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Arch. Min. Sci., Vol. 60 (2015), No 1, p. 39–50

Electronic version (in color) of this paper is available: http://mining.archives.pl

DOI 10.1515/amsc-2015-0003

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APPLICATION OF MULTIDIMENSIONAL DATA VISUALIZATION BY MEANS OF SELF-ORGANIZING KOHONEN MAPS TO EVALUATE CLASSIFICATION POSSIBILITIES OF VARIOUS COAL TYPES

ZASTOSOWANIE WIZUALIZACJI WIELOWYMIAROWYCH DANYCH ZA POMOCĄ SIECI KOHONENA DO OCENY MOŻLIWOŚCI KLASYFIKACJI RÓŻNYCH TYPÓW WĘGLA

Multidimensional data visualization methods are a modern tool allowing to classify some analysed objects. In the case of grained materials e.g. coal, many characteristics have an influence on the material quality. The paper presents the possibility of applying visualization techniques for coal type identification and determination of significant differences between various types of coal. To achieve this purpose, the method of Kohonen maps was applied by means of which three types of coal – 31, 34.2 and 35 (according to Polish classification of coal types) were investigated. It was stated that the applied methodology allows to identify certain coal types efficiently and can be used as a qualitative criterion for grained materials.

Keywords: Kohonen maps, grained material analysis, coal, multidimensional data, multidimensional visualization methods

Metody wizualizacji wielowymiarowych danych są nowoczesnym narzędziem umożliwiającym klasyfikację analizowanych obiektów, którymi mogą być różnego typu dane opisujące wybrane zjawisko lub materiał. W przypadku materiałów uziarnionych, jakim jest np. węgiel, wiele cech ma wpływ na jakość materiału, tj. np. gęstość, wielkość ziaren, ciepło spalania, zawartość popiołu, zawartość siarki itp. Na potrzeby artykułu przeprowadzono rozdział węgli z trzech wybranych kopalni węgla kamiennego, zlokalizowanych w Górnośląskim Okręgu Przemysłowym. Każda z tych kopalni pracuje na innego typu węglu. W tym przypadku były to węgle o typach 31, 34.2 oraz 35 (według polskiej klasyfikacji typów węgla). Najpierw, materiał został podzielony na klasy ziarnowe a następnie za pomocą rozdziale w cieczy ciężkiej (roztwór chlorku cynku) na frakcje gęstościowe. Dla tak przygotowanego materiału przeprowadzono następnie analizy chemiczne mające na celu określenie takich parametrów, jak zawartość siarki, zawartość popiołu, zawartość części lotnych, ciepło spalania oraz wilgotność analityczną. W ten sposób, dla każdej klaso-frakcji uzyskano bogate charakterystyki badanego materiału. Nasuwa się więc pytanie, czy możliwa jest identyfikacja typu węgla za pomocą dostępnych danych. W tym celu zastosowano

