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APPLICATION OF MULTI-PARAMETER DATA VISUALIZATION BY MEANS OF AUTOASSOCIATIVE NEURAL NETWORKS TO EVALUATE CLASSIFICATION POSSIBILITIES OF VARIOUS COAL TYPES

Dariusz JAMROZ

AGH University of Science and Technology, Faculty of Electrical Engineering, Automatics, Computer Science and Biomedical Engineering, Department of Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland, jamroz@agh.edu.pl

Abstract: The significance of data visualization in modern research is growing steadily. In mineral processing scientists have to face many problems with understanding data and finding essential variables from a large amount of data registered for material or process. Hence it is necessary to apply visualization of such data, especially when a set of data is multi-parameter and very complex. This paper puts forward a proposal to introduce the autoassociative neural networks for visualization of data concerning three various types of hard coal. Apart from theoretical discussion of the method, the empirical applications of the method are presented. The results revealed that it is a useful tool for a researcher facing a complicated set of data which allows for its proper classification. The optimal neural network parameters to successfully separate the analyzed three types of coal were found out for the analyzed example.

Keywords: *autoassociative neural networks, coal types, multidimensional visualization, multi-parameter, identification of data, pattern recognition, neural networks*

Introduction

Multidimensional statistical analysis can be divided into many types. Besides typical approximations or searching for a regressive equation with the use of numerous modern methods (Ahmed and Drzymala, 2005; Brozek and Surowiak, 2005; 2007; 2010; Drzymala, 2007; 2009; Gawenda et al., 2005; Niedoba, 2009; 2011; 2013b; Niedoba and Surowiak, 2012; Saramak, 2011; 2013; Snopkowski and Napieraj, 2012; Tumidajski, 1997; Tumidajski and Saramak, 2009), there are also many data-mining methods which are widely used. One of them includes visualization methods aimed at recognition of differences and similarities between analyzed sets of data. This is

frequently a very significant issue in mineral processing where processes are feature-dependent.

Owing to the methods of multidimensional data visualization through the transformation of multidimensional space into two-dimensional, it is possible to show multi-parameter data on the computer screen, thus making it possible to carry out a qualitative data analysis in the most natural way for a human being – by a sense of sight. One of the methods involves using autoassociative neural networks. This method was used in the paper to present and analyze a set of seven-parameter data describing samples of three various coal types: 31, 34.2 and 35 (according to Polish classification of coal types). It was decided to examine whether the amount of data is sufficient for the proper classification of coal types. The application of various methods to analyze recognition possibilities of various coal features is becoming an interesting issue. Recently, different visualization methods have been investigated such as observational tunnels method (Jamroz and Niedoba, 2014; Niedoba and Jamroz 2013). However, the application of autoassociative neural networks to evaluate the possibility of proper identification of coal type is a novel sort of approach.

Previous investigations conducted by means of observational tunnels method (Jamroz and Niedoba 2014) showed that not only analyzed data are correlated but also that only three parameters are sufficient to correct recognition of coal type. Furthermore, it was stated that occurrence of high linear correlation coefficient between two parameters does not mean the possibility of replacing one parameter by another one. However, the main reason of applying autoassociative neural networks in this paper is that this method allows some significant parameters without any additional analysis. It is not necessary to check which parameters are significant or to check which of them are correlated – in fact any additional analyzes are not necessary. The result is achieved immediately in the very suitable way for the researcher – by sight sense. This is because for neural network is not important if it has 3, 7 or 20 inputs. Sight sense is a mechanism which was developed by nature during many thousands of years. Everyone who performs image recognition knows that it is easier to observe, for example, a figure and state if it presents, for example, a giraffe than to write a program (using many various known or unknown methods) which is capable to recognize this animal on the basis of a photo. That is why connection of autoassociative neural network creating two-dimensional figure and our personal neural network (brain) analyzing this figure by sense of sight can give more readable results. So, it is much easier to check whether the points being part of various fractions can be separated by not complicated curve (like polynomial of low degree) or not than check it by means of selected analysis. Additionally, because autoassociative neural networks are non-linear methods then their abilities and clearness of results are much bigger than the ones of simple linear methods. Within previously conducted works the analyzes of multi-parameter coal data were performed by means of many methods: observational tunnels method (Niedoba and Jamroz 2013; Jamroz and Niedoba 2014), Kohonen network, multidimensional scaling (Jamroz 2014b), relevance maps, PCA

(Niedoba 2014) and autoassociative neural networks. By means of all these methods the satisfying results were obtained for coal and they are described in several papers. The detailed comparison of these methods efficiency is in progress.

