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VISUALIZATION OF SELF-ORGANIZING MAPS AND ESTIMATION OF THEIR QUALITY

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VILNIAUS UNIVERSITETAS

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SAVIORGANIZUOJANČIŲ NEURONINIŲ TINKLŲ VIZUALIZAVIMAS IR JO KOKYBĖS NUSTATYMAS

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1. Introduction

1.1. Research area and relevance of the problem

Nowadays technologies allow us to accumulate large amounts of different information and save it in the computer memory, external media or on the Internet. In the course of time, collection and storage become a load of rubbish which often makes it difficult to find the required data and other useful information. Modern technology enables us to quickly find a big amount of information about one or other thing you want, but the information found is often useless, distorted, and irrelevant. Therefore, it is becoming a serious problem and a challenge for every user. One of the solutions to solve this problem is data mining methods, which allow us to structure data by clustering, classifying them and, if there is a possibility, presenting the results visually.

One of the data mining methods is self-organizing networks. Usually this data mining method is called a self-organizing map (SOM), and sometimes by the name of the creator the Kohonen map. SOM can be used to cluster and visualize multidimensional data, as well as find the multidimensional data projection into a smaller number of dimensions of space. Despite that more than 40 years have passed after the appearance of SOM, it is still intensively researched and applied. Over time, a lot of various extensions and modifications of SOM have appeared, starting from the learning rules for different ways of SOM visualization techniques, but the main principle of the original self-organizing map remains the same. For many years, SOM has been applied to clustering and classifying of the numerical data, but currently, the scope of investigation has extended to the analysis of the textual data or other type of data.

One of SOM advantages as compared with other data mining methods is that, as a result SOM gives not only numerical estimates, like most other data mining methods, but the also results are presented in a visual form, and the visual information enables a user to understand it faster than the textual or numerical information. Mostly SOM is used to cluster the datasets. Comparing SOM with other clustering methods, there are no precisely defined clusters, i. e. the data are not unambiguously assigned to one or other cluster. Clustering of results can be variously interpreted by researchers, when watching a visual image of SOM. It allows us to notice the similarity between the data and groups that are not known in advance, which can be an advantage over other clustering methods. SOM also can be applied to data, assigned to different classes. In this case, a researcher can investigate how classes match up to the clusters obtained in SOM, and explain the reasons for such differences, one of which may be related to the fact that the data were incorrectly assigned to classes.

Currently, there is a variety of software systems, that implement the SOM visualization techniques, but there is a lack of systems in which SOM shows the number of data in each cell of SOM and what class of data is assigned to each cell of SOM. Also, the problem is that there are no numerical estimates showing data classes and SOM clustering overlaps.

In addition, the SOM result highly depends on a variety of learning parameters, so there is a problem, which values of a parameter should be chosen for analyzed datasets. It is also important to investigate which learning parameters allow us to get more accurate results when analyzing different types of data: textual and numerical.

So, the dissertation deals with two major problems:

1. Visualization of data, assigned to a specific class by self-organizing maps and estimation of the obtained results.
2. Dependence of the results obtained by the self-organizing maps on learning parameters.

1.2. Research object

The object of dissertation is data clustering, classification and visualization using self-organizing maps and estimation of their quality

1.3. The Aim and Tasks of the Research

The aim of this work is to propose a new visualization technique of self-organizing maps, which allows us to visualize textual and numerical data as classes are known in advance, and to observe the coincidence of the obtained clusters and data classes, as well to propose and investigate errors evaluating the coincidence.

To realize the aim of research, it is necessary to solve the following tasks:

1. To perform an analytical review of the existing SOM visualization techniques.
2. To propose errors, in order to evaluate the coincidence of the obtained SOM clusters and data classes.

3. To propose a SOM visualization technique, with a view to investigate the data when classes are known in advance.
4. To create a software system in which the proposed SOM visualization technique and proposed errors to evaluate the obtained SOM quality would be implemented.
5. To investigate experimentally the proposed SOM visualization technique and errors, depending on the values of the selected SOM learning parameters, analyzing the numerical and textual data.

1.4. Scientific novelty

1. The new SOM visualization technique is proposed, allowing us to see the ratio between different members of both textual and numerical data classes in the same SOM cell.
2. Two errors are proposed for estimation the SOM quality, which are suitable for data when their classes are known in advance.
3. It is investigated how different factors of text document conversion to numerical expression influence the SOM results obtained.

1.5. The defended statements

1. The proposed SOM visualization technique allows us to see the ratio between different data class members in the same SOM cell for both textual and numerical datasets.
2. The proposed errors for estimating the SOM quality allows us to estimate the coincidence between data classes and clusters obtained by SOM.
3. The appropriate of selected factors conversion of text documents into a numerical expression improve the results obtained by SOM.

1.6. The practical value of the study results

The new SOM system has been developed. Not only the proposed SOM visualization technique and errors to estimate the SOM quality are implemented in the new SOM system, but also there is a possibility to choose various neighboring functions and learning rates, which values can be changed in each iteration or epoch. It is also possible to split the analyzed dataset into two subsets: training and testing. For this reason, the new SOM

system can be used not only to analyze the data, but also to investigate the SOM features.
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1.7. Approbation and Publications of the Research

The main results of the dissertation were published in 7 scientific publications: five are published in periodicals, reviewed scientific journals, two of them are refereed in the ‘Thomson Reuters Web of Science’ database with an impact factor; other two publications are published in conference proceedings. Besides two abstracts were published in international conference abstracts proceedings. The main results of the work have been presented and discussed at 4 national and 3 international conferences.

1.8. Outline of the Dissertation

The dissertation consists of 5 chapters and references. The chapters of the dissertation are as follows: ‘Introduction’, ‘Review of self-organizing maps’, ‘The proposed errors for estimation of SOM quality’, ‘The experimental results’, ‘Summary’, and ‘General Conclusions’. The dissertation also includes the list of notation and abbreviations. The scope of the work is 132 pages that include 49 figures and 27 tables. The list of references consists of 87 sources.

2. Review of self-organizing maps

T. Kohonen began to explore self-organizing maps (SOMs) in 1982. More than 30 years have passed since that time, but SOM does not lose its popularity. New extensions and modifications are developed constantly. The main target of SOM is to preserve the topology of multidimensional data, i. e., to get a new set of data from the input data such that the new set preserved the structure (clusters, relationships, etc.) of the input data (Kohonen, 2001). SOM is applied to cluster and visualize data. The self-organizing map is a set of nodes, connected to one another via a rectangular or hexagonal topology. The rectangular topology of SOM is presented in Figure 1. The learning starts from setting the initial values of components of the codebook vectors M_{ij}. Usually these values are random numbers in the interval $(0, 1)$. The codebook vectors of neurons M_{ij}, $i = 1, \dots, k_x$, $j = 1, \dots, k_y$, are adapted according to the learning rule (1):

$$M_{ij}(t+1) = M_{ij}(t) + h_{ij}^{w}(t)\left(X_p - M_{ij}(t)\right). \qquad (1)$$

Here k_x is the number of rows, and k_y is the number of columns on a rectangular topology of SOM; t is the order number of the current learning steps; $h_{ij}^{w}(t)$ is a neighboring function. The neuron, the codebook vector M_w of which is with the minimal Euclidean distance to X_p, is designated as a winner (the so-called best matching unit, BMU). So, w is a pair of indices of the neuron-winner for the vector X_p. The learning is repeated until the maximum number of iterations T is reached. After SOM learning, the data $X_1, X_2, \dots, X_m$ or other data are presented to SOM, and neurons-winners for each X_i, $p = 1, \dots, m$, are found. In such a way, the data items are distributed on SOM, and some data clusters can be observed.

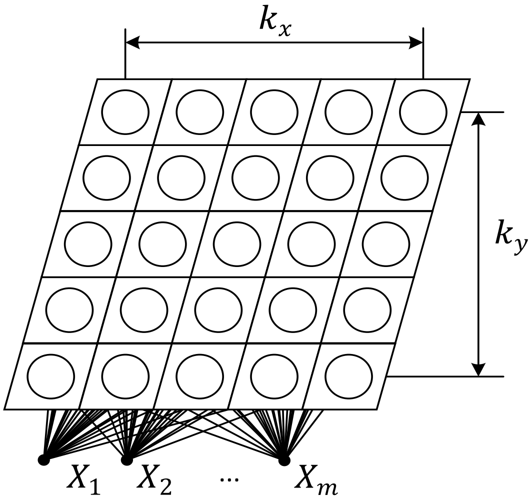


Figure 1. Two-dimensional SOM (rectangular topology)

2.1. Creation of text document matrices for self-organizing maps

In order to analyze text documents by SOM, it is necessary to convert them into numerical data. A so-called text document matrix needs to be created. First of all, document files are converted to the text files – only the text and digits remain, figures and formulas are rejected. Afterwards, we can choose control factors: remove the digits from the text files, choose a word length limit, word frequency, common word list, and stemming algorithm. According to the control factors, a so-called text document dictionary is created. The document dictionary is a list of words from text files excluding the words that do not satisfy the conditions defined by the control factors. Descriptions of the control factors, when a document dictionary is being created, are as follows:

- Almost in all text documents, there are digits. There is no need to include them into the document dictionary, because they do not characterize the text document.
- The word length limit is the number indicating the smallest length of words which will be included into the document dictionary. It is not advisable to include short words, such as the author's initials, articles 'a', 'an', 'the', or other not informative words into the dictionary.
- The common word list is a list of words that will not be included into the document dictionary. Often the words such as 'there', 'where', 'that', 'when', etc. compose the common word list. All of them are not important for document analysis, so these words just distort the results. However, the common word list can depend on the domain of text documents. For example, if we analyze scientific papers, the words such as 'describe', 'present', 'new', 'propose', 'method', etc. also do not characterize the papers and it is not purposeful to include them into the document dictionary.
- The stemming algorithm separates the stem from the word (Porter, 1980). For example, we have four words 'accepted', 'acceptation', 'acceptance', and 'acceptably'. The stem of the words is 'accept'. Only it is included into the document dictionary. All the other words are ignored.
- The word frequency is the number indicating how many times the word has to be repeated in the text so that it could be included into the dictionary. If a small frequency is chosen, rare words that do not characterize the text document will be included into the document dictionary. Otherwise, if a large frequency is chosen, frequent words will be included into the document dictionary, but not all of them characterize the text document.

Thus, the proper values of these control factors should be chosen in order to get a dictionary that characterizes the text documents as exactly as possible. According to the frequency of the document dictionary words in the text documents, a so-called text document matrix is created (2).

$$\begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \dots & x_{mn} \end{pmatrix} \quad (2)$$

Here x_{pl} is the frequency of the lth word in the pth text document, $p = 1, \dots, m,\ l = 1, \dots, n$. m is the number of the analyzed text documents, and n is the number of words in the text document dictionary. Therefore, the document matrix is a matrix the elements of which are equal to frequencies of the document dictionary words in the text documents. A row of matrix (2) is a vector, corresponding to a document. These vectors $X_1, X_2, \dots, X_m$ can be used for training SOM, $X_p = (x_{p1}, x_{p2}, \dots, x_{pn})$, $p = 1, \dots, m$. They are presented to SOM as input vectors. A set of the vectors $X_1, X_2, \dots, X_m$ composes a dataset analyzed. A data item corresponds to a vector, n is a dimensionality of the data item.

