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COMPARISON OF SELECTED METHODS OF MULTI-PARAMETER DATA VISUALIZATION USED FOR CLASSIFICATION OF COALS

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Abstract: Methods of multi-parameter data visualization through the transformation of multidimensional space into two-dimensional one allow to present multidimensional data on computer screen, thus making it possible to conduct a qualitative analysis of this data in the most natural way for human – by a sense of sight. In the paper a comparison was made to show the efficiency of selected seven methods of multidimensional visualization and further, to analyze data describing various coal type samples. Each of the methods was verified by checking how precisely a coal type can be classified when a given method is applied. For this purpose, a special criterion was designed to allow an evaluation of the results obtained by means of each of these methods. Detailed information included presentation of methods, elaborated algorithms, accepted parameters for best results as well the results. The framework for the comparison of the analyzed multi-parameter visualization methods includes: observational tunnels method multidimensional scaling MDS, principal component analysis PCA, relevance maps, autoassociative neural networks, Kohonen maps and parallel coordinates method.

Keywords*: multidimensional visualization, observational tunnels method, multidimensional scaling, MDS, principal component analysis, PCA, relevance maps, autoassociative neural networks, Kohonen maps, parallel coordinates method, grained material, coal*

Introduction

Multidimensional analysis of data is becoming an increasingly efficient statistical tool of data analysis. There are several methods of such approach which are being used much more often than in the past because of natural development of informatics. Modern statistical software allows the operator to analyze even huge sets of data

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relatively fast and with adequate precision. There are many books and articles in the field of mineral processing concerning such problems in many aspects such as (Ahmed and Drzymala, 2005; Gawenda et al., 2005; Brozek and Surowiak, 2005; 2007; 2010; Lyman, 1993; Niedoba 2009; 2011; 2013b; Niedoba and Surowiak, 2012; Saramak, 2011; 2013; Snopkowski and Napieraj, 2012; Tumidajski and Saramak, 2009). The precise description of processes and their characteristics may be found in (Drzymala, 2007; 2009). Among multidimensional statistical analysis methods, special attention should be given to multidimensional visualization methods which are the subject of this paper.

Owing to the methods of multidimensional data visualization through the transformation of multidimensional space into two-dimensional, it is possible to show multidimensional 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. Many methods had been used previously for analyzing multidimensional coal data, i.e. observational tunnels method (Niedoba and Jamroz, 2013; Jamroz and Niedoba, 2014), Kohonen network (Jamroz and Niedoba, 2015), multidimensional scaling (Jamroz, 2014b), relevance maps (Niedoba, 2015), PCA (Niedoba, 2014), autoassociative neural networks (Jamroz, 2014c) and parallel coordinates (Niedoba and Jamroz, 2013). Thanks to the above methods, results have been obtained for coal and they have been described in several papers. This paper presents a comparison of the above-mentioned multi-parameter visualization methods.

Apart from multi-parameter methods, there are also several other methods which can be applied to many purposes. These include: grand-tour method (Asimov, 1985), method of principal component analysis (Hotelling, 1933; Jolliffe, 2002), use of neural networks for data visualization (Aldrich, 1998; Jain and Mao, 1992; Kohonen, 1989), parallel coordinates method (Inselberg, 2009), multidimensional scaling (Kruskal, 1964), 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). Furthermore, the visualization of multidimensional solids is also possible (Jamroz, 2001; 2009).

Experiment

Three types of coal, 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 the coal type 31, 61 samples of the coal type 34.2 and 72 samples of the 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/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 type.

Methods

Observational tunnels method

Theoretical grounds of observational tunnels method were described in paper by Jamroz (2001). Intuitively, it may be said that the method of observational tunnels makes use of a parallel projection with a local orthogonal projection of an extent limited by the maximal radius of the tunnel. This solution makes it possible to observe selected parts of a space bearing important information~~,~~ which, for example, is not possible using an orthogonal projection. Detailed information concerning observation tunnels method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Niedoba and Jamroz (2013).