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wielowymiarową technikę wizualizacji statystycznej. Istnieje wiele metod takiej wizualizacji, z których kilka było już przedmiotem wcześniejszych publikacji autorów. W tym wypadku autorzy zdecydowali się zastosować metodę sieci Kohonena. Metoda ta została opisana w rozdziale 2 pracy, gdzie oprócz opisu teoretycznego podano również główne wzory stosowane podczas modelowania tą metodą (wzory (1)-(5)). Do zbadania postawionego problemu wykorzystano optymalną liczbę iteracji i optymalny czas uczenia sieci. Pewnym problemem pojawiającym się przy takiej wizualizacji jest konieczność doboru parametrów, w celu uzyskania widoku, który w sposób czytelny prezentuje poszukiwane przez nas informacje. Należy wspomnieć, że w trakcie prowadzonych eksperymentów uzyskiwano widoki przy użyciu sieci neuronowej o wielkości od 10 × 10 do 100 × 100 neuronów. Widoki były uzyskiwane przy wartości parametru MAX_DISTANCE od 1 do wielkości sieci oraz parametru ITER od 1 do 5000. Eksperymenty były prowadzone dla różnych wzorów określających modyfikację wag. Przedstawione w pracy wyniki stanowią najbardziej czytelne z uzyskanych. Wizualizacja wielowymiarowa przy użyciu sieci Kohonena pozwala stwierdzić, że informacje zawarte w analizowanych siedmiowymiarowych danych są wystarczające do prawidłowej klasyfikacji typów węgla 31, 34.2 oraz 35, przy czym nawet zobrazowanie 3 typów węgla na jednym rysunku pozwala stwierdzić, że neurony reprezentujące próbki węgla danego typu gromadzą się w skupiskach, które można od siebie odseparować. Z tego wynika, że dane zawierają informacje wystarczające do prawidłowej klasyfikacji węgla. Zauważyć jednak warto, że przedstawienie przy pomocy sieci Kohonena, danych reprezentujących różne typy węgla parami, pozwala uzyskać jeszcze bardziej czytelne wyniki. Najlepsze efekty osiągnięto dla sieci o 40 wierszach oraz 40 kolumnach neuronów, co łącznie dało liczbę 1600 neuronów, zaś czytelność wyników rośnie wraz z postępem uczenia sieci neuronowej (wzrostem parametru ITER). Przeprowadzone doświadczenia w pełni potwierdzają, że zastosowana metoda może być z powodzeniem wykorzystana w badaniach jakościowych związanych z różnego typu materiałami uziarnionymi, w tym również węglem. Badania w tym zakresie są kontynuowane.

Słowa kluczowe: sieci Kohonena, analiza materiału uziarnionego, dane wielowymiarowe, metody wizualizacji wielowymiarowej

1. Introduction

The qualitative analysis of multidimensional data (properties of material) obtained from the results of empirical experiments can be carried out by applying the multidimensional visualization method. The results of these analyses can be helpful thanks to materials characteristics as well as the construction of mineral processing models based on this data.

Attempts to depict multidimensional data have been undertaken on many occasions. Among many methods, the following ones can be selected: grand-tour method (Asimov, 1985; Cook et al., 1995), the method of principal component analysis (Li et al., 2000), use of neural networks for data visualization (Aldrich, 1998; Jain & Mao, 1992; Kraaijveld et al., 1995; Tadeusiewicz, 1993), parallel coordinates method (Chatterjee et al., 1993; Chou et al., 1999; Gennings et al., 1999; Inselberg, 1985), star graph method (Sobol & Klein, 1989), multidimensional scaling (Kim et al., 2000), scatter-plot matrices method (Cleveland, 1984), relevance maps method (Assa et al., 1999). Visualization of multidimensional solids is also possible (Jamróz, 2009). The observational tunnels method (Jamróz, 2001) makes it possible to achieve an external view of the observed multidimensional sets of points using tunnel radius, introduced by the author (Jamróz, 2014a; b; c; Jamróz & Niedoba, 2013; 2014; Niedoba, 2013).

In mineral processing applications the modern methods of data visualization is more and more important. The selection of proper groups of data to understand certain phenomena or process is one of the main goals which industrial plants desire to achieve. This is very important mainly when the set of data is very complex (Köse et al., 2012; Laine, 2002). Also, investigation of separation process occurring because of various features acting is often subject of interest of many scientific researchers (Brożek & Surowiak, 2005, 2007, 2010).

The methods of multidimensional data visualization through a transformation of multidimensional space into two-dimensional one allow to present multidimensional data on computer screen. Thanks to this, it is possible to conduct a qualitative analysis of this data in the most natural way for human being – by a sense of sight. One of such methods of multidimensional data visualization is the Kohonen maps method. It was used in the paper to present and analyze a seven-dimensional set of data describing samples of three various sorts of coal – types 31, 34.2 and 35. It was decided to check if this method allows to state that the amount of information contained in seven coal features is sufficient to classify a type of coal properly. The application of various methods to analyze possibilities of recognizing various coal features is becoming an interesting issue. Other methods of visualization were already used for the investigation (Jamróz & Niedoba, 2013, 2014; Niedoba, 2014). However, the application of Kohonen maps to evaluate the possibility of proper identification of coal type is a new approach.