Over the past decade, many researches dealing with text mining have been conducted. For this reason, various tools have been created to help analyze the textual data. We use the Text to Matrix Generator (TMG) toolbox implemented in Matlab (Zeimpekis, Gallopoulos, 2005) to create text document matrices. The toolbox allows us to construct text document matrices from text documents and to perform various data mining tasks: dimensionality reduction, clustering, classification, etc.

2.2. Learning parameters

The results of a self-organizing map depend on the selected learning parameters. Thus, it is important to choose the best learning parameters to get better results. The results are mostly affected by different neighboring functions h_{ij}^{w} (Table 1) and learning rates $\alpha(t)$ (Table 2). Usually, two neighboring functions – bubble (3) and Gaussian (4) are used. In our research, we analyze one more neighboring function, so-called heuristic (5) (Dzemyda, 2001).

Table 1. Neighboring functions

Bubble (3)	$h_{ij}^{w}(t) = \begin{cases} \alpha(t), (i,j) \in N_w \\ 0, (i,j) \in N_w \end{cases},$
Gaussian (4)	$h_{ij}^{w}(t) = \alpha(t) \cdot \exp\left(\frac{-\lVert R_w - R_{ij} \rVert^2}{2\left(\eta_{ij}^{w}(t)\right)^2}\right),$

Heuristic (5)	$h_{ij}^w = \frac{\alpha(t)}{\alpha(t) \cdot \eta_{ij}^w + 1}$.

In Table 1, N_w is the index set of neighboring nodes around the node with indices w. Two-dimensional vectors R_w and R_{ij} consist of indexes of M_w and M_{ij}, respectively. The indexes show a place of the neuron-winner, the codebook vector of which is M_w , for the vector X_p, and that of the neuron, the codebook vector of which is M_{ij}, in SOM. The parameter η_{ij}^w is the neighboring rank of M_{ij} according to M_w. As mentioned before, the learning rate $\alpha(t)$ also influences the results of the self-organizing map. Usually linear (6), inverse-of-time (7), and power series (8) learning rates are used for SOM training. In our investigation, we analyze one more learning rate, so-called heuristic (9). Four variants of learning rates are presented in Table 2.

Table 2. Learning rates

Linear (6)	$\alpha(t) = \left(1 - \frac{t}{T}\right)$,
Inverse-of-time (7)	$\alpha(t) = \frac{1}{t}$,
Power series (8)	$\alpha(t) = (0.005)^{\frac{t}{T}}$,
Heuristic (9)	$\alpha(t) = max\left(\frac{T+1-t}{T}, 0.01\right)$.

In this work, two cases are investigated:

- When the learning rate $\alpha(t)$ depends on the iteration number (in this case, t is the order number of the current iteration and T is the total number of iterations). One iteration is part of the training process, when one input vector is passed to the network and the neurons are changed.
- When the learning rate $\alpha(t)$ depends on the epoch number (in this case, t is the order number of the current epoch and T is the total number of epochs). An epoch is part of the training process, when all the vectors of the training dataset are passed to the network at once.

2.3. Estimation of the SOM quality

After training the SOM network, its quality must be evaluated. Usually two errors (quantization and topographic) are calculated. The quantization error E_{QE} shows how well neurons of the trained network adapt to the input vectors. Quantization error (10) is the average distance between the data vectors X_p and their neuron-winners $M_{w(p)}$.

$$E_{\mathrm{QE}} = \frac{1}{m}\sum_{p=1}^{m}\left\|X_p - M_{w(p)}\right\|. \tag{10}$$

Topographic error E_{TE} shows how well the trained network keeps the topography of the data analyzed. The topographic error (11) is calculated by the formula:

$$E_{\mathrm{TE}} = \frac{1}{m}\sum_{p=1}^{m} u(X_p). \tag{11}$$

If the neuron-winner of vector X_p is near to the neuron, the distance from X_p to it is the smallest one, disregarding the neuron-winner, then $u(X_p) = 0$, otherwise, $u(X_p) = 1$.

2.4. Extensions and modification of self-organizing maps

More than 30 years have passed since the self-organizing maps has been introduced, so the new extensions and modifications are developed constantly. In the dissertation a review of commonly used SOM modifications and extensions is presented, namely: merge self-organizing map (Strickert, Hammer, 2005), recursive self-organizing map (Voegtlin, 2002), WEBSOM (Kaski and other, 1998), etc. Mostly all of them are created to speed-up the learning algorithm or to perform specific tasks. For example, WEBSOM is the first SOM extension created for the textual document analysis.

Now a lot of researchers are still using SOM for different problem solutions. One of the newest SOM modifications is the batch-learning self-organizing map (BLSOM), used in the bioinformatics area (Iwasaki, 2013). In this method, SOM has been modified for gene informatics to make the learning process and resulting map independent of the data input. BLSOM is a powerful tool for big data analysis. It allows us to visualize and classify big sequences, obtained from genomes (millions of metagenomics sequences).

Also, we can find SOM extensions with an unusual visualization technique suitable for unstructured data. This visualization technique (Prakash, 2013) helps us to analyze several features at once, so it is much more suitable for a big data visual analysis. As a result, we get SOM as a spider graph, where we can find a large number of analyzed features in each graph.

2.5. Self-organizing map systems

In the dissertation an analytical overview of the most popular SOM systems is made. In order to demonstrate visualization techniques, implemented into SOM systems (SOM-Toolbox, Databionic ESOM, Viscovery SOMine, NeNet), experiments have been carried out using two datasets and these systems. Other SOM systems have also been reviewed, such as: Orange, SOM-analyzer, R package for SOM and others. In the review, the advantages and disadvantages of systems are highlighted.

One of the main disadvantages of all the reviewed systems is that there is no possibility to see the number of all vectors which fall in the same cell of SOM. It is important, because only showing a single class member in the cell, it is not clear how many and which class members are in the same cell of SOM, so the researcher cannot say which SOM cluster obtained is 'stronger'. It is also purposeful to propose new errors that would enable to estimate the SOM quality considering the coincidence of data classes and clusters obtained in SOM.

3. The proposed errors for estimation of SOM quality

As mentioned before, after training SOM, usually the quantization E_{QE} and topographic E_{TE} errors are calculated. However, these two errors do not show whether the analyzed dataset classes correspond to the clusters formed in the SOM. Often, when we analyze the classified data by the clustering methods, there is a need to evaluate the coincidence between data classes and the obtained clusters. The coincidence indicates that the data are assigned to appropriate classes. In a mismatch case, the researcher must to seek causes of the data mismatch. One of the possible reason is that the data are assigned to unsuitable classes. There are some errors, that help evaluate the coincidences between classes and the obtained clusters (Manning and others, 2008), but then the data must be unambiguously assigned to one of the clusters. SOM uniqueness, comparing with other clustering methods is that in the SOM results there is no strictly expressed cluster, i. e. it is not specified which data item is assigned to which cluster, only the formed clusters we can usually see in the SOM. The researcher, observing the maps, can see and estimate the coincidence (and mismatch) of data classes and clusters. The problem arises when you have to view and explore a lot of SOM maps. As it is known, the SOM results can depend on different learning parameters and factors of the text document conversion into numerical expression, – various factors yield different SOM results. Therefore, the researcher has to view many SOM maps. Furthermore, there may be cases where the visual differences between the results (coincidences of classes and clusters) are not obvious, so it is very difficult to determine in which SOM the clusters are far from one other, and in which they are close to each other. For these reasons, in the dissertation two new heuristic errors are proposed to estimate the SOM quality when the classified data are analyzed. The proposed errors can be applied to compare several SOM maps, that are analyzing the same dataset and SOM sizes are the same.

3.1. The first proposed error – evaluation of the same class members

If we analyze the data when classes are known in advance, it is important to verify how the data of the same class are located in SOM. Thus, the first proposed error estimates how close the same class members are in SOM and the SOM clusters coincide. It allows us to estimate if all the data from the same class are similar to one other. The error value is calculated for each class separately. The proposed error E_c is calculated by the following formula:

$$E_c = \frac{1}{N_c}\sum_{i=1}^{n_c-1}\sum_{j=i+1}^{n_c}\left(\left\|Z_i^c - Z_j^c\right\|k_i^c k_j^c + b_{ij}\right). \qquad (12)$$

Here c is a class label; N_c is the number of data items from the cth class; n_c is the total number of neurons (cells) corresponding to the data from the cth class; Z_i^c is a vector, consisting of indices of the SOM cells, corresponding to the data from the cth class, $Z_i^c \in R^2$; k_i^c is the number of the data items from the cth class in the SOM cell, the indices of which are Z_i^c. There may be cases, where the members of different classes fall into the same SOM cell. In such a case, the penalty b_{ij} is calculated by formula (13). The penalty is used in formula (14). If only the same class members are in one SOM cell, the penalty is equal to $b_{ij} = 0$.

$$b_{ij} = \frac{l_i^{c'}}{k_i} + \frac{l_j^{c'}}{k_j}. \qquad (13)$$

Here k_i (k_j) is the number of data vectors, that are in the cell with the indices Z_i^c (Z_j^c). $l_i^{c'}$ ($l_j^{c'}$) is the number of data vectors from another class than of the cth vectors, in the cell with the indices Z_i^c (Z_j^c).

Purposefully, the sum of errors in (12) is not divided by the number of sum members $n_c(n_c-1)/2$, because such a division unifies the results of errors if we compare several SOMs. If data vectors of the same class are more widely distributed in the SOM, the number n_c is larger than that where the data vectors are grouped in one place. Therefore, when we evaluate the results of several SOMs it is purposeful to divide the proposed error by the same number, for example, by the number N_c of the cth class data vectors.

The smaller value of the error E_c means that the data from the same class are clustered better on SOM. In that case, it can be said that the SOM cluster is coincident with the data class. Thus, the researcher can not only assess the coincidence between clusters and classes visually, but also observe the values of errors.

3.2 Second proposed error – evaluation of class centers

The first error is calculated for each class separately. However, it is also important to evaluate how far or close the data clusters are, which correspond to the analyzed data from the same classes in SOM. So, the second proposed error evaluates how far the different class centers are in SOM. Observing the value of this error together with the first error values, the researcher cannot only visually assess the coincidence of the SOM clusters and data classes. First of all, the indices of data centers Y^c of each class on SOM have to be found:

$$Y^c = \frac{1}{n_c}\sum_{i=1}^{n_c} Z_i^c. \tag{14}$$

Here n_c is the total number of neurons (cells) corresponding to the data from the cth class; Z_i^c is a vector that consists of indices of the SOM cells, corresponding to the data from the cth class, $Z_i^c \in R^2$. Then the value of the error E_{center} is calculated by the formula:

$$E_{\text{center}} = \frac{1}{m'}\sum_{c=1}^{k-1}\sum_{d=c+1}^{k}\|Y^c - Y^d\|. \tag{15}$$

Here $m' = \frac{k(k-1)}{2}$, k is the number of data classes.