Multidimensional scaling

Multidimensional scaling (MDS) is the method based on mapping of *n*-dimensional space into *m*-dimensional space. It is based on calculation of a distance between each pair of *n*-dimensional points. On the basis of these distances the considered method determines mutual location of these points images in destined *m*-dimensional space. Let d_{ij} mean distance between *n*-dimensional points of no. *i* and *j*. Multidimensional scaling is based on such location of points in *m*-dimensional space that distance D_{ij} calculated in this space between mapped points of no. *i* and *j* is possibly closest to d_{ij}. The operation of algorithm MDS can be based on iterative change of location of randomly (initially) located points in *m*-dimensional space in the way assuring the function $S = \sqrt{\sum_{i>j}\left(D_{ij} - d_{ij}\right)^2}$ achieving the smallest possible value. For *m*=2 this method allows to watch multidimensional data directly on two-dimensional computer screen. Detailed information concerning MDS method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Jamroz (2014b).

Principal Component Analysis

PCA method is one of the statistical methods of factor analysis. It consists of perpendicular projection of multidimensional data on the plane represented by properly selected eigenvectors V_1 and V_2, which are related to the highest eigenvalues of covariance matrix of observational set. The selection of vectors V_1 and V_2 allows to obtain an image on plane representing the biggest number of data changes whose mutual distance is the biggest. Detailed information concerning PCA method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Niedoba (2014).

Relevance maps

Relevance maps method on plane serving for data visualization is based on placing special points called relevance points which represent individual features of the considered object (Assa, 1999). For each feature (coordinate) the relevance point representing this feature is assigned. That means that by seven-dimensional data set 7 such points are placed on plane which represent individual coordinates. The distribution of the points representing presented multidimensional data shows relations between these data and features. The more i^{th} feature is present in a certain object (which means that i^{th} coordinate is higher), the closest the point representing certain object according to relevance representing i^{th} feature (coordinate) should be. Thus, each relevance point representing a certain feature divides the plane into areas more or less dependent on i^{th} feature (more or less distanced from relevance point representing the i^{th} feature). Detailed information concerning relevance maps method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Niedoba (2015).

Autoassociative neural networks

Autoassociative neural networks are an example of self-organizing neural networks whose 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. 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*~~,~~ are 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 start. 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*. Detailed information concerning autoassociative neural networks method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Jamroz (2014c).

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 term of neighborhood 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 teaching series is 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). Detailed information concerning Kohonen maps method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Jamroz and Niedoba (2015).

Parallel Coordinates

In parallel coordinates method, there are n parallel axes located on plane, related to n dimensions of space. One point of space is represented by broken curve. This curve is passing through each i^{th} axis in place related to value of i^{th} coordinate of the point. Detailed information concerning parallel coordinates method, applied algorithm and obtained results for visualization of 7-parameter data describing three coal types were presented in paper by Niedoba and Jamroz (2013).

Results and discussion

As part of previous works, for each of the compared methods a computer program was created to obtain views of analyzed multidimensional data. In this way, seven systems were created. All of them were created by means of C++ language with application of Microsoft Visual Studio. All these methods were described in detail in the authors' previous papers, including detailed information about individual methods, elaborated algorithms and accepted parameters allowing to obtain best results. For the purpose of obtaining clear results, the data representing various coal types were analyzed in pairs. Such an approach made it possible to state if images of points representing various coal samples were located in easily separated areas of the figure or otherwise.

Having results obtained in the previous works, it is possible to compare multidimensional data visualization methods in this paper. For evaluation purposes, it is necessary to test each of the methods by verifying how clearly they allow to state if the amount of information contained in seven coal features is sufficient to classify coal types properly. For this purpose a special criterion must be determined allowing to evaluate the transparency of results. The definition of appropriate criterion is not a simple task. The result of each working program is a view (two-dimensional one) of seven-parameter data describing coal. Here is where the most difficult thing occurs: how to evaluate separated areas of the particular figure when compared to others. Therefore, let us assume that areas of the figure occupied by points representing various coal types will be separated by curve. Furthermore, let us assume that the parameter evaluating the level of complexity of the curve is the number of inflection points. Curve consists of arcs, where arc is the fragment of curve turning in the same direction. Curvature within one arc can change even by transferring into a fragment of straight line. The inflection points are the points connecting arcs turning in various directions. For inflection points determined in this way the second differential is equal to zero. It is assumed that part of the straight line is treated as inflection point only if it connects arcs turning in various directions (although, the second differential for the whole part of line is equal to zero).