2. Coal characteristics

Three types of coal, types 31 (energetic coal), 34.2 (semi-coking coal) and 35 (coking coal) in the Polish classification were used in the investigation. They originated from three various Polish coal mines and 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/cm^3). 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. The examples of such data were presented in tables 1-3 showing the data for size fractions 14.00-12.50 mm for each type of coal.

TABLE 1

Data for size fraction 14.00-12.50 mm – coal, type 31

Density [Mg/m^3]	Mass [g]	Combustion heat [cal]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	308.6	7048	6.41	0.72	34.32	3.23
1.3-1.4	292.5	5859	19.61	0.7	29.22	3.36
1.4-1.5	36.1	2948	16.55	0.76	28.92	3.87
1.5-1.6	10.7	5117	26.10	1.55	31.08	3.40
1.6-1.7	25.6	4467	35.78	2.28	26.71	2.40
1.7-1.8	139	3920	37.20	1.23	29.24	2.19
1.8-1.9	12.7	3078	48.20	1.13	24.05	2.23
>1.9	601.2	457	86.53	0.40	9.30	0.91

TABLE 2

Data for size fraction 14.00-12.50 mm – coal, type 34.2

Density [Mg/m^3]	Mass [g]	Combustion heat [cal]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	360.5	8227	2	0.32	28.96	1.04
1.3-1.4	57	7647	7.67	0.71	24.16	1.87
1.4-1.5	25.5	6901	15.33	0.83	24.58	1.34
1.5-1.6	12.2	5798	33.73	0.17	27.85	0.95
1.6-1.7	3.2	4830	34.3	0.34	No data	No data
1.7-1.8	15	4152	36.15	0.34	27.93	0.37
1.8-1.9	3.6	4415	27	0.05	31.75	1.01
>1.9	68.9	693	79.33	0.91	12.08	0.52

TABLE 3

Data for size fraction 14.00-12.50 mm – coal, type 35

Density [Mg/m^3]	Mass [g]	Combustion heat [cal]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	268.7	8327	2.38	0.28	20.28	1.45
1.3-1.4	89.3	7610	8.97	0.36	20.10	1.21
1.4-1.5	39.8	6567	19.61	0.56	18.83	1.28
1.5-1.6	22.0	5031	35.68	0.39	16.22	1.32
1.6-1.7	25.7	4988	34.62	1.26	19.42	1.47
1.7-1.8	29.0	4589	40.60	0.38	18.86	1.61
1.8-1.9	28.1	3286	52.24	1.14	17.95	1.51
>1.9	589.5	702	80.57	0.20	10.84	1.37

3. Kohonen maps

Kohonen maps are an example of self-organizing neural networks in which the learning process occurs without the teacher. They are one-layer networks with competitive learning rules to which the neighborhood term was introduced. Each network input is connected to each neuron. During the learning process the weights are modified for the neuron – winner, whose output signal that is a response to part of teaching series is the biggest, and, to a lesser degree, for the weights neighboring the neuron winners. The modification of weights occurs in a way so that the neuron response (winner and winner's neighbors) to a given part of the teaching series was even bigger.

By accepting the two-dimensional neighborhood (neurons positioned in lines and web columns), it is possible to represent network output directly on the screen in a way that a signal of neuron located in i^{th} line and j^{th} column is shown on the screen as a point of coordinates (i, j). Figure 1 presents a simple example of such network. It is composed of two lines and three columns of neurons. Each of the neurons has three inputs in this Figure.

Each input of a neuron is associated with weight. The signal impact of certain input on output neuron signal depends on it. So, the n-dimensional weight vector is assigned to each neuron,

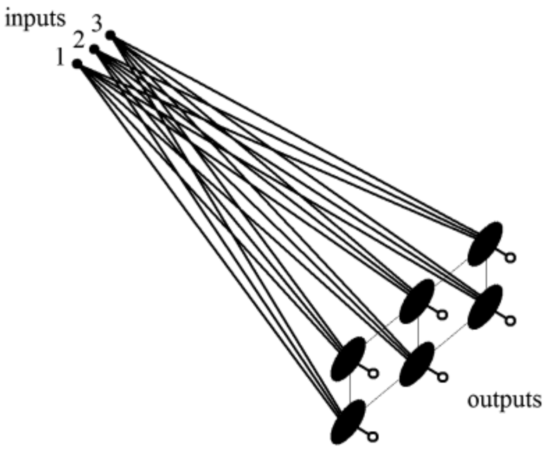

Fig. 1. Example of simple Kohonen map compound of two lines and three columns of neurons. Each of the neurons has three inputs