The higher value of the error E_{center} means that the centers of classes in SOM are more separated from one other than in the case of a lower error. The larger value of the error means better results (the distance between different class centers is larger).

Both proposed errors E_{c} and E_{center} can be used to evaluate the coincidence of data classes and clusters of several SOMs of the same size, when the same data are differently visualized in SOM. The following simple example illustrates it.

Suppose we have two SOM maps of the same size which are assigned to one of three classes (Figure 2), in which the same data are differently visualized.

1 (3, 1)	(3, 2)	**3** (3, 3)
1, 1 (2, 1)	**2, 3, 3** (2, 2)	**3** (2, 3)
(1, 1)	(1, 2)	**2** (1, 3)

a)

1 (3, 1)	**1** (3, 2)	**3, 3** (3, 3)
1 (2, 1)	**2** (2, 2)	**3, 3** (2, 3)
(1, 1)	(1, 2)	**2** (1, 3)

b)

Figure 2. Example of two SOMs: a) $E_1 = 0{,}67$, $E_2 = 1{,}04$, $E_3 = 1{,}63$, $E_{\mathrm{center}} = 1{,}32$, b) $E_1 = 1{,}13$, $E_2 = 0{,}71$, $E_3 = 1$, $E_{\mathrm{center}} = 1{,}48$

In the example of SOMs, the highlighted numbers 1, 2, 3 denote the analyzed data class labels ($c = 1, 2, 3$). The pairs of numbers, in the corner of each cell indicate the cell indices. As we can see in Figure 2a, the members of class I are located on two cells and, in Figure 2b, the first class members are located on three cells. It is obvious that the data are clustered more in Figure 2a. This fact is confirmed by the first error ($E_1 = 0{,}67$ for SOM in Figure 2a and $E_1 = 1{,}32$ for SOM in Figure 2b). The lower value of the first error means that the class members are close to one other. The value of the first error for the class II data of SOM in Figure 2a is larger ($E_2 = 1{,}04$) than that of SOM in Figure 2b ($E_2 = 0{,}71$), because not only the data from the class II, but also from the class III are in a cell. So, when we calculate the first error for the class II, we add a penalty $b = \frac{2}{3}$. Analogous results of the first error are obtained for the class III data. In this case, a penalty $b = \frac{1}{3}$ is added.

The value of the error E_{center} in both cases is similar: a) $E_{\mathrm{center}} = 1{,}32$, b) $E_{\mathrm{center}} = 1{,}48$. However, a slightly higher value is obtained in Figure 2b, which means, that in this case, the centers of different classes are a little bit farther from one other.

It is obvious that such an estimation of SOM is a multicriteria problem, because, at the same time, we need to find the values of several criteria (4 criteria are estimated in

Figure 2). A simple solution of this problem is to use the weighted sum method, i.e. to sum the values of errors and multiply them by the weights. However, the selection of weights depends on the decision maker and the specificity of the problem. For example, there is a possibility that the values of one class are more important than that of the other. In the dissertation, such a multicriteria problem is not solved, and the values of the errors are estimated separately.

3.3. The proposed visualization technique of SOM

The analysis of SOM systems has showed that the systems have many different visualization techniques. However, the systems have a common disadvantage. If the classes, which the data belong to, are known, and the labels of the classes are displayed in the map, it is difficult to understand how many data vectors from one or other class correspond to a cell (neuron), because usually only different (but not the same) labels are shown. It is especially important, when the vectors from different classes fall into a SOM cell. Also, we do not know how many data vectors are from the same class and how many data vectors are from the different classes, and what their proportions are.

In order to solve the problem, some techniques have been developed in the SOM systems. For example, a histogram map is implemented in the system NeNet (Figure 3). The histogram shows how many data vectors fall into a cell, but it is not obvious how many vectors are from one or another class. It is possible to create a map, where all the labels (not only different) are shown in SOM-Toolbox (Figure 4). The view of such a map is very complicate, because the labels overlap, it is not clear which label corresponds to which cell. The Databionic ESOM and Viscovery SOMine systems do not even have such abilities.

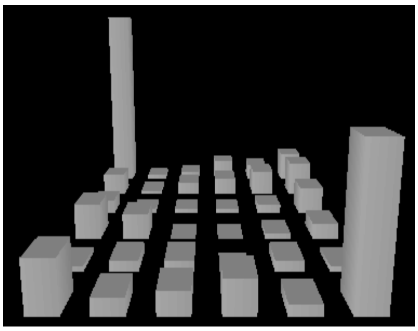


Figure 3. Histogram map, obtained by the system NeNet

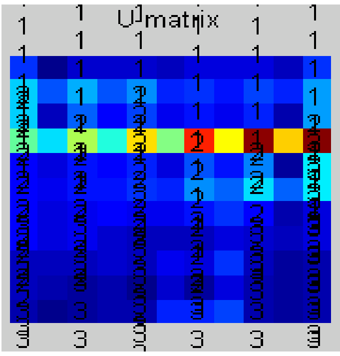


Figure 4. SOM, obtained by SOM-Toolbox, where all labels are shown

In order to avoid draw batches, in the dissertation the visualization technique for SOM is proposed, which is used for data where classes are known in advance. It is purposeful to draw the pie charts in each cell of SOM. The pie chart will show a proportion between the data vectors that are assigned to the different classes and fall into a cell. In addition, it is right to show different classes in different colors.

Suppose we have a SOM, as shown in Figure 2a. When we apply the proposed visualization technique, we get a SOM shown in Figure 5.

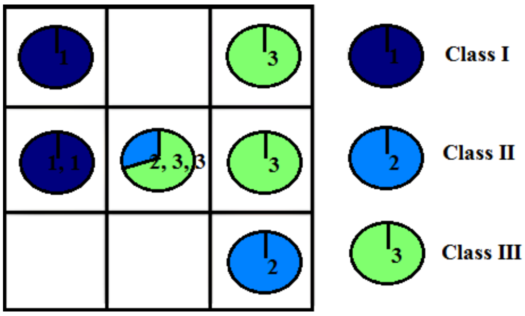


Figure 5. Proposed visualization technique of SOM

As we can see, in the middle cell of SOM two different class vectors (a total of three vectors) fall, where two vectors belong to class III, and one vector belongs to class II. The parts of the pie chart are colored respectively by showing a ratio: $\frac{1}{3}$ – II class (blue color) and $\frac{2}{3}$ – III class (green color). The pie chart, only the same class vectors are colored by the same color.

It is worth mentioning, that such a visualization technique of SOM was proposed in 2011, in the paper of the dissertation author [2]. At that time, according to information, no system had such a visualization technique. However, in 2013 a similar visualization technique of SOM was implemented in the Orange system (Demšar et all., 2013).

3.4. The new SOM system

In the dissertation, the new SOM system is developed, in which the proposed SOM visualization technique and the proposed error for estimation of SOM quality are implemented. In this system, there is a possibility to choose not only the usually used neighboring functions (bubble and Gaussian), but also the heuristic neighboring function. Also, in the system it is possible to choose different learning rates (linear, inverse-of-time, power series, and heuristic) and the way in which the learning rate values will be changed: in each iteration or each epoch. Two SOMs (for the training and testing datasets) are presented in the results. These properties of the system are suitable not only for the analysis of the data, but also for the investigation of self-organizing maps.

The general scheme of system workflow is presented in Figure 6. Before starting the experiment, it is necessary to load the dataset. The dataset is split into two subsets: the training and testing, i. e. one part of the data is used to train SOM, and the other to test it. When we select the learning parameters, we can start training the SOM using the training dataset. As a result we obtain trained SOM, and now the testing dataset is used to estimate how much dataset not used in SOM training, is suitable for the trained SOM. Also, the quality of SOM is estimated of both datasets (training and testing) by four errors: quantization E_{QE}, topographic E_{TE}, error between the same class members E_c and error between different class centers E_{center}. If the quality of SOM results obtained is not satisfy, the researcher can back to selection of a new learning parameters step. The cycle is repeated until the values of analyzed errors corresponds to the desired researcher's results.

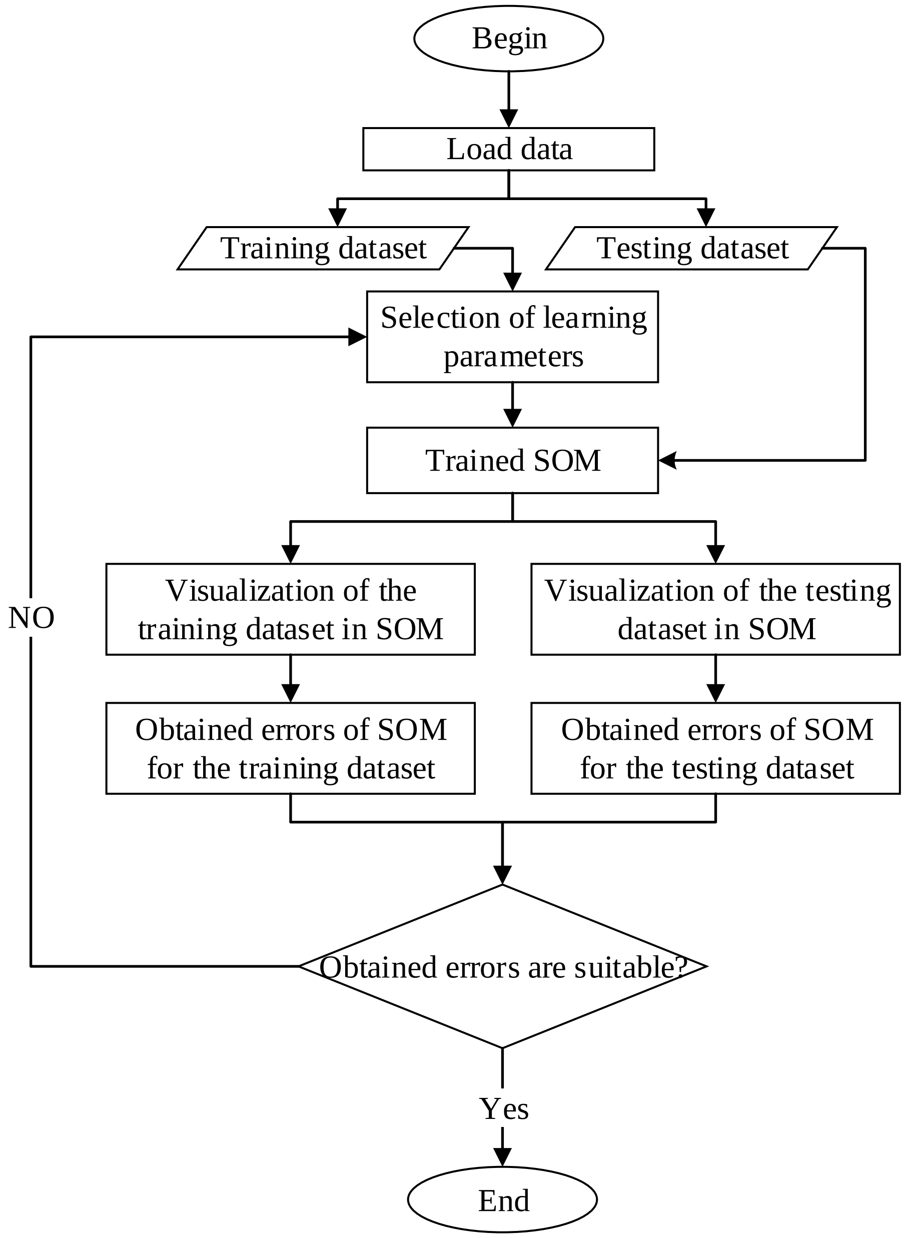


Figure 6. The workflow scheme of the new SOM system

A graphical user interface of the new system is presented in Figure 7. The system is designed in Matlab, so it can be used as an additional toolbox. The proposed system can be used for data assigned more than to five classes, but this limitation is not a problem, because, in most cases, there is no need to classify data having more classes than five. In addition, if it is necessary, it can be simply expanded to analysis of more than five classes.