The following criterion is accepted: result obtained as the effect of visualization is clearer if the separating curve consists of a lower number of inflection points.

On all figures black spots on curves represent inflection points.

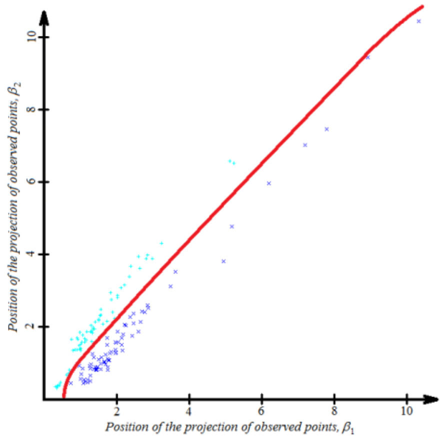

Fig. 1. Curve which separates points representing coal type 31 (x) and coal type 34.2 (+) with application of observational tunnels method. The curve has no inflection points

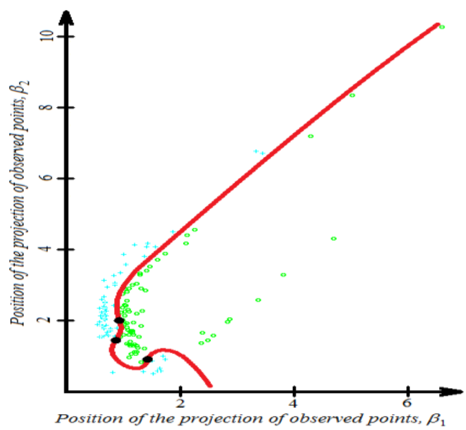

Fig. 2. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of observational tunnels method. The curve has three inflection points

Figures 1-3 present the views of curves obtained for observational tunnels method. These curves separate areas of the figures occupied by images of points representing various coal types. Figure 1 shows that curve separating points of coal type 31 from coal type 34.2 has no inflection points. This is an example of the least complicated curve (best separated areas) for the accepted criterion. Figure 2. shows a situation in which curve separating coal type 34.2 and coal type 35 had 3 inflection points. From Fig. 3 it can be observed that curve separating coal type 31 from coal type 35 has only one inflection point. It means that four inflection points were used to obtain three views allowing to state that each coal type can be separated from each other. This value will be the evaluation of observational tunnels method used to create Figs. 1–3.

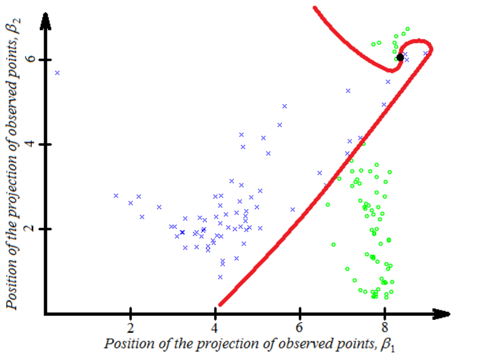

Fig. 3. Curve which separates points representing coal type 31 (x) and coal type 35 (o) with application of observational tunnels method. The curve has one inflection point

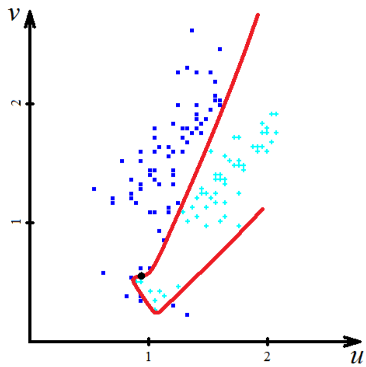

Fig. 4. Curve which separates points representing coal type 31 (■) and coal type 34.2 (+) with application of multidimensional scaling. The curve has one inflection point