where n is the number of network inputs. The value of neuron output is calculated according to the formula:

$$y_{i,j} = \sum_{k=1}^{n} w_{i,j,k} x_{k,w} \tag{1}$$

where:

n — number of network inputs,
$y_{i,j}$ — output value of neuron number (i, j), so located in i^{th} line and j^{th} network column,
$w_{i,j,k}$ — weight of k^{th} input of neuron number (i, j),
$x_{k,w}$ — k^{th} feature of w^{th} part of input data set.

The input data set consists of parts described by n features. It can be then treated as a set of n-dimensional vectors.

The operation of Kohonen maps consists of two stages:

I. Self-organization of network. At this stage all weights are calculated on the basis of input data. The algorithm used for this stage consists of several steps:
   1. Scaling of input data in a way assuring that the length of each data vector is equal to 1, so each of n values of each input data vector is changed:

$$\tilde{x}_{k,w} = \frac{x_{k,w}}{\sqrt{\sum_{i=1}^{n} \left(x_{i,w}\right)^2}} \tag{2}$$

   where
   $x_{k,w}$ — k^{th} coordinate (feature) of w^{th} vector of input data set,
   $\tilde{x}_{k,w}$ — $x_{k,w}$ after change.
   2. Random selecting of all weights $w_{i,j,k}$. It was accepted that each weight is assigned to a random value from the range (0, 0.5) by application of flat probability distribution.

Subsequently, points 3-5 are realized for each input data vector ITER times (where ITER is a parameter accepted in certain moment):

3. For the next w^{th} input data vector, the input values of each neuron are calculated according to formula (1). On the basis of results the winner neuron is accepted, which is the neuron with the highest indicated value.
4. Modification of weights for the winner neuron and its neighbors. The following modification was accepted:

$$\tilde{w}_{i,j,k} = w_{i,j,k} + \eta(x_{k,w} - w_{i,j,k}) \tag{3}$$

where:

$$\eta = \begin{cases} \dfrac{0.01}{dist+1} & \text{for} \quad dist < MAX\_DISTANCE \\ 0 & \quad else \end{cases} \tag{4}$$

where:

$dist$	—	distance in Euclidean metrics of neuron number (i, j) from the winner neuron,
$MAX\_DISTANCE$	—	parameter accepted in a certain moment,
$w_{i,j,k}$	—	weight of k^{th} neuron input of number (i, j),
$\tilde{w}_{i,j,k}$	—	is $w_{i,j,k}$ after change,
$x_{k,w}$	—	is k^{th} coordinate (feature) of w^{th} vector of input data set.

As it can be seen the weights of neurons which are closer than MAX_DISTANCE from the winner neuron are modified. It was accepted that these modifications lower hyperbolically with the distance from the winner neuron.

5. Weight vectors of each neuron which was changed are normalized, which means that:

$$\tilde{w}_{i,j,k} = \frac{w_{i,j,k}}{\sqrt{\sum_{p=1}^{n} \left(w_{i,j,p}\right)^2}} \tag{5}$$

where:

$w_{i,j,k}$ — weight of k^{th} neuron input number (i, j),
$\tilde{w}_{i,j,k}$ — is $w_{i,j,k}$ after change.

II. Projection of image. Points 1-2 are realized for each input data vector:

1. For following w^{th} input data vector the values of every neuron output are calculated (according to formula 1). On the basis of results the neuron which is the winner is found, which means the neuron with the highest output value. Let us accept that this is the neuron numbered (u, v), located in u^{th} line and v^{th} column of the network.
2. It must be examined if the symbol representing fraction other than the fraction of w^{th} data vector was previously drawn in the spot of coordinates (u, v):
   - If yes, it means that the neuron numbered (u, v) represents more than one fraction. This means that a network cannot recognize at least two vectors of data originated from two fractions. This is error and the procedure must be stopped. The network is subjected to further teaching by determining higher ITER value or changing other parameters.