General visualization principles of multi-parameter data

Only multi-parameter analysis of many features describing grained material gives sufficient information about the researched material. A number of methods can be applied for this purpose, including visualization methods. Based on a big collection of data it is often impossible to observe significant differences. Multi-parameter visualization, by contrast, gives a chance to do it. There are many techniques of multi-parameter visualization. The following methods of data visualization should be mentioned: grand-tour method (Asimov 1985), the method of principal component analysis (Hotelling, 1933; Jolliffe, 2002; Niedoba, 2014), the use of neural networks for data visualization (Kohonen, 1989; Jain and Mao, 1992; Aldrich, 1998), a parallel coordinates method (Inselberg 2009), multidimensional scaling (Kruskal, 1964; Jamroz, 2014b), the scatter-plot matrices method (Cleveland, 1984), method using the so-called relevance maps (Assa et al., 1999), method of observational tunnels (Jamroz, 2001; 2014a; Jamroz and Niedoba, 2013; 2014). The visualization of multidimensional solids is also possible (Jamroz, 2001; 2009).

Experiment

Three types of coal, types 31 (energetic coal), 34.2 (semi-coking coal) and 35 (coking coal) according to the Polish classification, were used in the investigation (Olejnik et al., 2010). Seven-parameter data consisted of 205 samples, including 72 samples of coal, type 31, 61 samples of coal, type 34.2 and 72 samples of coal, type 35. The whole set of data used in this paper can be found in (Niedoba, 2013a). They were obtained from three different Polish coal mines. Subsequently, all of them were initially screened on a set of sieves of the following sizes: -1.00, -3.15, -6.30, -8.00, -10.00, -12.50, -14.00, -16.00 and -20.00 mm. Then, the size fractions were additionally separated into density fractions by separation in dense media using zinc chloride aqueous solution of various densities (1.3, 1.4, 1.5, 1.6, 1.7, 1.8 and 1.9 g/cm³). The fractions were used as a basis for further consideration and additional coal features were determined by means of chemical analysis. For each density-size fraction such parameters as combustion heat, ash contents, sulfur contents, volatile parts contents and analytical moisture were determined, making up, together with the mass of these fractions, seven various features for each coal type. Examples of data were presented in Table 1 showing the data for density-size fractions 1.00-0.50 mm for type 31 of coal.

Table 1. Data for density-size fraction 1.00-0.50 mm – coal type 31

Density [g/cm ³]	Mass	Combustion heat [cal]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents v^a	Analytical moisture W_a
<1.3	4187.8	7367	1.25	0.63	36.02	4.15
1.3–1.4	2864	7021	3.35	0.66	32.14	4.33
1.4–1.5	310	5939	18.78	1.33	27.54	2.55
1.5–1.6	102.3	5547	23.83	1.66	26.87	2.80
1.6–1.7	111.9	4911	30.54	1.91	25.98	2.65
1.7–1.8	91.3	4177	39.94	1.93	25.17	2.35
1.8–1.9	80.9	3462	47.43	1.74	24.00	2.29
>1.9	1051.8	762	82.20	1.72	13.05	1.14

Autoassociative neural networks

Method description

Autoassociative neural networks are an example of self-organizing neural networks which learning process occurs without the teacher. When applied to visualization of multi-parameter data, the network has n inputs, one of indirect layers consisting of 2 neurons and n outputs. The number of network inputs and outputs is equal to the number of parameters of the analyzed data. The network is learnt by error backward propagation method.

