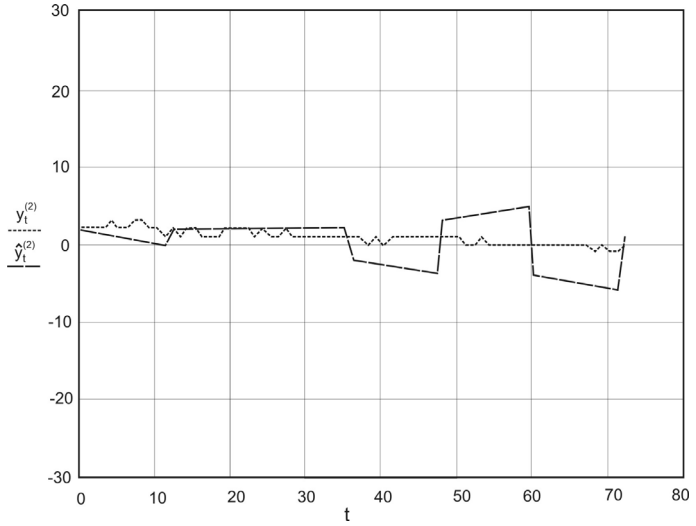

Figure 3. Data approximation by 2nd sensor

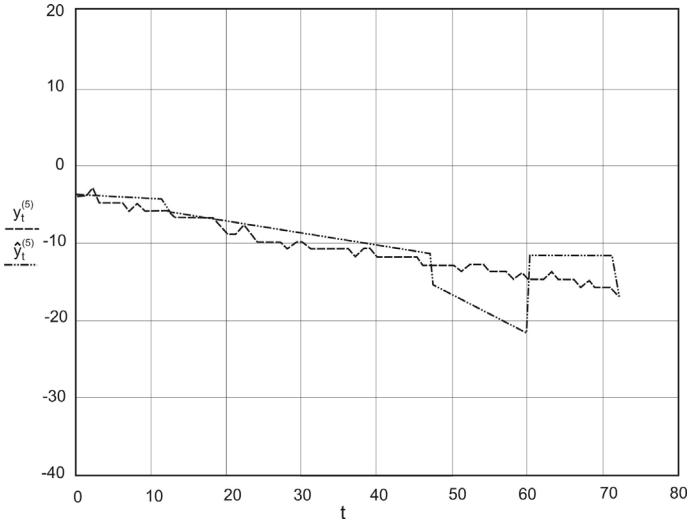

Figure 4. Data approximation by 5th sensor

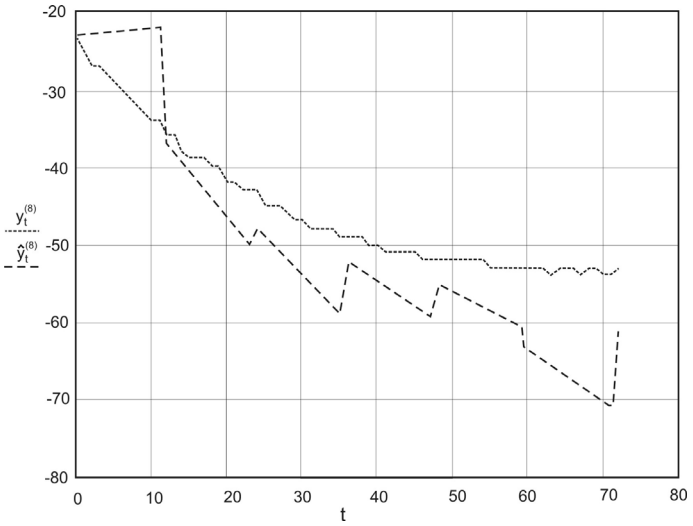

Figure 5. Data approximation by 8th sensor

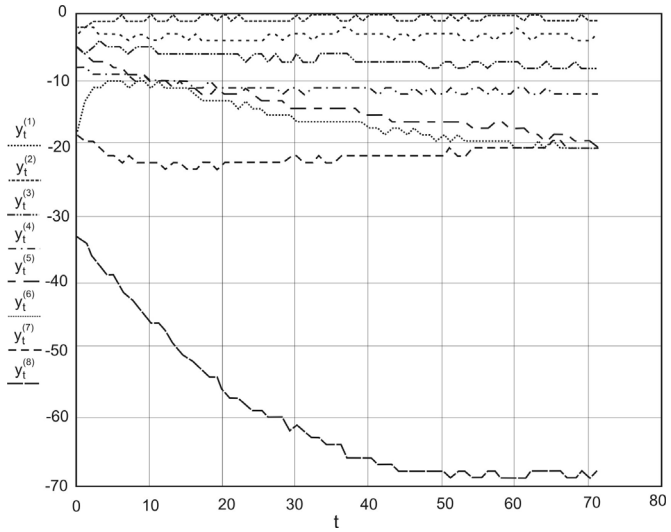

Figure 6. Measurement results for matter chlorine (second measurement)

After that we consider the problem of recognition of two matters. We should measure the matter chlorine once more and obtain other experimental data at the output of the gas analyzer (see Fig. 6). This data do not differs very much from the data presented in Fig. 1, and also the expected model should not differ very much from the previous one.