– If not, then in spot (u, v) the symbol representing fraction of w^{th} data vector is being drawn.

In this way the image of neurons representing individual data fractions is created on the computer screen.

4. Experiment results

As part of the research program a computer system was elaborated based on assumptions presented in the previous chapter whose purpose was to visualize seven-dimensional data describing coal. As a result of experiments, it occurred that the best results were obtained by a neural network composed of 40 lines and 40 columns of neurons, which makes up 1600 neurons all together. Figures 2-7 present obtained results. Figure 2 presents the view of answer of a learnt neural network to one of input data vectors representing coal type 31. Brighter spots indicate neurons with higher value occurring on the output and darker spots indicate neurons with lower value occurring on the output. The neuron winner was marked with symbol "x", which means the one with highest indicated value. This result was obtained by determining parameters *MAX_DISTANCE* = 5 and *ITER* = 260. The accepted *MAX_DISTANCE* means that during self-organization the weights of neurons located in the distance lower than 5 from the winner neuron were modified. The accepted *ITER* means that the network self-learning process was conducted for each input data vector 260 times.

After joining such neural network answers for all vectors from the data set, Figure 3 was obtained. It presents the way how neurons divided between themselves the data representing individual

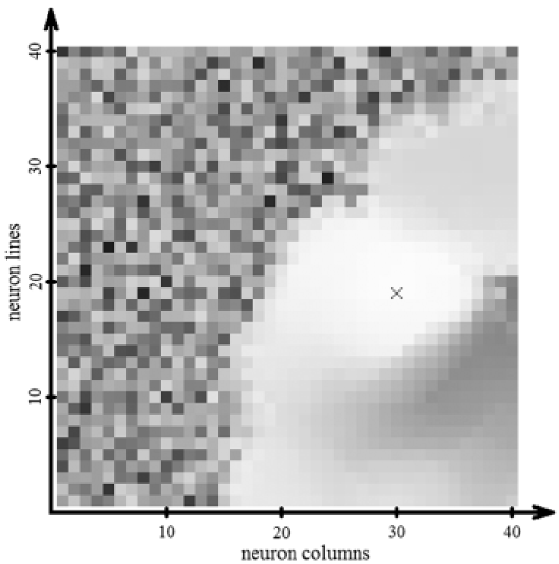

Fig. 2. View of the answer of learnt neural network for one of input data vectors representing coal type 31. Brighter fields mean neurons with higher value occurring on the output and darker fields – lower value. Symbol "x" – the winner neuron

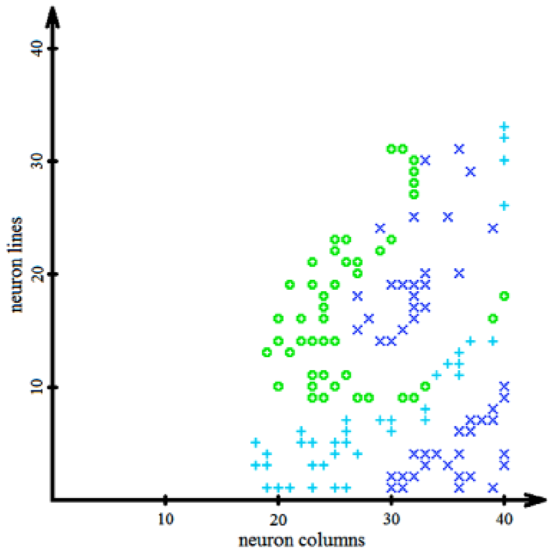

Fig. 3. Neurons' impact on the division of data representing three various types of coal by parameters *MAX_DISTANCE* = 5 and *ITER* = 260. Symbol (×) was used for marking neurons recognizing coal samples, type 31, (+) – coal samples, type 34.2, (○) – coal samples, type 35

types of coals. It can be seen that neurons representing coal samples of certain types aggregate and that these aggregations can be separated. It is worth noticing that the information on data vectors affiliation to certain fractions is not used to self-learning of network (to calculate weights). In this situation the grouping of neurons representing certain fraction depends only on certain properties of this data noticed by the network. For comparison, the way how neurons divided data representing individual types of coals was presented in Figure 4, accepting values of *MAX_DISTANCE* = 4 and *ITER* = 262. It can be noticed that the change of parameters causes a different way of neural network allotment of individual parameters to data representing various types of coal.