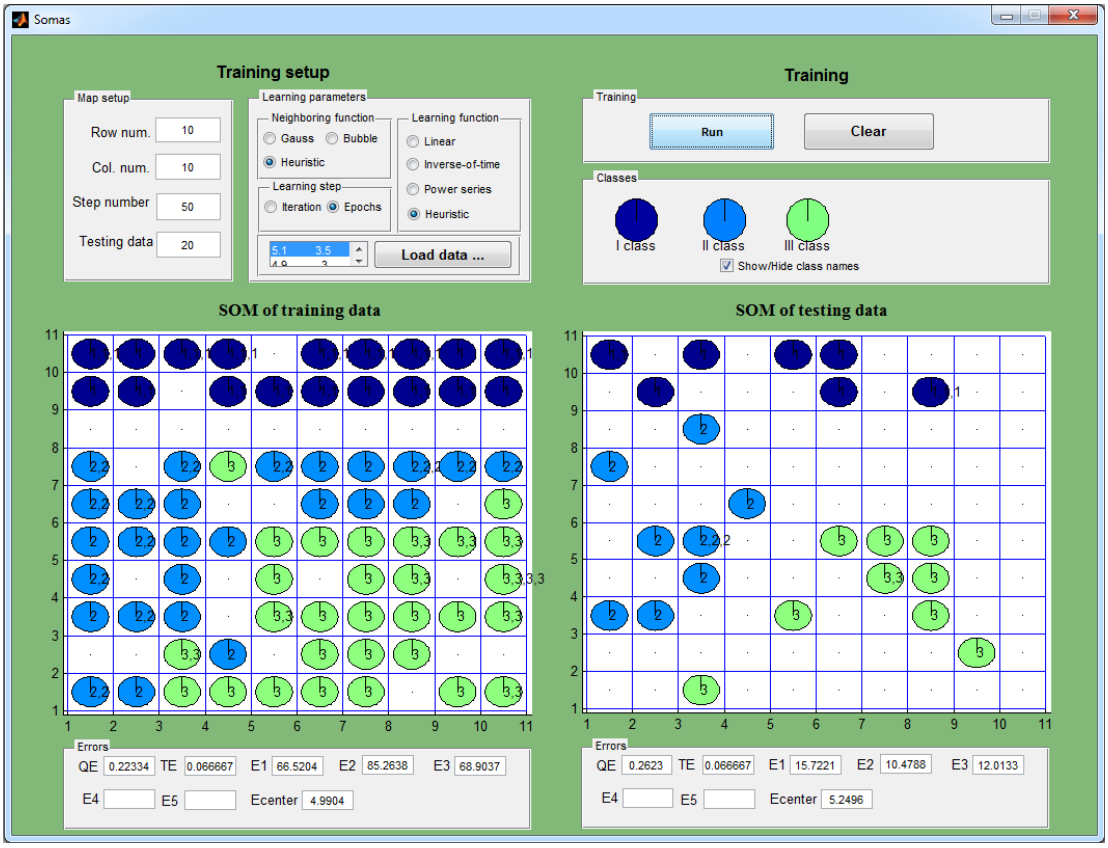
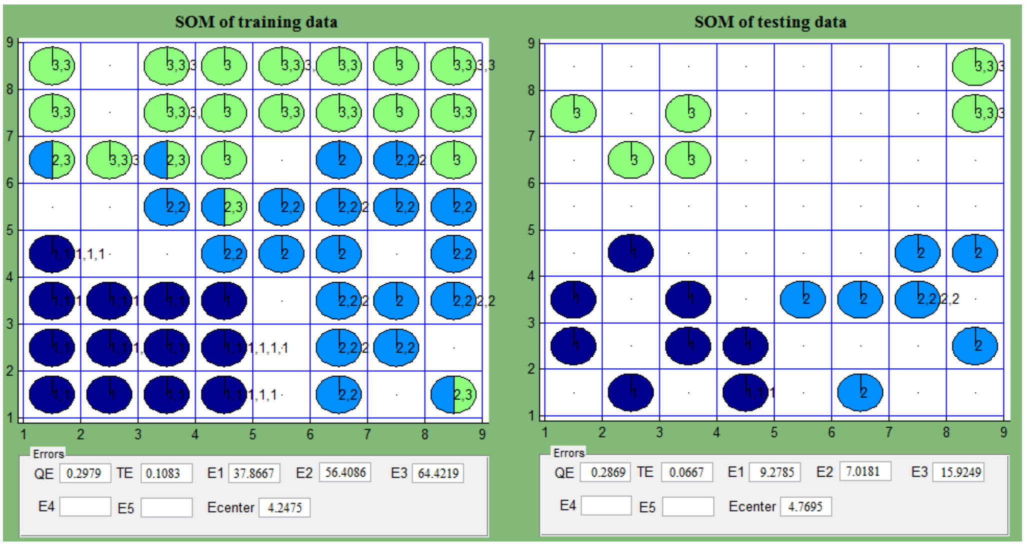


Figure 7. Graphical user interface of the new SOM system

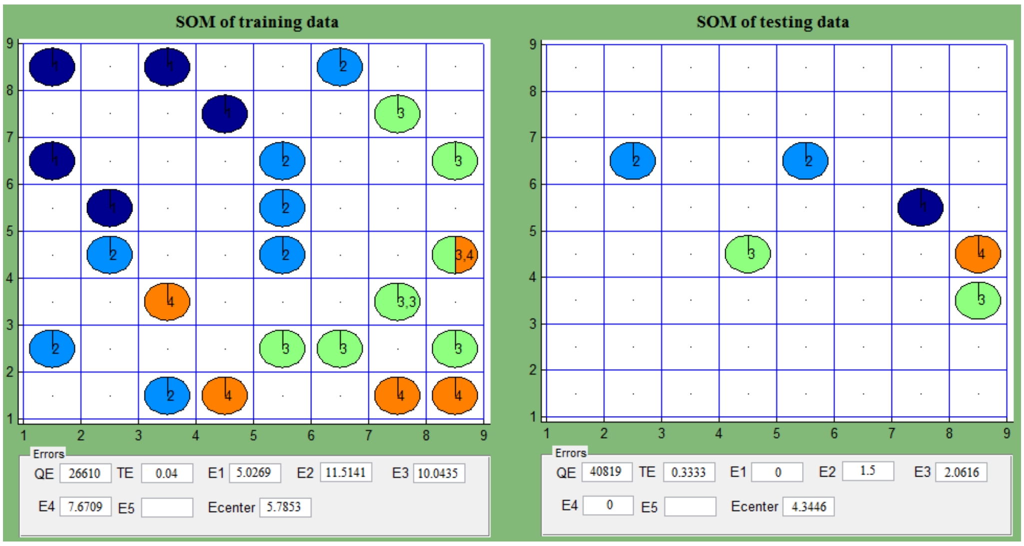
Suppose we train SOM using two datasets: iris and economic (see more about data in section 4.1). As we can see in Figure 8, in the case of the iris dataset, all class I members are located in the bottom left corner of SOM. The members of class II and III are separated from class I by empty cells. Some of the members of class II and III fall into the same cell, so the pie chart is divided into slices, which corresponds to the ratio among all the members and specific class in the cell. On the right side of the system graphical user interface we can the map of the testing dataset. It is obvious that the testing dataset adapts to the trained SOM network and the different class members are located in the same places as in the case of the training dataset.



a) **b)**

Figure 8. Iris dataset in 8×8 SOM, obtained by the new SOM system: a) training dataset, b) testing dataset

The trained SOM with an economic dataset is presented in Figure 9. As we can see, all the members of class I are located in the left top corner. The members of class II make small clusters, one of them is at the top of the map and the others in the left bottom corner of SOM.



a) **b)**

Figure 9. Economic dataset in 8×8 SOM, obtained by the new SOM system: a) training dataset, b) testing dataset

The members of class III and IV are located in the right bottom corner, some of the members fall in the same cell of SOM. In the case of the testing dataset, as we can see in

Figure 9, only the member of class I is located not in the same place of SOM, as shown in SOM of the training dataset. Other class members are located in the right places.

4. The experimental results

4.1. Analyzed datasets

Different datasets with different specific features are used in the experimental part of the dissertation. Some of the datasets were taken from the database 'UCI Repository of Machine Learning Databases' (Asuncion and Newman 2007):

1. **Iris dataset**. The iris dataset consists of the values of some features of three species of flowers: Iris Setosa, Iris Versicolor, and Iris Virginica. Four features were measured, so four-dimensional vectors $X_1, X_2, \dots, X_{150}$ are formed, where $X_p = (x_{p1}, x_{p2}, x_{p3}, x_{p4})$, $p = 1, \dots, 150$. The dataset is divided to three classes: class I – Iris Setosa, class II – Iris Versicolor, and class III – Iris Virginica.
2. **Glass dataset**. The glass dataset was collected by a scientist, who wanted to help criminalists to recognize glass slivers found. Nine-dimensional vectors $X_1, X_2, \dots, X_{214}$ are formed, where $X_p = (x_{p1}, x_{p2}, \dots, x_{p9})$, $p = 1, \dots 214$. The dataset is divided into five classes: class I – building windows, class II – vehicle windows, class III – containers, class IV – tableware, and class V – headlamps.
3. **Zoo dataset.** The zoological dataset is about animals and their characteristics. Sixteen-dimensional vectors $X_1, X_2, \dots, X_{92}$ are formed, where $X_p = (x_{p1}, x_{p2}, \dots, x_{p16}), p = 1, \dots 92$. The dataset is divided into five classes: class I – mammals, class II – birds, class III – fish, class IV – insects, and class V – invertebrates.

The **economic dataset** consists of the values of some features of the European Union (EU) countries, and some countries, that strive to become EU members. We have chosen economic indices of the EU countries in 2009 (Eurostat, 2010). Six-dimensional vectors $X_1, X_2, \dots, X_{31}$ are formed, where $X_p = (x_{p1}, x_{p2}, \dots, x_{p6})$, $p = 1, \dots 214$. The dataset is divided into four classes: class I – the countries that established the European Union (Belgium, German, France, Italy, Luxemburg, and the Netherlands), class II – the countries that joined EU in 1957-1995 (Denmark, Ireland, Greece, Spain, Austria, Portugal, Finland, Sweden, United Kingdom), class III – the countries that joined EU in

2004-2007 (Czech Republic, Estonia, Cyprus, Latvia, Lithuania, Hungary, Malta, Poland, Slovenia, Slovakia, Bulgaria, Romania), and class IV – the countries that are seeking to be EU members (Macedonia, Turkey, Iceland, Croatia).