Let us construct the vector $\bar{a}^{CHLOR\_2}$ by the second measurement of chlorine and find the deviation of one measurement from another by their characteristic vectors $\bar{a}^{CHLOR}$ and $\bar{a}^{CHLOR\_2}$: $|| \bar{a}^{CHLOR} - \bar{a}^{CHLOR\_2} ||= 28.833$.

Then we input the matter from another class which differs very much from chlorine, for example, brandy, into the gas-analyser. The measurement results are shown in Fig. 7.

After constructing the vector $\bar{a}^{TAW}$ by measurements of the matter brandy we should find the deviation $\bar{a}^{CHLOR}$ from $\bar{a}^{TAW}$: $|| \bar{a}^{CHLOR} - \bar{a}^{TAW} ||= 290.927$. One can see that difference between the characteristics of chlorine and brandy is by an order greater than the difference between the characteristics of the different measurements of chlorine, i.e. at the low δ chlorine and brandy differ by the algorithm, which confirms the efficiency of its use.

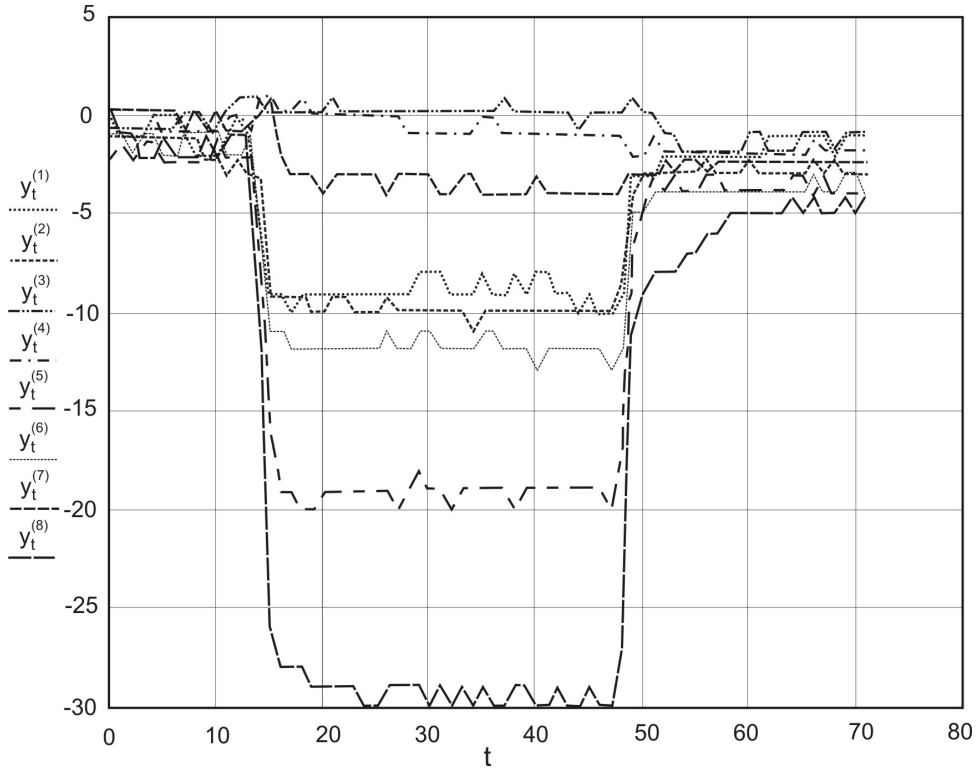

Figure 7. Measurement results for matter brandy

We would like to mention that the recognition of brandy has been chosen only as an example. In much the same way, one can recognize other odorants and mixtures of odorants, classify the odorants to classes, naturally, after the corresponding measurements, and under certain conditions it is also possible to recognize volatile matters, previously conducted a stage of training on the components of these compounds.

Conclusion

Thus, the method of piece-linear approximation by fuzzy data proposed in the paper allows recognizing the odors regardless of the concrete sensory systems. It has become possible thanks to the stage of training, during which we use the information only on the results of the test measurements without taking into account the complex internal self-structure of the gas-analysis sensory system – the data provider. Another advantage of this method is the fact that from the very beginning the method has supposed an occurrence of errors in the data, and the recognition is conceptually focused on minimizing the need of errors (the estimates of maximum possibility should be constructed).

The method proposed in this paper is quite simple to implement and it allows recognizing in real time. Thus, the use of this method together with optimally selected sensitive coatings of sensors can improve very much the process of recognizing the volatile matters and molecules by gas-analysers.

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Authors' Information

Veda Kasyanyuk *– PhD, Head of Scientific Sector, theoretical cybernetics sector, theoretical cybernetics department, faculty of cybernetics, Kyiv National Taras Shevchenko University, Glushkov av. 4-D, Kyiv-03127, Ukraine.*

Iryna Volchyna *– Engineer; theoretical cybernetics sector, theoretical cybernetics department, faculty of cybernetics, Kyiv National Taras Shevchenko University, Glushkov av. 4-D, Kyiv-03127, Ukraine, e-mail: volchyn@voliacable.com*