With a view to obtaining even clearer results, it was decided to present the same data by means of Kohonen maps in another way. It was verified how the network would assign its neurons for data representing coal types in pairs. Figure 5 presents the way how neurons divided data representing samples of coal type 31 and 34.2. Here, it is even more clear that neurons representing samples of coal 31 aggregate, which can be easily separated from neuron aggregation representing samples of coal, type 34.2. Figure 6 presents the way how neurons divided data representing coal types 34.2 and 35. It can be seen that neuron representing coal samples, type 34.2 gather in clusters which can be easily separated from neuron aggregations representing coal samples, type 35. Figure 7 shows the way how neurons divided data representing samples of coals 31 and 35. It is clearly visible that neurons representing coal samples, type 31 gather in clusters which can be easily separated from neuron aggregations representing coal samples, type 35.

If it is possible to ascertain the possibility of separation of coal samples type 31 from coal samples type 34.5 (Fig. 5), the coal samples type 34.2 from coal samples type 35 (Fig. 6) and coal samples type 34.2 from coal samples type 35 (Fig. 7), then it can be stated that it is possible to separate samples of each type of coal from the others. By application of the multidimensional

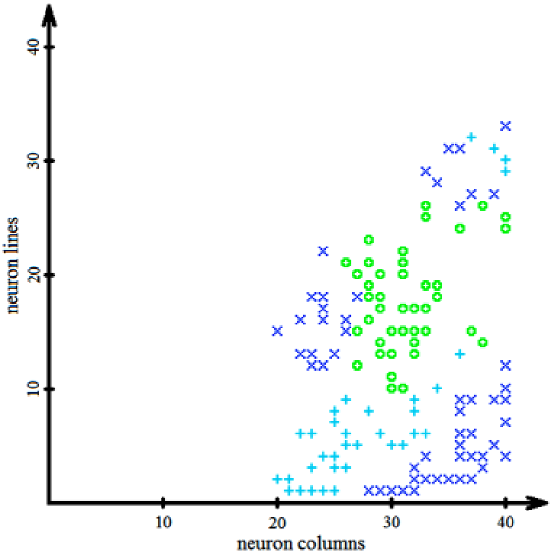

Fig. 4. Neurons' impact on the division of data representing three various types of coal by parameters *MAX_DISTANCE* = 4 and *ITER* = 262. Symbol (×) was used for marking neurons recognizing coal samples, type 31, (+) – coal samples, type 34.2, (○) – coal samples, type 35

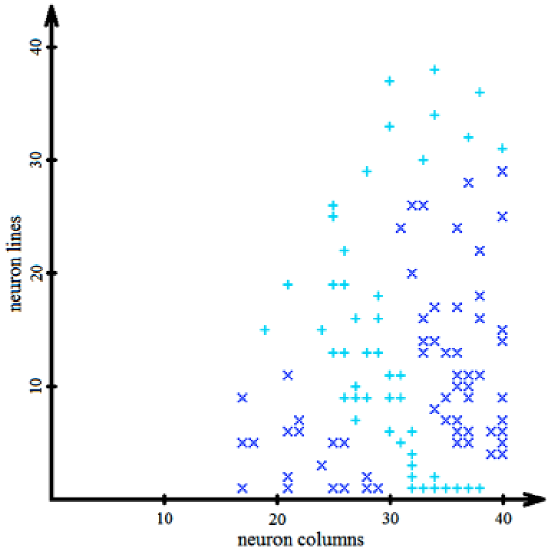

Fig. 5. Neurons' impact on the division of data representing two various types of coal by parameters *MAX_DISTANCE* = 4 and *ITER* = 3050. Symbol (×) was used for marking neurons recognizing coal samples, type 31, (+) – coal samples, type 34.2