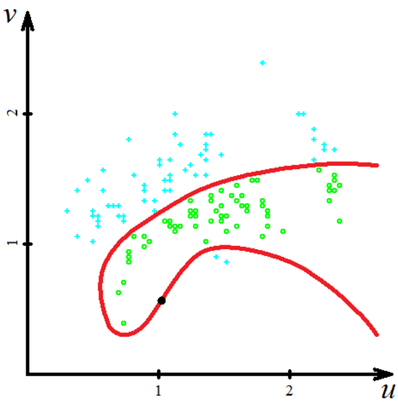

Fig. 5. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of multidimensional scaling. The curve has one inflection point

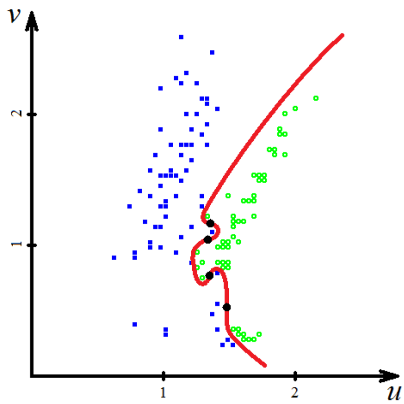

Fig. 6. Curve which separates points representing coal type 31 (■) and coal type 35 (o) with application of multidimensional scaling. Curve has four inflection points

Figures 4–6 present views of curves obtained for multidimensional scaling. Figure 4 shows that curve separating points of coal type 31 from coal type 34.2 has only one inflection point. Figure 5 shows a situation in which curve separating coal type 34.2 and coal type 35 has also 1 inflection point. From Fig. 6 it can be observed that curve separating coal type 31 from coal type 35 has four inflection points. This is an example of a complicated curve for the accepted criterion. It can be noticed that in this case the possibility of separating points which represent various coal types is not so clear as in the case of, for example, Fig. 1. To use multidimensional scaling for obtaining three views that allow to state that each coal type can be separated from others, curves with 6 inflection points have to be used.

Figures from 7 to 9 present views of curves obtained for PCA method. Figure 7 shows that curve separating points of coal type 31 from coal type 34.2 has even five inflection points. Fig. 8 shows a situation in which curve separating coal type 34.2 and coal type 35 had four inflection points. From Fig. 9 it can be observed that curve separating coal type 31 from coal type 35 had also 4 inflection points. To obtain three views allowing to state that each coal type can be separated from others with the use of PCA method, curves containing a total of 13 inflection points were used.

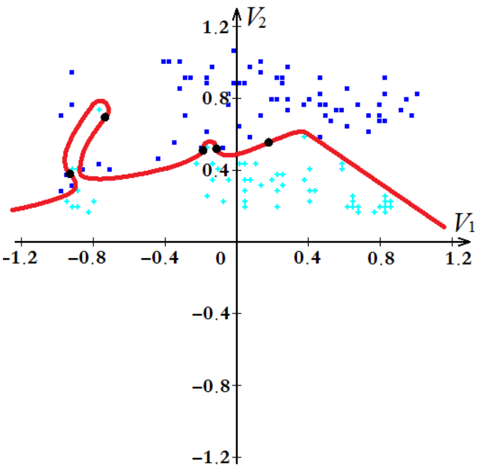

Fig. 7. Curve which separates points representing coal type 31 (■) and coal type 34.2 (+) with application of PCA method. The curve has five inflection points

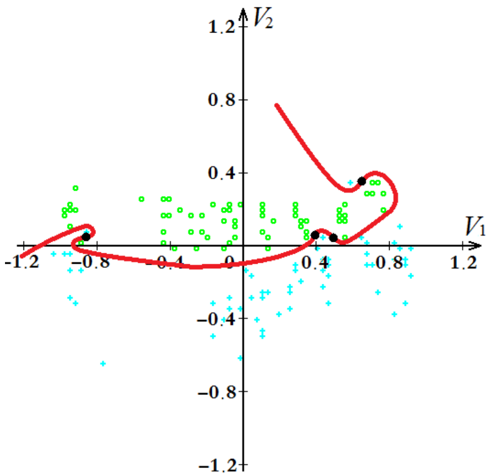

Fig. 8. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of PCA method. The curve has four inflection points