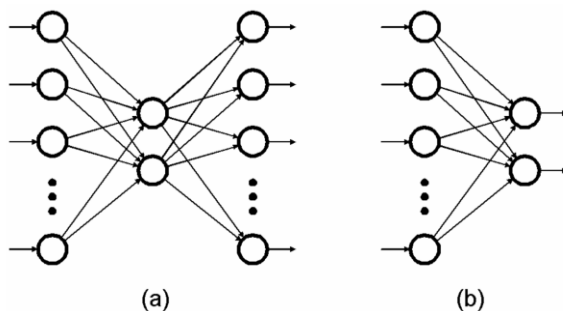


Fig. 1. Structure of autoassociative neural network used for multi-parameter data visualization.
 (a) network training for receiving signals on outputs possibly closest to signals on inputs,
 (b) transformation of input signal in location on two-dimensional screen with the use of a fragment of previously learnt network

As a result of learning process, the same signals should impact both the outputs and inputs of neural networks. The described network is based on a change of input n -dimensional space B into two-dimensional space Y and then back into n -dimensional space B^* in the most similar way to B . The data going through the layer of two neurons, which outputs represent two-dimensional space Y , is compressed by network,

thus resulting in a two-dimensional preservation of certain individual features of original data from space B, which allows for reconstruction of the data.

When the learning process is over, the data visualization can be started. It consists in providing input to each data vector x on the neural network and projecting two-dimensional point representing it (on the basis of data from hidden layer consisting of two neurons). The location of this point is determined by two coordinates taken directly from the outputs of two neurons which constitute indirect layer and represent (in a compressed way) space B . A general working scheme by learning and visualization of such network has been presented in Figure 1.

Algorithm

A set of input data consists of elements described by n features. It can be then treated as a set of n -parameter vectors. The visualization based on autoassociative neural networks involves two stages.

- D) Self-organization of network. In this stage all neuron weights are calculated on the basis of input data (Fig. 1a). The algorithm developed to fulfill this stage includes:
 - 1. scaling of input data in order to ensure that the neural network can reproduce it as a result of the learning process. Individual features representing data parameters were scaled so fit the network output permissible range. In order to calculate the value of neuron output the function of hyperbolic tangent was used (described in equations (1) and (2)). So, the values of network outputs are within the range (-1, 1). It was decided then to scale the individual coordinates (features) of data sets to range (-0.9, 0.9),
 - 2. randomization of all weights $w_{i,j,k}$ for all neurons (where $w_{i,j,k}$ is the weight of k^{th} input of neuron located in i^{th} network layer on j^{th} position). Each weight was assigned to a value within the range (-0.5, 0.5) by applying plate probability distribution.

The next points 3-7 are carried out for each of input data vector ITER times (ITER is a parameter accepted in a given moment):

- 3. the output values for all neurons located in first layer are calculated for the next w^{th} vector of input data. The weight is associated for an input of every neuron in the network. An input signal has an influence upon output signal. Additionally, the value of output signal depends on an additional weight (with adopted index 0) which determines component constant. To each neuron the $n+1$ -parameter weight vector is assigned, where n is the number of network inputs. The value of output of first layer neuron is calculated according to the formula:

$$y_{1,j} = g \left(w_{1,j,0} + \sum_{k=1}^n w_{1,j,k} x_{k,w} \right) \tag{1}$$

where: g – adopted non-linear function, n – number of network inputs, $y_{i,j}$ – value of output of neuron located on i^{th} layer of network on j^{th} position (for the first layer of neurons the value of i is equal to 1), $w_{i,j,k}$ – weight of k^{th} input of neuron located on i^{th} network layer on j^{th} position, $x_{k,w}$ – k^{th} feature of w^{th} part of input data set (k^{th} coordinate of w^{th} data vector). Application of non-linear function g in Eq. (1) allows to increase the calculating possibilities of neural network. In conducted experiments the hyperbolic tangens function was used as this function.

4. The values are calculated for all neurons' outputs located in all individual network layers. The calculations of neurons' outputs in the next layer can always be followed by the calculation of neuron values from the previous layer. This can take place because the values of previous layer outputs constitute at same time inputs for the next layer of neurons. In this way the values of all neurons in all layers are calculated.

$$y_{i,j} = g \left(w_{i,j,0} + \sum_{k=1}^{\text{size}(i-1)} w_{i,j,k} y_{i-1,k} \right) \quad (2)$$

where: $\text{size}(i-1)$ – number of neurons in $i-1$ layer, $y_{i,j}$ – output value of neuron located in i^{th} network layer on j^{th} position, $w_{i,j,k}$ – weight of k^{th} input of neuron located in i^{th} network layer on j^{th} position, g – adopted non-linear function, the same as in equation (1).