The dataset of different text documents was also used in the experimental investigation. The dimension of vectors is different, because it depends on the length of the text document dictionary.

1. **Orders of the Ministries.** The document of eight text areas taken from the document database of Seimas of the Republic of Lithuania (LRS, 2013) have been analyzed in the experimental investigation. 15 similar size orders were selected randomly from Ministries of Finance, Culture, Transport and Communication, Health, Education and Science, Economy, the Interior and Agriculture. Using these orders, three dataset have been created: $X^1 = \{X_1^1,\ X_2^1, \dots, X_{60}^1\}$, $X^2 = \{X_1^2,$ $X_2^2, \dots, X_{60}^2\}$, and $X^3 = \{X_1^3,\ X_2^3, \dots, X_{60}^3\}$. All the datasets were divided into four classes.

   The first dataset represents: class I – Health, class II – Education and Science, class III – the Interior, and class IV – Agriculture ministries. The second dataset represents: class I – Finance, class II – Culture, class III – Transport and Communication, and IV class – Agriculture ministries. The third dataset represents: class I – Finance, class II – Economy, class III – the Interior, and class IV – Agriculture ministries.
2. **Scientific papers I.** 60 scientific papers$X_1, X_2, \dots, X_{60}$ have been taken randomly from the Internet freely accessible databases (SpringerLink, ScienceDirect, etc.). The dataset is divided into four classes: class I – papers about artificial neural networks (ANN), class II – papers about bioinformatics, class III – papers about optimization, and class IV – papers about self-organizing maps.
3. **Scientific papers II.** 45 scientific papers $X_1, X_2, \dots, X_{60}$ have been taken randomly from the Internet freely accessible databases (SpringerLink, ScienceDirect, etc.). The dataset is divided into three classes: class I – papers about Pareto optimization, class II – papers about simplex optimization, and class III – papers about genetic optimization.

Such a dataset distribution and class assignment has been performed by the author of the dissertation.

4.1. Comparative analysis of SOM systems

The proposed SOM system in subsection 3.4 has been compared with other SOM systems reviewed in subsection 2.5: NeNet, SOM-Toolbox, Databionic ESOM, Viscovery SOMine, and Orange. After a comparative analysis has been made, we can see advantages and disadvantages of various systems (Table 3). The systems are compared according to the following:

K1. There is a possibility to analyze data sets of different sizes.

K2. It is easy to prepare data to the system, there is a possibility to prepare data in the form of a simple text file.

K3. There is a possibility to split the data into training and testing datasets.

K4. It is possible to use more than two learning parameters.

K5. There is a possibility to use more than one neighboring function.

K6. There is a possibility to change learning rate values in each epoch or each iteration.

K7. There is a possibility to visualize all data vectors labels in the same cell of SOM.

K8. There is a possibility to see the ratio among different data vectors in the same cell of SOM.

K9. The distance between neurons are displayed in the SOM.

K10. There is a possibility to choose different SOM visualization techniques.

In Table 3, we can see which criteria are satisfied by all the analyzed systems. The last column indicates the number of criteria satisfied by the system. The sign '+' means that the system satisfies the criteria and the sign '-' means that criteria are not satisfied. As we can see, the systems NeNet and Databionic satisfy the least number of criteria (3 criteria). These two systems have only the basic functions and control parameters, so if we want to carry out a more detailed investigation we have to deal with one or other restriction. The Viscovery SOMine system (4 criteria) has various visualization techniques, but we can also select only the basic learning parameters. A similar visualization technique, proposed in the dissertation was implemented in Orange system, but there are no other important parameters that could help for deeper investigation, such as various neighboring functions and learning parameters, so the system satisfies only 6 criteria. The most criteria are satisfied by the SOM-Toolbox system (9 criteria) and the new here proposed system (8 criteria). SOM-Toolbox is created by a T. Kohonen who is SOM originator, so in this system, a lot of different functions and parameters are realized, which facilitates a deeper investigation. However, there is no possibility to see the ratio between the different vectors in the same cell of SOM. This option is implemented in the new SOM system.

Table 3. Comparative analysis of SOM systems

System \ Criteria	K1	K2	K3	K4	K5	K6	K7	K8	K9	K10	Totally
NeNet	–	+	–	–	–	–	–	–	+	+	3
SOM-Toolbox	+	+	+	+	+	+	+	–	+	+	9
Databionic ESOM	+	–	–	–	–	–	–	–	+	+	3
Viscovery SOMine	+	+	–	–	–	–	–	–	+	+	4
Orange	+	+	–	–	+	–	–	+*	+	+	6
New SOM system	+	+	+	+	+	+	+	+	–	–	8

* – a similar visualization technique was implemented later than the author of the dissertation has proposed.

4.2. Investigation of learning parameters of self-organizing maps

The main target of this investigation is to find out how different neighboring functions, learning parameters, and the way of changes of the learning parameter values (in each iteration or epoch) influence the SOM results. The quantization E_{QE} and two proposed errors E_c, E_{center} are used to evaluate the SOM quality.

The experimental investigation was carried out with 'Orders of Ministry', glass, and zoo datasets. First of all, 60 documents of the 'Orders of Ministry' dataset are converted to numerical expressions. When creating the text document matrix, some control factors are fixed. The numbers are removed, because this information is not informative and does not define the documents. The primary research has shown that the total number of frequencies for this dataset is five, because, if we use a larger number, some documents did not have such words, that were repeated five times, and the documents simply rejected them. Therefore, we created five different text document matrices which have 60 rows and a different number of columns: 3812 (when the frequency is equal to 1), 1494 (when the frequency is equal to 2), 769 (when the frequency is equal to 3), 446 (when the frequency is equal to 4), and 287 (when the frequency is equal to 5).

The primary research has shown that the size of the map and a larger epoch or iteration number do not affect the results essentially. Therefore in all the experiments the map size is 10×10 and the epoch numbers are equal to 50. The number of epochs multiplied by the number of data items N corresponds to the number of iterations. Each experiment is repeated 10 times with different initial values of neurons M_{ij}. The averages of the quantization error and all the other errors are calculated. The self-organizing map is trained using 80% of the whole dataset, and the rest 20% of the dataset are used for testing in order to see how well the testing dataset adapts to the trained SOM.

The summarized results of numerical and textual document datasets are presented in Figure 10 and Figure 11. The percentages shown in the diagrams are calculated by summarizing the training and testing dataset results. In the case of the textual dataset, we can see that 49% of the smallest error values are obtained using the heuristic neighboring function, and only 20% using the bubble neighboring function. It can be assumed that the lower heuristic neighboring function values allows us to get better results when we analyze the textual dataset, and the larger neighboring function values (bubble neighboring function) make the results worse. In the case of the numerical dataset, we can see that slightly better results are obtained when the Gaussian neighboring function is used (37%).

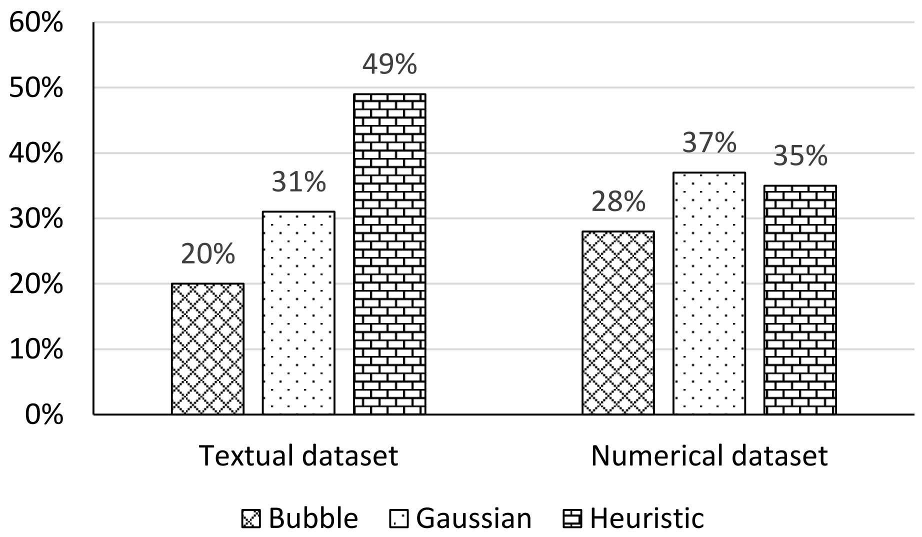


Figure 10. Summarized results of neighboring functions

As we can see (Figure 12), in the case of the textual document dataset, when comparing neighboring functions, the best results are obtained using the inverse-of-time learning rate and the values are changed in each epoch (16%), while the worst results are obtained when the linear learning rate is used and the values are changed in each epoch (7%). In the case of the numerical dataset, the best results are obtained when the linear learning rate is used and the values are changed in each iteration (17%). The worst results are obtained when the heuristic learning rate is used and the values are changed in each iteration (9%).

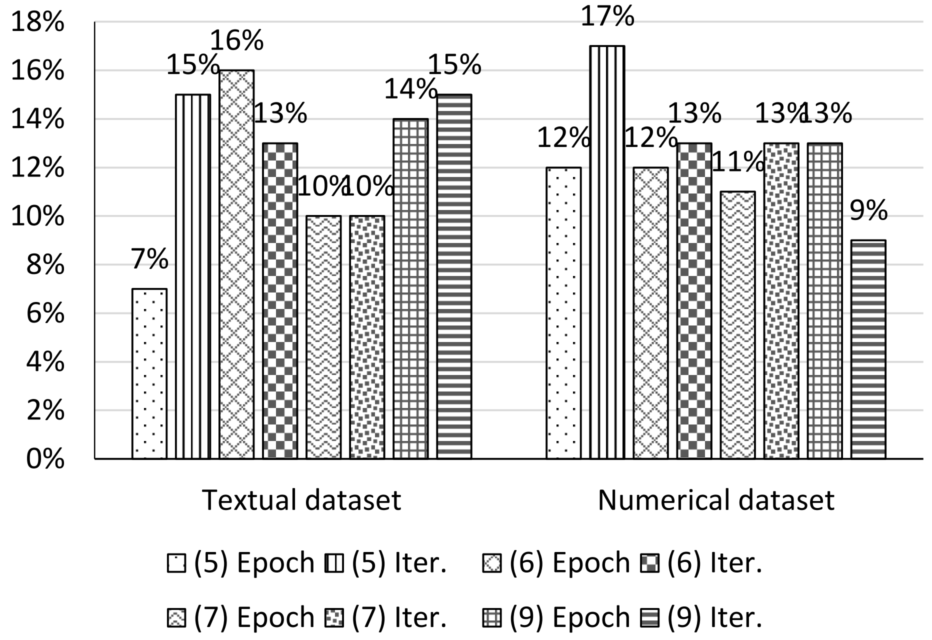
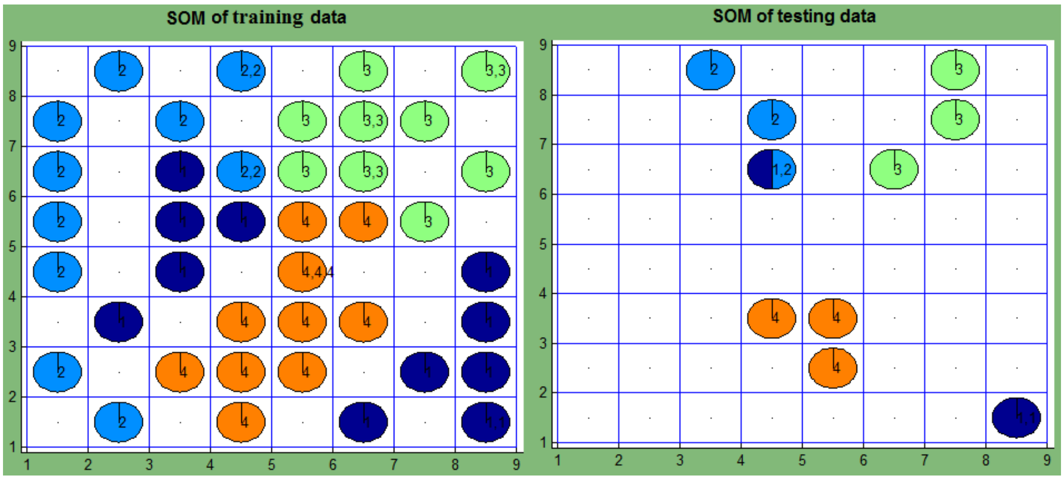