Figure 10 presents, only for additional information, graph with sorted absolute values of covariance matrix eigenvalues. Eigenvectors related to the largest eigenvalues were used to construct Figs. 7, 8 and 9. In general case, it is possible to evaluate efficiency of PCA method on the basis of these eigenvalues distributions – how much information would be preserved during n-dimensional space mapping into the space determined by k eigenvectors related to k biggest absolute values of covariance matrix eigenvalues obtained by means of PCA method. As it can be seen in the Fig. 10 two first eigenvalues for all three coal pairs are much bigger than the others. So, it can be stated that majority of the information is mapped on two-dimensional figures presented above which were created as the result of projecting data on two appropriate eigenvectors.

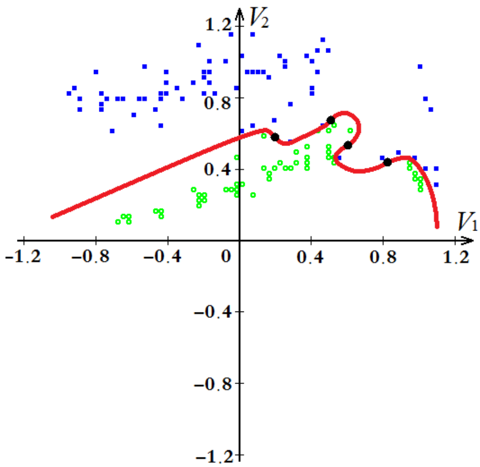

Fig. 9. Curve which separates points representing coal type 31 (■) and coal type 35 (o) with application of PCA method. The curve has four inflection points

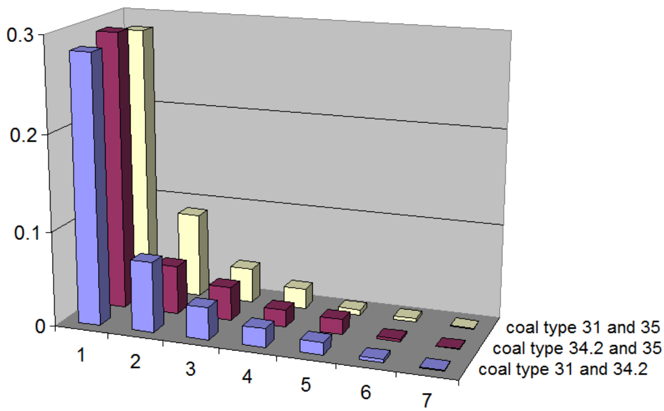

Fig. 10. Sorted absolute values of covariance matrix eigenvalues calculated for data being source for Figs 7-9

Figures 11–13 present views of curves obtained for the relevance maps method. Figure 11 shows that curve separating points of coal type 31 from coal type 34.2 has three inflection points. Figure 12 shows a situation in which curve separating coal type 34.2 and coal type 35 has four inflection points. From Fig. 13 it can be observed that curve separating coal type 31 from coal type 35 has four inflection points. To obtain three views allowing to state that each coal type can be separated from others with the use of relevance maps, curves containing a total of 11 inflection points were used.