5. For the purpose of calculating the errors of network output, it is necessary to obtain the difference between network input values (what is supposed to be obtained) and output values obtained on the last layer of neurons. This difference is then multiplied by a derivative of function g adopted in equations (1) and (2), which is the derivative of hyperbolic tangens function, obtaining:

$$\delta_{i,j} = (1 - y_{i,j}^2) (x_{j,w} - y_{i,j}) \quad (3)$$

where: $\delta_{i,j}$ – calculated error value of output of neuron located in i^{th} network layer on j^{th} position (in this equation i means the number of last network layer), $y_{i,j}$ – output value of j^{th} neuron of i^{th} layer, $x_{j,w}$ – j^{th} feature of w^{th} part of input data set.

6. The errors of neurons' outputs from other network layers, individually from the penultimate to the first layer, are calculated as following:

$$\delta_{i,j} = (1 - y_{i,j}^2) \sum_{k=1}^{\text{size}(j+1)} (\delta_{i+1,k} w_{i+1,k,j}) \quad (4)$$

where: $\delta_{i,j}$ – calculated error value of output of neuron located on i^{th} network layer on j^{th} position, $w_{i+1,k,j}$ – weight of j^{th} input of k^{th} neuron from $i+1$ layer, $\text{size}(j+1)$ – number of neurons located in layer $j+1$, $y_{i,j}$ – output value of j^{th} neuron from i^{th} layer.

7. Modification of neuron network weights on the basis of previously calculated errors. The modification was adopted according to the formula:

$$\tilde{w}_{i,j,k} = w_{i,j,k} + \eta \delta_{i,j} y_{i-1,k} \quad (5)$$

where: $w_{i,j,k}$ – weight of k^{th} input of j^{th} neuron from i^{th} layer, $\tilde{w}_{i,j,k}$ – weight $w_{i,j,k}$ after change, $\delta_{i,j}$ – value of error of j^{th} neuron output from i^{th} layer, $y_{i-1,k}$ – value of output of k^{th} neuron from $i+1$ layer, η – speed of learning, the constant 0.01 was adopted.

II) Projection of image (Fig. 1b). Points 1-2 are realized for each input data vector.

1. The values of outputs of following neuron layers are calculated for next w^{th} input data vector. The calculations of the values of next neuron layers are conducted until the output value of determined two-neuron layer is found. Which layer it is should be assumed at the beginning during the construction of neural network. Let us assume that values obtained from outputs of these two neurons are u and v .
2. The symbol representing fraction of w^{th} data vector is drawn on screen in point of coordinates (u, v) . The values u and v are within the range $(-1, 1)$ – it occurs from the previously accepted hyperbolic tangent function in equations (1) and (2).

The image of “locations” through which the data representing individual coal fractions flow is created in this way.

Results and discussion

During investigation the analysis was performed for various parameters. Such parameters were searched by which neural network is able to group coal data in the possibly best way. Some obtained parameters need to be accepted as constants – for example, number of network layers and non-linear function g (on which basis neuron outputs are calculated). For further analysis of coal data is sufficient to select initial, random values of all neurons weights generated by pseudo-random generator of values and value of parameter ITER – meaning number of learning repeats. Choice of other set of values generated by random numbers generator is not a problem. However, choice of the moment of stopping learning process requires experience and knowledge of neural networks functioning way.

Neural networks are very specific. They are being learnt till the moment when they will recognize correctly. If learning process is too short then it will be insufficiently well prepared. However, in practice of artificial neural networks the phenomenon of network “over-learning” exists when the learning process lasts too long. It happens because algorithm tries more and more adequately fit function realized by network to samples and this causes that this function becomes very complex, with large number of extremes – as a result it will recognize samples being outside learning set incorrectly. Example of function being realized by correctly learnt network and by “over-learnt” network is presented on Figure 2. That is why at certain moment when

neural network is already learnt, the learning process should be stopped. In purpose of checking if network was learnt, various criteria can be searched. Figure 3 shows relation between network error and parameter ITER. This error is calculated as mean squared error of difference between individual inputs and outputs of the network for all samples and network inputs. This graph was obtained for data containing 3 types of coal, showed on Figs 5–6. In case of this data for ITER = 5 this error was equal to 0.104462, for ITER = 30 it was equal to 0.028714 and for ITER = 9000 it was equal to 0.006332.