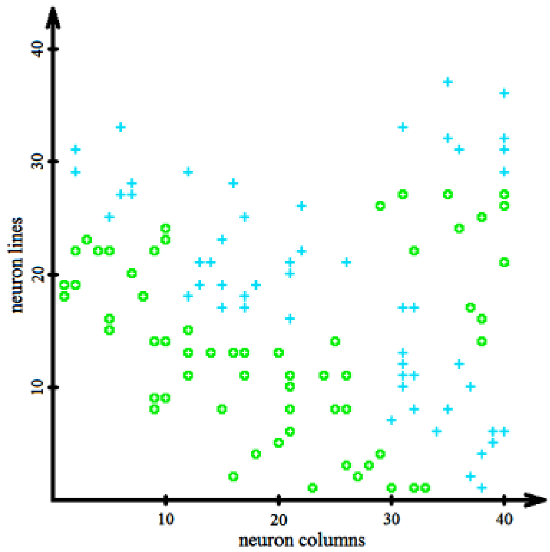

Fig. 6. Neurons' impact on the division of data representing two various types of coal by parameters *MAX_DISTANCE* = 5 and *ITER* = 1300. Symbol (+) was used for marking neurons recognizing coal samples, type 34.2, (○) – coal samples, type 35

data visualization by means of Kohonen map, it can be noticed that information gathered in the analyzed seven-dimensional data describing samples of three types of coal is sufficient for the proper classification.

5. Conclusions

The conducted experiments based on visualization of seven-dimensional data by means of Kohonen map allowed to conclude that:

1. Multidimensional visualization by means of Kohonen map allows to state that information gathered in the analyzed seven-dimensional 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 neurons representing coal samples of certain type gather in aggregations, which can be separated. It indicates that the data contains enough information for the proper classification of coal.
3. The presentation of data representing various coal types in pairs by means of Kohonen map allows to obtain even clearer results.
4. The best results were obtained by means of neural network comprised of 40 lines and 40 columns of neurons, which makes up 1600 neurons all together.
5. The transparency of results is growing with the progress of neural network learning process (growth of the ITER parameter value).
6. The transparency of obtained results depends highly on accepted parameters. A change of these parameters results in a different allotment of individual neurons in the neural network to data representing various types of coal.

7. One of the problems related to such visualization is the necessity of selecting parameters for the purpose of obtaining view which presents the searched information clearly. It is worth mentioning that during the conducted experiments the views obtained by means of neural network of size 10 × 10 till 100 × 100 were provided. The views were obtained from the value of parameter *MAX_DISTANCE* starting from 1 to the limit size of the network and parameter *ITER* starting from 1 to 5000. The experiments were conducted for various patterns determining modification of weights. The results presented in the paper are the clearest from the obtained ones.

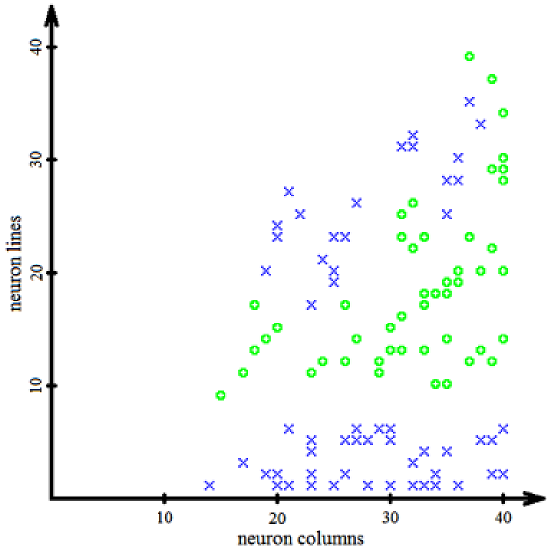

Fig. 7. Neurons' impact on division of data representing two various types of coal by parameters *MAX_DISTANCE* = 6 and *ITER* = 550. Symbol (×) was used for marking the neurons recognizing samples of coal, type 31, (○) – samples of coal, type 35

Acknowledgement

The paper is the result of a scientific project no. *N N524 339040*, agreement no. *3390/B/T02/2011/40*.

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Received: 27 February 2014