Figure 11. Summarized results of learning parameters

4.3. The influence of text document conversion factors on the SOM results

The main target of this investigation is to find out how different text document conversion factors influence the SOM results. The quantization E_{QE} and two proposed errors E_c, E_{center} are used to evaluate the SOM quality.

The first testing experiment is carried out with the 'Scientific paper I' dataset to find out how SOM clusters and visualizes the documents from different areas. Figure 13 shows that some clusters are obvious.



a) **b)**

Figure 13. SOM of the data, corresponding to the scientific papers on ANN, bioinformatics, optimization, and SOM

Most data items of the same classes form clusters, only some data items are separated from their class clusters. All the data of the class IV (SOM) form one cluster. All the data of the class III (optimization) form another cluster. Some data items of the class I are mixed with the clusters of the class II, because in fact, many words can be the same in the papers on artificial neural networks and bioinformatics.

In order to find tendencies how the control factors affect the results, we choose the scientific papers from rather close areas: the papers about the optimization based on Pareto, simplex, and genetic algorithms (Scientific papers dataset II). Then the papers are converted to text documents, and a document dictionary is created. It can be done in two ways: 1) a researcher manually refers to the words that must be included into the document dictionary; 2) the document dictionary is created automatically from the text documents analyzed. The description of included control factors used to create the text document dictionary in experiments are as follows:

No. 1. At first, we create the text document matrix for the dataset that corresponds to the optimization papers, where only three words – ‘simplex’, ‘genetic’, and ‘Pareto’ – are included into the dictionary.

No. 2. The dictionary consists of the following words: ‘simplex’, ‘programming’, ‘convex’, ‘corner’, ‘vertices’, ‘genetic’, ‘mutation’, ‘crossover’, ‘chromosome’, ‘fitness’, ‘Pareto’, ‘multiobjective’, ‘front’, ‘dominate’, ‘decision’.

No. 3. The experiment is carried out disregarding the common word list as a document dictionary is being created.

No. 4. The common word list created by the Text to Matrix Generator toolbox (TMG), is used. This common word list has more than 300 words, such as ‘there’, ‘where’, ‘here’, ‘some’, etc.

No. 5. The TMG toolbox has a common word list unsuitable for scientific papers. So, considering that the papers about optimization are analyzed here, we create a new common word list including the words such as ‘function’, ‘fig’, ‘table’, ‘formula’, ‘optimization’, ‘present’, ‘minimum’, ‘maximum’, ‘function’, ‘variable’, etc.

No. 6-8. The experiments analogous to **No. 3-5**, only the stemming algorithm used in addition.

The experimental investigation results are presented in Tables 4 and 5.

Table 4. The values of SOM quality errors for training data

No.	Experiment	E_{QE}	E_1	E_2	E_3	E_{center}
1	Manual dictionary creation I, $n = 3$	2,26	2,84	2,81	3,11	4,01
2	Manual dictionary creation II, $n = 15$	7,55	4,25	2,30	2,38	4,02
3	Without the common word list, $n = 3441$	96,18	4,49	4,13	4,74	1,57
4	Common word list obtained by TMG, $n = 3198$	77,12	2,86	4,67	4,68	1,64
5	New common word list, $n = 3157$	69,19	3,25	4,00	2,91	3,40
6	Without the common word list, but with the stemming algorithm, $n = 2685$	105,76	4,59	3,81	3,71	2,32
7	Common word list obtained by TMG and the stemming algorithm, $n = 2486$	88,47	3,57	4,07	4,84	2,05
8	New common word list and the stemming algorithm, $n = 2471$	82,70	3,48	3,95	4,60	2,75

Table 5. The values of SOM quality errors for testing data

No.	Experiment	E_{QE}	E_1	E_2	E_3	E_{center}
1	Manual dictionary creation I, $n = 3$	2,92	3,28	1,33	2,95	4,37
2	Manual dictionary creation II, $n = 15$	14,45	5,90	2,42	3,20	3,26
3	Without the common word list, $n = 3441$	143,68	2,75	3,24	4,90	1,76
4	Common word list obtained by TMG, $n = 3198$	122,06	1,33	0,83	1,94	2,40
5	New common word list, $n = 3157$	117,46	1,05	0,67	3,48	3,13
6	Without the common word list, but with the stemming algorithm, $n = 2685$	155,64	3,70	3,41	4,47	1,63
7	Common word list obtained by TMG and the stemming algorithm, $n = 2486$	137,27	0,67	1,80	5,34	2,69
8	New common word list and the stemming algorithm, $n = 2471$	134,03	0,83	3,82	1,14	2,27

The summarized results of ‘Scientific paper II’ datasets are presented in Figure 14. The percentages shown in the diagrams are calculated by summarizing the training and testing dataset results (Tables 4-5). As we can see, the best results are obtained using manual dictionary I (18%). Similar results are obtained when the new common words list (16%) and manual dictionary II (15%) are used. The worst results are obtained without the use of any common word list (6%).

So when there is a pre-known information about the data analyzed, the best way is to create the text document dictionary manually. If we do not have information about the analyzed data, the text document dictionary has to be created automatically. In this case, it is advisable to include the main words from the analyzed area, because otherwise the results can be distorted.

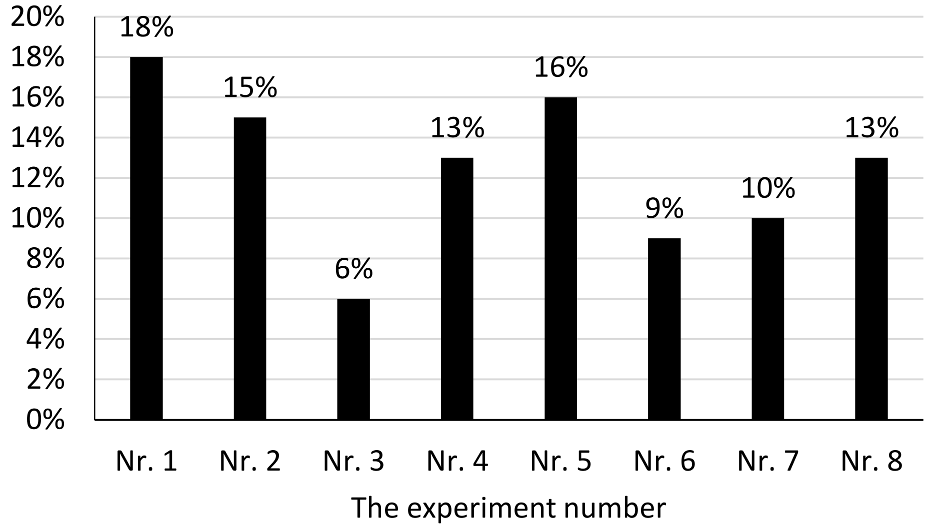


Figure 14. Summarized results of Tables 4 and 5

4.4. The influence of word frequency on SOM results

In this research, the word frequency used to create the text document dictionary is investigated. The experimental investigation is performed with 'Orders of Ministry' dataset. The primary research has shown that the total number of frequencies for this dataset is 5, because, if we use a larger number, some documents do not have such words, that were repeated five times, and the documents simply rejected them. So, in total 10 text document matrices are created: the word frequency is from 1 to 5 and the common word list is used and not used. The text document matrixes are analyzed by self-organizing maps and k-means methods. Each experiment is repeated 5 times with different initial values of neurons M_{ij}. The averages of the proposed errors are calculated and presented in Tables 6 and 7.

Table 6. The overall SOM results of the training dataset

Frequency of words / Errors	1	2	3	4	5
The common word list is not used					
E_1	25,28	27,94	27,26	26,46	28,36
E_2	19,95	22,55	21,86	23,81	24,55
E_3	20,23	22,04	22,36	21,34	23,3
E_4	21,75	23,85	24,23	28,10	26,59
E_{center}	4,20	3,47	3,46	3,11	2,93
The common word list is used					
E_1	27,77	27,10	26,88	25,42	25,94

E_2	20,13	22,85	21,40	23,31	23,29
E_3	17,43	19,39	20,77	23,1	26,26
E_4	23,11	23,87	25,58	24,69	26,78
E_{center}	4,10	3,79	3,34	3,54	3,10

Table 7. The overall SOM results of the testing dataset

Errors \ Frequency of words	1	2	3	4	5
The common word list is not used					
E_1	2,04	3,56	3,47	3,52	4,60
E_2	1,93	2,96	2,59	2,66	3,34
E_3	3,33	3,45	4,27	3,32	5,12
E_4	1,68	2,92	2,46	3,31	2,18
E_{center}	4,67	4,45	3,78	3,41	3,37
The common word list is used					
E_1	2,99	2,98	2,76	3,71	3,86
E_2	2,38	2,53	2,59	3,17	2,92
E_3	3,06	3,16	3,43	3,99	6,28
E_4	2,56	2,51	3,26	2,14	2,22
E_{center}	4,59	4,54	3,76	3,88	3,07

The percentages shown in the diagram (Figure 15) are calculated by summarizing the training and testing dataset results (Tables 6-7).