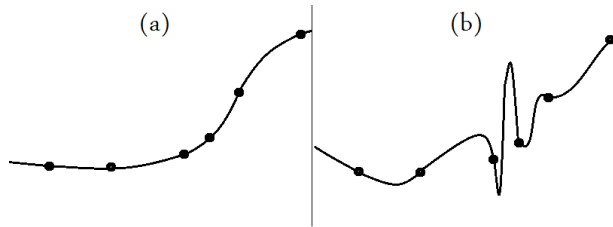


Fig. 2. Examples of two functions of one variable being realized by the same neural network learnt on the basis of the same set consisted of 6 points. Part (a) shows function realized by network learnt correctly, part (b) shows function realized by “over-learnt” network

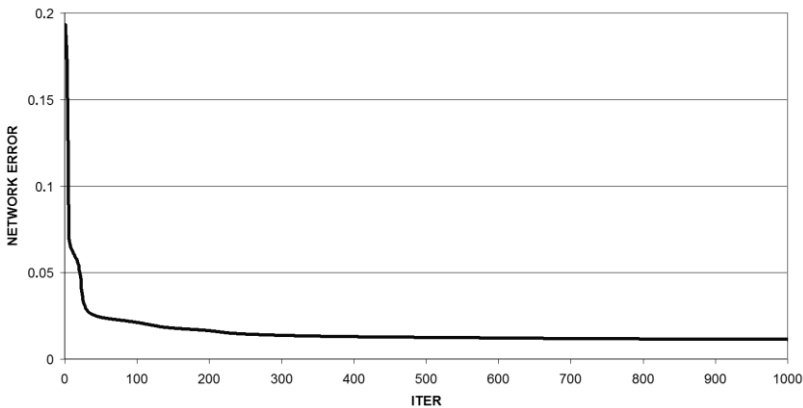


Fig. 3. Relation between network error and ITER parameter. Error is calculated as mean square error of difference between individual inputs and outputs of the network for all samples and network inputs

In practice, this graph does not give much because it always presents function which lowers till certain limit. Additionally, in case of neural networks, as it was mentioned before, during learning process till certain moment we achieve better and better results and then, despite that error still lowers, network becomes “over-learnt”. Thus, if views from which occurs that separation is possible were obtained it means that in analyzed data (in chosen parameters) information allowing proper recognition gathers. In case if analyzed data (containing chosen 7 parameters) do not contain information necessary to identify coal type then independently on learning process

length is not possible to achieve views showing that data of various fractions are located in other part of the figure. It should be remembered that during network learning no information about what fraction is represented by the sample is provided. That means that during learning process network does not know if any two samples represent the same fraction or various ones. Only after ending of learning process (during plotting) each sample is assigned with number of fraction of which it is part. This is done in purpose of checking if network assigned to each fraction other part of the 2-D space (graph).

Based on assumptions put forward in the previous chapter a computer software was developed to visualize seven-parameter data describing various types of coal. The software was developed C++ language by means of Microsoft Visual Studio. The experiment led to a conclusion that the best results from the analysis of data describing various coal types were yielded by a 6-layer neural network. Three layers serve to compress data from seven to two parameters while the other three serve to decompress from two to seven parameters. The third layer consists of two neurons (their outputs serve to visualization) and each of the remaining layers consists of 7 neurons. In Figure 4 the topology of network was shown. The outputs of neurons $y_{3,1}$ and $y_{3,2}$ are the outputs of two-neuron layer on which the visualization was based. Full information is transferred through these two signal outputs, which is necessary to reconstruct seven-parameter input data. This is why on the basis of these outputs, it is possible to read the coordinate values of the point located on plane which represent seven-parameter input data vector.