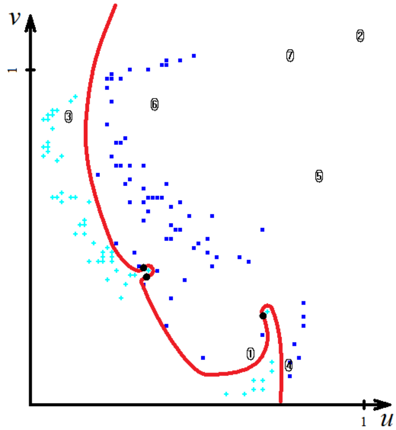

Fig. 11. Curve which separates points representing coal type 31 (■) and coal type 34.2 (+) with application of relevance maps. The curve has three inflection points

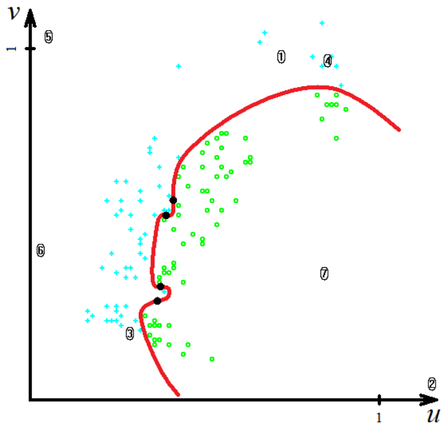

Fig. 12. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of relevance maps. The curve has four inflection points

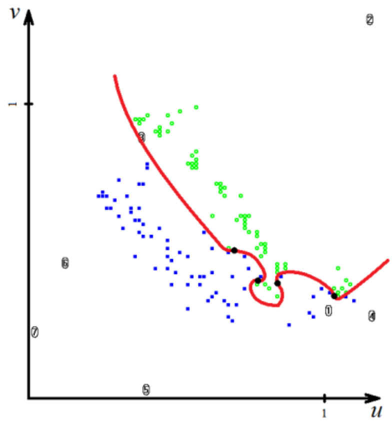

Fig. 13. Curve which separates points representing coal type 31 (■) and coal type 35 (o) with application of relevance maps. The curve has four inflection points

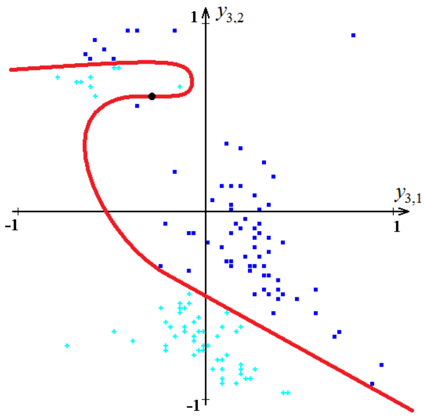

Fig. 14. Curve which separates points representing coal type 31 (■) and coal type 34.2 (+) with application of autoassociative neural networks. The curve has one inflection point

Figures 14–16 present views of curves obtained for autoassociative neural networks. Figure 14 shows that curve separating points of coal type 31 from coal type 34.2 has only one inflection point. Figure 15 shows a situation in which curve separating coal type 34.2 from coal type 35 has no inflection points. From Fig. 16 it can be observed that curve separating coal type 31 and coal type 35 has 2 inflection points. To obtain three views allowing to state that each coal type can be separated from others with the use of autoassociative neural networks, curves containing a total of 3 inflection points were used. These curves gave the best result. Visualization by means of autoassociative neural networks allows to obtain the clearest results.

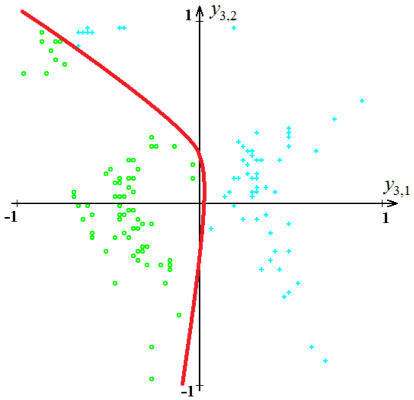

Fig. 15. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of autoassociative neural networks. The curve has no inflection points

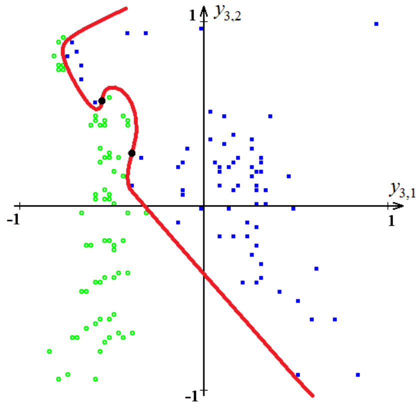

Fig. 16. Curve which separates points representing coal type 31 (■) and coal type 35 (o) with application of autoassociative neural networks. The curve has two inflection points