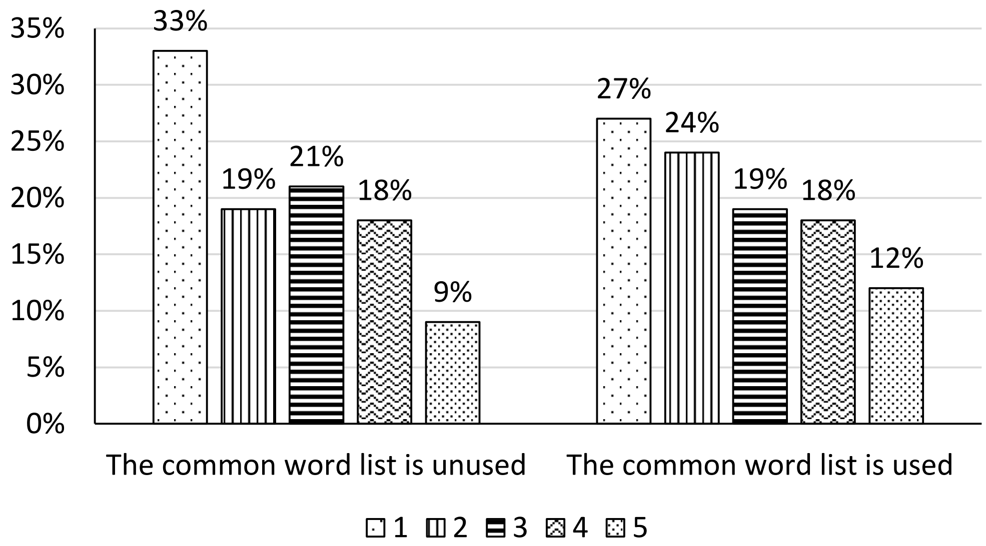


Figure 14. Summarized results of Tables 4 and 5

As we can see, the best results are obtained when the smallest word frequency is selected (33% when the common word list is used and 27% when the common word list is not used). When the word frequency is increased, the values of the proposed errors $E_1, E_2, E_3, E_4,\ E_{\text{center}}$ become worse. The worst results are obtained when the common word list is not used and the word frequency is equal to 5, i. e. all the words are included in the text document dictionary (9% of all cases).

It is useful to compare the SOM results to that obtained by one of the most popular clustering method k-means (MacQueen, 1967). At first, the number K of desired clusters is selected and initial values of cluster centers are assigned. Then, each data item is assigned to the cluster with the closest centers, and new centers for each cluster are computed. The steps are repeated iteratively until the stop or convergence criterion is satisfied. The convergence criterion can be based on the squared error (averaged difference between the cluster centers and the items assigned to the clusters). The stop criterion can be a high number of iteration steps. Usually the k-means method quality is estimated by calculating the square error between the center of the cluster and the cluster assigned to the data:

$$E_{AKS} = \sum_{i=1}^{K} \sum_{j=1}^{\mu} \left\| X_j^i - C^i \right\|^2.$$

In the experimental investigation the data are assigned to the classes, so it is important to evaluate whether obtained clusters match the vector classes. First of all, the data are clustered into clusters the number of which corresponds to the class number of the data. Later, the overlaps of the classes and obtained clusters are determined, i. e. the vectors of some dataset class have to be assigned to the cluster which has the largest number of members of that class. Then the number of vectors wrongly assigned to the cluster is calculated. The average results of 10 experiments are presented in Table 8.

Table 8. The overall k-means results

Error \ Frequency of words	1	2	3	4	5
The common word list is not used					
The number of vectors wrongly assigned to the cluster	20,0	22,9	26,3	30,7	32,1
E_{AKS}	39929	37438	33185	28885	24589
The common word list is used					
The number of vectors wrongly assigned to the cluster	23,2	24,3	24,1	28,8	31,7
E_{AKS}	37656	34775	30982	26690	22693

Each time when the word frequency is increased, the number of vector wrongly assigned to the cluster results are the larger, except only the case, where the word frequency is equal to 2 and the common word list is used. In all cases, where the frequency of the words is decreasing, the values of error E_{AKS} are decreasing too. However, evaluation of the results, obtained by error E_{AKS}, is not appropriate, since the size of a dataset is various, and the lower value of E_{AKS} does not show the clustering accuracy. In most cases, the accurate results are obtained where the minimal frequency of the word is selected, and the worst results are where the frequency of the word is equal to 5.

5. Summary and General Conclusions

The investigation of self-organizing maps yield the following results: the new SOM visualization technique is proposed; new errors for estimation of SOM quality are proposed, which allows us to compare the coincidence between classes and clusters of several SOMs; the new SOM system is created in which the proposed visualization technique, errors and various learning parameters are implemented; the influence of different SOM learning parameters and text document conversion to numerical expression factors on the obtained SOM results has been investigated.

The experimental investigation has shown that the proposed visualization technique and proposed errors are useful for dataset analysis, when data classes are known in advance. The experimental results led to the following conclusions:

1. The proposed errors properly estimate the coincidence of the data classes and clusters obtained in SOM.
2. The proposed visualization technique allows us to visualize the ratio between different class members which fall in the same cell of SOM.
3. In the case of the textual document dataset, more accurate results are obtained according to the proposed errors when heuristic neighboring function is used (49% of all cases), the Gaussian neighboring function – 31%, and bubble – 20% of all cases; in the case of the numerical dataset, better SOM results are obtained when the Gaussian neighboring function is used (37% of all cases), but they do not differ very much from the results obtained using the heuristic neighboring function (35% of all cases).

4. Depending on the learning rate selection, the best SOM results for the textual document dataset (in the case of proposed errors) are obtained, when the inverse-of-time learning rate is used and the values are changed in each epoch (16% of all cases). The worst results are obtained when the linear learning rate is used and the values are changed in each epoch (7% of all cases). In the case of the numerical dataset, the best results are obtained when the linear learning rate is used and the values are changed in each iteration (17% of all cases), and the worse results when heuristic learning rate is used and the values are changed in each iteration (9% of all cases).
5. Investigations of the text document, used when the text document dataset is converted into the numerical expression show that more accurate results (in the case of proposed errors) are obtained, if the text document dictionary is created manually (18% and 15% of all cases), i. e. the researcher by himself includes the words to the text document dictionary. When the automatic text document dictionary creation is used, the accurate results are obtained when the new common word list is used (16% of all cases) to create the text document dictionary and the stemming algorithm is not used.
6. The investigation of the word frequency influence on the SOM results shows that by increasing the minimum number of word frequencies, the overall accuracy of the SOM results declines; the most accurate results are obtained when the minimum number of word frequencies is equal to 1 (approximately 30%), and the worst results are when the number of word frequencies is equal to 5 (approximately 10,5%).

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About the Author

Pavel Stefanovič was born on the 25th of July, 1985 in Varėna, Lithuania. In 2004, he graduated from the Varėnos Ryto secondary school. He received a Bachelor’s degree in Education and Teacher training from Vilnius Pedagogical University. He received a Bachelor’s degree in Informatics and Teacher training from Vilnius Pedagogical University in 2008, and a Master’s degree in Informatics from Vilnius Pedagogical University in 2010. From 2007 till now he is working in Vilnius Simono Daukanto progymnasium as an informatics teacher and informatics technology specialist. From 2010 to 2014 he was a PhD student of Vilnius University, Institute of Mathematics and Informatics. Also, from 2012 till now he is working as a researcher in Vilnius University, Institute of Mathematics and Informatics.

SAVIORGANIZUOJANČIŲ NEURONINIŲ TINKLŲ VIZUALIZAVIMAS IR JO KOKYBĖS NUSTATYMAS

Tyrimo sritis ir problemos aktualumas

Šių laikų technologijos leidžia kaupti didelius kiekius įvairialypės informacijos bei ją talpinti kompiuterio atmintyje, išorinėse laikmenose arba internete. Ilgą laiką kaupiant informaciją, saugyklos tampa dideliu šiukšlynu, kuriame dažnai tampa sunku rasti reikalingus duomenis ar kitą naudingą informaciją. Šiuolaikinės technologijos mums leidžia surasti iš gausybės informacijos vieną ar kitą norimą dalyką greitai, tačiau rasta informacija dažnai būna nenaudinga, iškraipyta ar neesminė. Todėl tai tampa didele problema ir iššūkiu kiekvienam naudotojui. Vienas iš šios problemos sprendimų būdų yra panaudoti duomenų tyrybos metodus (angl. *data mining*), kurie leidžia duomenis susisteminti juos klasterizuojant, klasifikuojant bei esant galimybei jų rezultatus pateikti vizualiai.

Vienas iš duomenų tyrybos metodų yra saviorganizuojantis neuroninis tinklas (SOM). SOM dažnai vadinamas saviorganizuojančiu žemėlapiu, o kartais pradininko pavarde – Kohoneno žemėlapiu (Kohonen, 2001). SOM tinklai gali būti naudojami duomenims klasterizuoti ir vizualizuoti. SOM gali pagelbėti ieškant daugiamačių duomenų projekcijų mažesnio skaičiaus matmenų erdvėje. Nors jau praėjo daugiau nei 40 metų nuo SOM tinklų atsiradimo, tačiau jie ir toliau intensyviai tiriami ir taikomi. Laikui bėgant atsirado daug įvairių SOM praplėtimų ir modifikacijų, pradedant nuo mokymo taisyklėje įvestų naujų pakeitimų iki skirtingų SOM vizualizavimo būdų. Tačiau pagrindinis mokymo principas išlieka tas pats. Daug metų SOM tinklai buvo taikomi įvairiems skaitinės išraiškos duomenims klasifikuoti ir klasterizuoti, bet šiuo metu taikymų sritis yra plečiama tiriant tekstinius ar kito tipo duomenis.

Vienas iš SOM tinklų privalumų, lyginant su kitais duomenų tyrybos metodais yra tai, kad gaunami ne tik skaitiniai įverčiai, kaip būna daugumoje kitų duomenų tyrybos metodų, bet ir jų rezultatai pateikiami vizualia forma, o vizualią informaciją žmogus suvokia greičiau nei tekstinę ar skaitinę. SOM tinklai dažnai taikomi duomenims klasterizuoti. Lyginant su kitais klasterizavimo metodais, jie pasižymi tuo, kad čia nėra gaunami tiksliai apibrėžti klasteriai, t. y. duomenys nėra vienareikšmiškai priskiriami vienam ar kitam klasteriui. Klasterizavimo rezultatus gali įvairiai interpretuoti pats tyrėjas, stebėdamas vizualų SOM vaizdą. Tai leidžia pastebėti duomenų tarpusavio panašumą ir grupes, kurios iš anksto nėra žinomos, o tai gali būti privalumu prieš kitus klasterizavimo metodus. SOM tinklai gali būti taikomi ir duomenims, kurie jau yra priskirti klasėms, klasterizuoti. Tuomet tyrėjas gali matyti, ar klasės sutampa su SOM gautais klasteriais, ir aiškintis to nesutapimo priežastis, kurių viena gali būti susijusi su tuo, kad duomenys buvo netiksliai priskirti klasėms.

Šiuo metu yra sukurta įvairių programinių sistemų, kuriose įgyvendinti įvairūs SOM vizualizavimo būdai, tačiau trūksta sistemų, kuriose, vizualizuojant SOM tinklą, būtų matoma, kiek ir kokios klasės duomenų priskirta kiekvienam SOM tinklo langeliui. Problema yra ir ta, kad nėra skaitinių įverčių, parodančių duomenų klasių ir SOM gautų klasterių sutapimą.