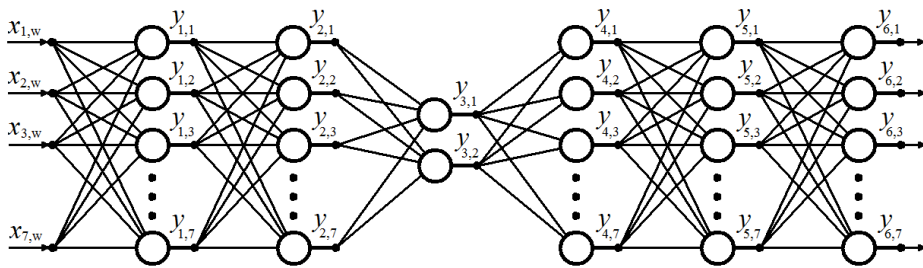


Fig. 4. Topology of autoassociative neural network with the best results. Three layers serve to compress data and three to reproduce data. Outputs $y_{3,1}$ and $y_{3,2}$ of the layer consisting of two neurons serve to visualize seven-parameter data

The obtained results were presented in Figures 5-9. The views show a way of compression of seven-parameter data by neural network to two parameters determined by outputs $y_{3,1}$ and $y_{3,2}$ of the network. The compression must allow for a reconstruction of seven-parameter input data by the last three network layers, hence it should contain all information needed for this purpose. In this way it is possible to see all significant features of seven-parameter data on two-dimensional screen.

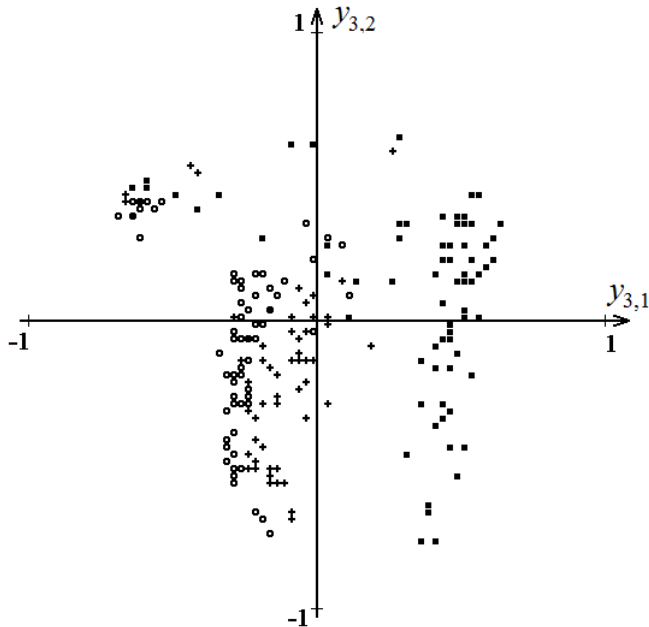


Fig. 5. A presentation of seven- parameter data representing three various coal types by parameter ITER=30 shown by neural network with two signals $y_{3,1}$ and $y_{3,2}$. Signals representing samples of coal type 31 were marked with (■), (+) – samples of coal type 34.2, (o) – samples of coal type 35

Figure 5 shows the view obtained by parameter ITER=30. The adopted ITER value means that the self-learning process network was conducted for each input data vector 30 times. Figures 5-6 show how the network evolves. It can be seen that the signals which are a reply to data representing the same coal types start to occupy separated subareas and groups. In Figure 5 it can be noticed that by small value of parameter ITER=30, the signals representing the same types start to group. However, in some parts of the space, the signals of various coal types still overlap. In Figure 6 (ITER=9000) it can be observed that signals which are a reply to data representing samples of certain coal type gather. It can be seen that these gatherings can be separated. The clearness of the signal space division grows along with the increase of ITER parameter, so with the network learning process. It should be pointed out that the information of data vectors affiliation to certain fractions was not taken into account during self-learning of the network (calculating of weights). Therefore, the grouping of signals (i.e. those that go through layer consisting of two neurons) representing a certain fraction depends only on certain data properties noticed by the network.

In order to achieve even more clear results, it was decided to make a presentation of the same data in other way by means of autoassociative neural network. An examination was conducted how network will allocate signals to data representing coal types in pairs. Figure 7 depicts network data on coal types 34.2 and 35. It is even

more clear that signals representing coal type 34.2 gather in aggregations which can be easily separated from signals representing samples of coal type 35.