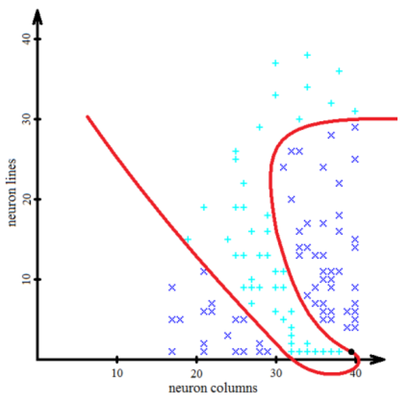

Fig. 17. Curve which separates points representing coal type 31 (x) and coal type 34.2 (+) with application of Kohonen maps. The curve has one inflection point

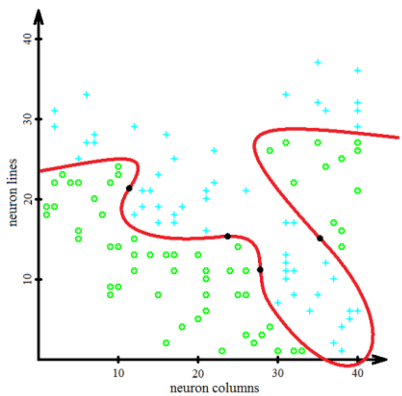

Fig. 18. Curve which separates points representing coal type 34.2 (+) and coal type 35 (o) with application of Kohonen maps. The curve has four inflection points

Figures 17–19 present views of curves obtained for Kohonen maps. Figure 17 shows that curve separating points of coal type 31 from coal type 34.2 has only one inflection point. Figure 18 presents a situation in which curve separating coal type

34.2 and coal type 35 has 4 inflection points. From Fig. 19 it can be observed that curve separating coal type 31 from coal type 35 has three inflection points. To obtain three views allowing to state that each coal type can be separated from others with the use of Kohonen maps, curves containing a total of 8 inflection points were used.

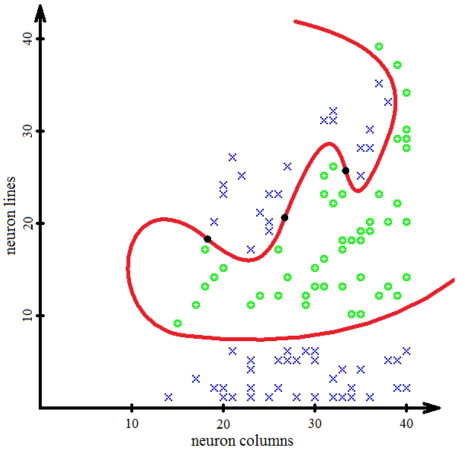

Fig. 19. Curve which separates points representing coal type 31 (x) and coal type 35 (o) with application of Kohonen maps. The curve has three inflection points

The visualization of analyzed coal samples by means of parallel coordinates method did not allow to conclude that 7-parameter data, the subject of analysis, was sufficient to classify coal types properly (Niedoba and Jamroz, 2013). It means that this method cannot be used efficiently for analyses concerning coal samples.

Table 1 contains the juxtaposition of obtained results for the seven analyzed methods of multidimensional visualization. Column "View 31/34.2" presents a number of inflection points for curves separating images of points representing coal types 31 and 34.2. The clearest result for these two coal types was obtained by means of observational tunnels method (no inflection points). Column "View 34.2/35" presents a number of inflection points for curves separating images of points representing coal types 34.2 and 35. The clearest view in this case was obtained by means of autoassociative neural networks (no inflection points). Column "View 31/35" presents a number of inflection points for curves separating images of points representing coal types 31 and 35. The clearest result comparing these two types of coal was obtained by means of observational tunnels method (one inflection point). The last column shows the sum of inflection points indicated in the previous columns.