Be to, SOM rezultatas labai priklauso nuo įvairių mokymo faktorių parinkimo, todėl iškyla problema, kokias faktorių reikšmes parinkti analizuojamiems duomenis. Taip pat svarbu ištirti, kokios reikšmės leidžia gauti tikslesnius rezultatus, kai analizuojami skirtingo tipo duomenys: tekstiniai ir skaitiniai.

Taigi šioje disertacijoje sprendžiamos dvi pagrindinės problemos:

1. Duomenų, priskirtų tam tikroms klasėms, vizualizavimas, taikant saviorganizuojančius neuroninius tinklus, ir gautų rezultatų kokybės vertinimas.
2. Gautų rezultatų priklausomybė nuo saviorganizuojančio tinklo mokymo faktorių reikšmių parinkimo.

Tyrimo objektas

Disertacijos tyrimo objektas – duomenų klasterizavimas, klasifikavimas ir vizualizavimas, naudojant saviorganizuojančius neuroninius tinklus, bei jų kokybės vertinimas.

Darbo tikslas ir uždaviniai

Darbo tikslas – sukurti saviorganizuojančių neuroninių tinklų vizualizavimo būdą, leisiantį vizualizuoti skaitinius ir tekstinius duomenis, kurių klasės iš anksto žinomos, ir stebėti gautų klasterių ir duomenų klasių sutapimą bei pasiūlyti ir ištirti šiuos sutapimus įvertinančias paklaidas.

Siekiant tikslo būtina spręsti šiuos uždavinius:

1. Atlikti esamų SOM vizualizavimo būdų analitinę apžvalgą.
2. Pasiūlyti paklaidas, įvertinančias SOM gautų klasterių ir duomenų klasių sutapimą.
3. Pasiūlyti SOM vizualizavimo būdą duomenims, kurių klasės yra žinomos, tirti.
4. Sukurti programinę sistemą, kurioje įgyvendintas pasiūlytas SOM vizualizavimo būdas, bei SOM kokybę įvertinančias paklaidas.
5. Eksperimentiškai ištirti pasiūlytą SOM vizualizavimo būdą, paklaidas, priklausomai nuo SOM mokymo faktorių reikšmių, tiriant skaitinius ir tekstinius duomenis.

Tyrimo metodai

Analizuojant mokslinius ir eksperimentinius pasiekimus saviorganizuojančių neuroninių tinklų srityje, buvo naudoti informacijos paieškos, sisteminimo, analizės, lyginamosios analizės ir apibendrinimo metodai. Remiantis eksperimentinio tyrimo metodu, atlikta statistinė duomenų ir tyrimų rezultatų analizė, kurios rezultatams įvertinti naudotas apibendrinimo metodas.

Darbo mokslinis naujumas

1. Pasiūlytas SOM vizualizavimo būdas, skirtas skirtingų klasių tiek tekstinių, tiek skaitinių duomenų, pakliuvusių į vieną SOM langelį, santykiui pavaizduoti.
2. Pasiūlyti naujas SOM kokybę įvertinančias paklaidas, kai analizuojami duomenys, priskirti iš anksto žinomoms klasėms.
3. Ištirta tekstinių dokumentų konvertavimo į skaitinę išraišką faktorių įtaka gautiems SOM žemėlapio rezultatams.

Ginamieji teiginiai

1. Pasiūlytas SOM vizualizavimo būdas leidžia pavaizduoti skirtingų klasių duomenų, pakliuvusių į tą patį SOM žemėlapio langelį, santykius.
2. Pasiūlytos SOM kokybės įvertinimo paklaidos leidžia įvertinti duomenų klasių ir SOM gautų klasterių atitikimą.
3. Tekstinių dokumentų konvertavimo į skaitinę išraišką tinkamas faktorių parinkimas pagerina gautus SOM rezultatus.

Darbo rezultatų praktinė reikšmė

Sukurta SOM programinė sistema, kurioje įgyvendintas ne tik pasiūlytas SOM vizualizavimo būdas bei SOM kokybę nustatančios paklaidos, bet ir yra galimybė pasirinkti įvairias kaimynystės funkcijas bei mokymo parametrus, kurių reikšmės gali keistis arba kiekvienoje iteracijoje, arba kiekvienoje epochoje. Taip pat yra galimybė išskaidyti nagrinėjamą duomenų aibę į du poaibius: mokymo ir testavimo. Dėl šių priežasčių sukurta SOM sistema gali būti naudojama ne tik duomenims analizuoti, bet ir SOM tinklui tirti. Dalis tyrimų rezultatų gauti vykdant Europos socialinio fondo finansuojamą projektą „Paslaugų interneto technologijų kūrimo ir panaudojimo našių skaičiavimų platformose teoriniai ir inžineriniai aspektai" (Nr. VP1-3.1-ŠMM-08-K-01-010).

Darbo rezultatų aprobavimas

Tyrimų rezultatai publikuoti 7 moksliniuose leidiniuose: 5 periodiniuose recenzuojamuose mokslo žurnaluose, iš jų – 2 leidiniuose, referuojamuose „Thomson Reuters Web of Science" duomenų bazėje ir turinčiuose citavimo indeksą; bei 2 straipsniai – konferencijų pranešimų medžiagoje. Taip pat publikuotos 2 santraukos tarptautinių konferencijų santraukų rinkiniuose. Tyrimų rezultatai buvo pristatyti ir aptarti šiose nacionalinėse ir tarptautinėse konferencijose Lietuvoje ir užsienyje:

Disertacijos struktūra

Disertaciją sudaro 5 skyriai ir literatūros sąrašas. Pirmas disertacijos skyrius yra „Įvadas". Šioje dalyje yra pateiktos disertacijoje sprendžiamos problemos, tikslas, uždaviniai, naudoti tyrimo metodai, ginamieji teiginiai, mokslinis naujumas, disertacijos praktinė reikšmė bei darbo rezultatų aprobavimas. Antras skyrius „Saviorganizuojančių neuroninių tinklų apžvalga" skirtas saviorganizuojančių neuroninių tinklų metodui bei jo mokymo faktoriams pristatyti. Aprašytas būdas, kaip yra konvertuojami tekstiniai duomenys į skaitinę išraišką. Apžvelgtos šio metodo modifikacijos bei praplėtimai. Pateiktos populiariausių saviorganizuojančių neuroninių tinklų sistemų vizualizavimo galimybės. Trečiame skyriuje „Naujas SOM vizualizavimo būdas bei jo kokybę nustatančios paklaidos" pateiktas naujai pasiūlytas SOM vizualizavimo būdas, aprašytas jo pranašumas, lyginant su kitais antrame skyriuje aprašytais sistemų vizualizavimo būdais. Taip pat pasiūlyti matai, kurie leidžia įvertinti gauto SOM žemėlapio kokybę, kai yra nagrinėjami duomenys, kurių klasės yra iš anksto žinomos. Skyriuje „Eksperimentinių tyrimų rezultatai“ pateikti eksperimentiniai tyrimai, jų aprašymai bei gauti rezultatai. Paskutiniame skyriuje „Bendrosios išvados“ yra disertacijos išvados bei rezultatai. Papildomai disertacijoje pateiktas naudotų žymėjimų sąrašas. Bendra disertacijos apimtis – 132 puslapiai, kuriuose – 49 paveikslai ir 27 lentelės. Disertacijoje remtasi 87 literatūros šaltiniais.

Bendrosios išvados

Tiriant saviorganizuojančius neuroninius tinklus, gauti šie rezultatai: sukurtas naujas SOM vizualizavimo būdas; pasiūlytos paklaidos, leidžiančios įvertinti (tarpusavyje palyginti) keliuose SOM žemėlapiuose susidariusių klasterių atitikimą su duomenų klasėmis; sukurta nauja SOM sistema, kurioje įgyvendintas pasiūlytas SOM vizualizavimo būdas, SOM kokybę įvertinančios paklaidos bei galimybė rinktis įvairius SOM mokymo faktorius; ištirta SOM mokymo faktorių bei tekstinių dokumentų konvertavimo į skaitinius duomenis įtaka gautiems SOM rezultatams.

Atlikti tyrimai atskleidė darbe pasiūlytų SOM rezultatų kokybę, vertintų paklaidų bei pasiūlyto SOM vizualizavimo būdo naudą, tiriant duomenis, kurių klasės iš anksto žinomos. Remiantis eksperimentinių tyrimų rezultatais, padarytos šios išvados:

1. Pasiūlytos SOM žemėlapio kokybę įvertinančios paklaidos tinkamai parodo duomenų klasių ir klasterių atitikimą žemėlapyje.
2. Pasiūlytas SOM vizualizavimo būdas leidžia pavaizduoti skirtingų klasių duomenų, pakliuvusių į tą patį SOM žemėlapio langelį, santykius.
3. Tiriant tekstinius duomenis, pasiūlytų SOM kokybę įvertinančių paklaidų prasme, euristinės funkcijos naudojimas, leidžia gauti tikslesnius rezultatus – 49 % tirtų atvejų, Gauso funkcijos – 31 %, burbuliuko – 20 %; tiriant skaitinius duomenis geriausi SOM rezultatai taikytų paklaidų prasme gauti, naudojant Gauso kaimynystės funkciją (37 % atvejų), tačiau jie mažai skiriasi nuo rezultatų, gautų naudojant euristinę funkciją (35 % atvejų).
4. Atsižvelgiant į naudotą mokymo parametrą, geriausi SOM rezultatai vertintų paklaidų prasme tekstinių duomenų aibei gauti, naudojant atvirkštinį laikui

mokymo parametrą, keičiant jo reikšmes kiekvienoje epochoje (16 % tirtų atvejų), o blogiausi, – naudojant tiesinį mokymo parametrą, keičiant jo reikšmes kiekvienoje epochoje (7 % tirtų atvejų); Skaitinių duomenų atveju geriausi rezultatai gauti, naudojant tiesinį mokymo parametrą, keičiant jo reikšmes kiekvienoje iteracijoje (17 % tirtų atvejų), o blogiausi, – naudojant euristinį mokymo parametrą, keičiant jo reikšmes kiekvienoje iteracijoje (9 % tirtų atvejų).

5. Tiriant žodyno, kuris naudojamas konvertuojant tekstinius dokumentus į skaitinius duomenis, sudarymo būdus, tiksliausi SOM rezultatai naudotų paklaidų prasme gauti žodyną sudarant rankiniu būdu (18 % ir 15 %), t. y. į jį įtraukiant norimus raktinius žodžius; Tiriant automatinius žodyno sudarymo būdus, tiksliausi SOM rezultatai gauti (16 %), kai sudarant žodyną atmetami dažniausiai vartojami žodžiai iš sąrašo, sudaryto atsižvelgiant į dokumente pateikiamą informaciją ir nenaudojamas joks žodžių kamieno išskyrimo algoritmas.
6. Tiriant žodžių pasikartojimo dokumente skaičiaus įtaką SOM rezultatams, didinant minimalų žodžių pasikartojimų skaičių, bendras SOM rezultatų tikslumas mažėja; tiksliausi rezultatai gauti, kai minimalus pasikartojimų skaičius lygus 1 (vidutiniškai 30 %), o blogiausi rezultatai, – kai minimalus pasikartojimų skaičius lygus 5 (vidutiniškai 10,5 %).

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