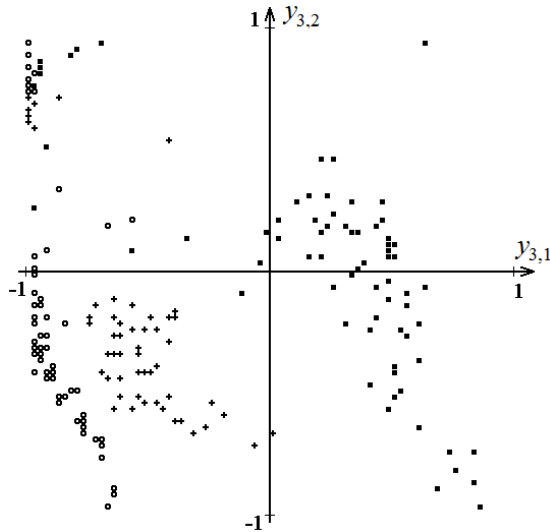


Fig. 6. A presentation of seven-parameter data representing three various coal types by parameter ITER = 9000 shown by neural network with two signals $y_{3,1}$ and $y_{3,2}$. Signals representing samples of coal type 31 were marked with (■), (+) – samples of coal type 34.2, (o) – samples of coal type 35

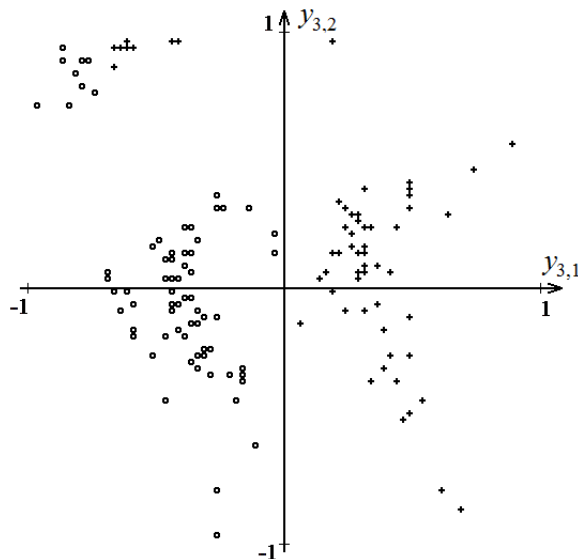


Fig. 7. A presentation of seven-parameter data representing three various coal types by parameter ITER=4000 shown by neural network with two signals $y_{3,1}$ and $y_{3,2}$. Signals representing samples of coal type 34.2 were marked with (+) –, (o) – samples of coal type 35

Figure 8 depicts the way how neural network presents data representing coal types 31 and 35. It is also clear that signals representing samples of coal type 31 gather in aggregations which can be easily separated from signals representing samples of coal type 35. Figure 9 shows the way how network presents data representing coal types 31 and 34.2. It can be clearly seen that signals representing samples of coal type 31 gather in aggregations which can be easily separated from signals representing samples of coal type 34.2.

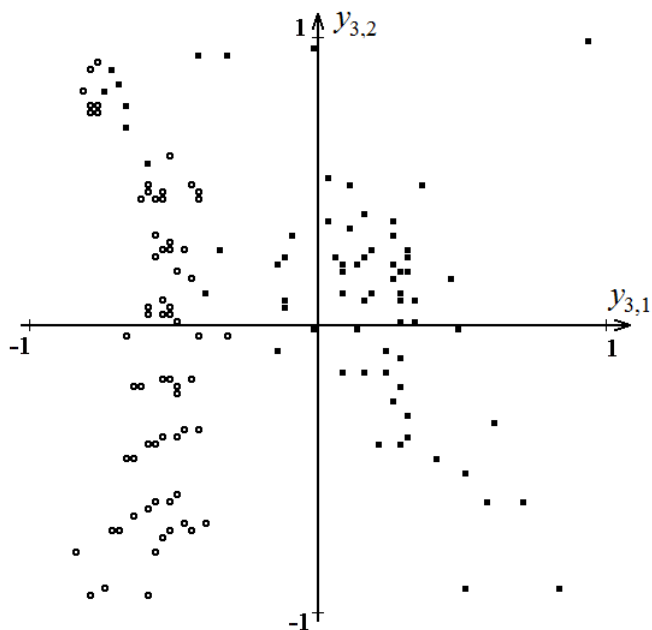


Fig. 8. A presentation of seven-parameter data representing three various coal types by parameter ITER=17120 shown by neural network with two signals $y_{3,1}$ and $y_{3,2}$. Signals representing samples of coal type 31 were marked with (■), (○) – samples of coal type 35