Finally, the autoassociative neural networks method with result of only 3 inflection points gives the best outcome. The worst outcome gave parallel coordinates method – on the basis of obtained views it was not possible to separate analyzed points representing various coal types. That is why this method was rejected from further analyses. Among methods allowing to obtain appropriate results, the worst was PCA method with the result of 13 inflection points all together.

Table 1. Final ranking of the compared multi-parameter visualization methods. For each method, a number of inflection points was indicated for curves separating images of points representing various coal types. Additionally, the sum of curves' inflection points from three views was presented

Location	Method	View 31/34.2	View 34.2/35	View 31/35	Sum
1	Autoassociative neural networks	1	0	2	3
2	Observational tunnels	0	3	1	4
3	Multidimensional scaling	1	1	4	6
4	Kohonen maps	1	4	3	8
5	Relevance maps	3	4	4	11
6	Principal component analysis	5	4	4	13
7	Parallel coordinates	Inefficient method			

While comparing visualization methods it is worth mentioning an additional fact. Almost all of the analyzed methods required a personal interference of the operator in the process of obtaining the clearest views. Particularly, it was based on the choice of appropriate parameters, randomization of initial random values and stopping algorithm when clear results were obtained. The exception was PCA method which does not require any interference of the operator during creation of multi-parameter data view.

Additionally, two of the described methods should be highlighted as the most efficients ones –these are autoassociative neural networks and Kohonen maps. Only these two methods allowed to obtain clear results showing on one figure the possibility of separating all three analyzed coal types (Jamroz, 2014c; Jamroz and Niedoba, 2015). In such cases views for pairs of coal types were given for better transparency.

Worth paying attention is the fact that multidimensional visualization can be used in 3D (Bondarev et al., 2011). However, in this case to observe data on the screen it is necessary to make projection from 3D into 2D (even three-dimensional screen is always flat). Thus, it requires additional observation of the obtained 3D data from various sides which are not always clear for each observation angle. The methods presented in the paper allow directly to notice some important features without any additional analysis by 2D projections – all what is needed is to observe and get result. It happens because the observer uses his most natural mechanism – sense of sight. Indeed, it is then connection between visualization methods creating two-dimensional figures and human personal neural network – brain, which analyzes this figures by sense of sight.

The criterion accepted in the paper which determines clearness of space division by samples representing various coal types is not the only possible one. Authors considered also possibility of evaluating clearness of figure division by means of broken line constructed from intervals. However, in this case there were situations which require complicated broken line, constructed from many intervals to obtain visually clear results. The interesting alternative could be also division of space with application of principal curves (Einbeck et al., 2007). The efficiency of such approach in practice should be verified.

Conclusions

As a result of conducted analysis of seven methods of multidimensional visualization used for evaluating the possibility of efficient classification of 7-parameter coal samples, the following conclusions can be drawn.

1. The criterion introduced to analysis allowed to evaluate the transparency of obtained results by individual methods of multidimensional visualization.
2. The autoassociative neural networks method turned out to be the best. Furthermore, this method showed in the most effective manner the possibility of separating points representing coal type 34.2 and coal type 35.
3. The clearest possibility of separating points representing coal type 31 and coal type 34.2 was presented by observational tunnels method. Also, this method presented in the most effective manner the possibility of separating points representing coal type 31 and coal type 35.
4. The worst method was parallel coordinates method – on the basis of obtained views, it was impossible to state whether the separation of points representing individual coal types is possible or not.
5. Among methods which allowed to obtain appropriate results the worst was PCA method.
6. Only the PCA method did not require any interference of the operator during creation of multidimensional data view. The other methods required such interference by choosing appropriate parameters, randomization of initial random values and stopping algorithm when clear results were obtained.
7. Only two of the tested methods: autoassociative neural networks and Kohonen maps allowed to obtain clear views, showing the possibility of separating all three coal types on one figure (Jamroz, 2014c; Jamroz and Niedoba, 2015). In such cases, views for pairs of coal types were obtained additionally only to increase the image quality.

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