If it is possible to confirm the possibility of separation of coal samples, type 34.2 from coal type 35 (Fig. 7), the possibility of separation of coal samples, type 31 from coal type 35 (Fig. 8) and, furthermore, the possibility of separation of coal samples, type 31 from coal type 34.2 (Fig. 9) is also confirmed, then it can be stated that the samples of all three types of coal can be separated from each other. The application of multi-parameter data visualization by means of autoassociative neural networks allows to arrive at a conclusion that the information about seven-parameter input data describing samples of three coal types is sufficient for their proper classification.

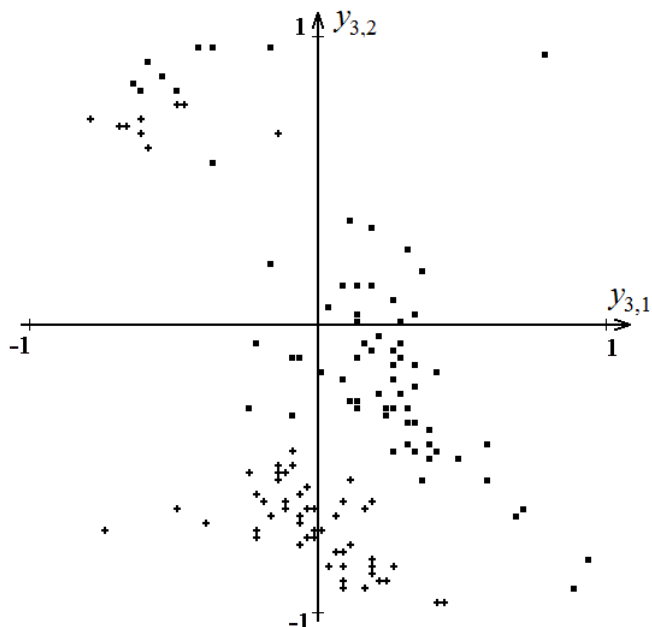


Fig. 9. A presentation of seven-parameter data representing three various coal types by parameter ITER =5230 shown by neural network with two signals $y_{3,1}$ and $y_{3,2}$, show. Signals representing samples of coal type 31 were marked with (■), (+) – samples of coal type 34.2

Conclusions

The conducted experiments involving the visualization of seven-parameter data visualization by means of autoassociative neural networks allowed to draw the following conclusions.

1. Visualization of seven-parameter data by means of autoassociative neural networks allows to state that the information in analyzed seven-parameter data is sufficient for the proper classification of coal types 31, 34.2 and 35.
2. Even the presentation of three types of coal in one Figure allows to state that signals representing samples of coal of certain type gather in aggregations which can be easily separated. It occurs that data contains information sufficient for the proper classification of coal types.
3. Presentation of data representing various coal types in pairs by means of autoassociative neural networks allows to obtain even more clear results.
4. The best results were obtained by means of neural network consisting of 6 layers. Three layers served to compress data from 7 to 2 parameters and three layers served to decompress from 2 to 7 parameters. Third layer which comprised two neurons, which outputs served for visualization purposes, and each of the remaining layers consisted of 7 neurons.

5. Clearness of results grows along with the learning progress of neural network (growth of parameter ITER value).
6. Whether the results are clear highly depends on adopted parameters. The change of these parameters results in different allotment of individual areas of signal space by neural network to data representing various types of coal.
7. Some sort of problem arising from such visualization is the necessity of selecting parameters in order to obtain a view which clearly presents the searched information. It should be noticed that during conducted experiments the views obtained by means of neural networks ranged from 3 to 8 layers. These views were obtained by ITER parameter value equal from 1 to 30000. The experiments were conducted for various initial ranges of weights. The results presented in the paper include the clearest ones from the all obtained.

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