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MULTI-PARAMETER DATA VISUALIZATION BY MEANS OF PRINCIPAL COMPONENT ANALYSIS (PCA) IN QUALITATIVE EVALUATION OF VARIOUS COAL TYPES

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Abstract: Multi-parameter data visualization methods are a modern tool allowing to classify some analyzed objects. When it comes to grained materials, e.g. coal, many characteristics have an influence on the material quality. Besides the most obvious features like particle size, particle density or ash contents, coal has many other qualities which show significant differences between the studied types of material. The paper presents the possibility of applying visualization techniques for coal type identification and determination of significant differences between various types of coal. The Principal Component Analysis was applied to achieve this purpose. Three types of coal 31, 34.2 and 35 (according to Polish classification of coal types) were investigated, which were initially screened on sieves and subsequently divided into density fractions. Next, each size-density fraction was analyzed chemically to obtain other characteristics. It was pointed out that the applied methodology allowed to identify certain coal types efficiently, which makes it useful as a qualitative criterion for grained materials. However, it was impossible to provide such identification based on contrastive comparisons of all three types of coal. The presented methodology is a new way of analyzing data concerning widely understood mineral processing.

Keywords: *Principal Component Analysis, PCA, multi-parameter data visualization, coal, identification of data, covariance matrix, pattern recognition*

Introduction

In mineral processing operations particle properties influence processing results (Drzymala, 2009; Kelly and Spottiswood, 1989). In the case of coal the most important parameters are size and density. But it is often not enough to classify coal type properly. In modern statistical research there is often a need of applying multi-parameter (called also as multidimensional) statistical methods. A simple regressive analysis is not enough in more complex cases (Brozek and Surowiak, 2005; 2007, 2010). That is why many new techniques are introduced in scientific works. Of course,

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there are many methods connected with regressive equations (Gawenda et al., 2005; Lyman, 1993; Niedoba, 2009; 2011; 2013a; 2013b; Niedoba and Surowiak, 2012; Saramak, 2011; 2013; Snopkowski and Napieraj, 2012; Tumidajski, 1997; Tumidajski and Saramak, 2009) or even fractals (Ahmed and Drzymala, 2005) but many methods of data-mining are also in use. A special type of statistical analysis involves multi-parameter data visualization methods geared towards recognizing differences and similarities between analyzed sets of data. Finding these differences is often a very important issue in mineral processing, where processes depend on many material features.

The qualitative analysis of multi-parameter data (properties of material) obtained from the results of empirical experiments can be carried out by applying the multi-parameter visualization method. The results of analyses can be helpful thanks to the characteristics of materials as well as the development of mineral processing models based on this data. Attempts to depict multi-parameter 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), use of neural networks for data visualization (Aldrich, 1998; Jain and Mao, 1992; Kraaijveld et al., 1995), parallel coordinates method (Chatterjee et al., 1993; Chou et al., 1999; Gennings et al., 1999; Inselberg, 1985), star graph method (Sobol and 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 (Jamroz, 2001; 2009). The observational tunnels method (Jamroz, 2001; 2014) makes it possible to obtain an external view of the observed multi-parameter sets of points using tunnel radius introduced by the present author (Jamroz and Niedoba, 2014; Niedoba and Jamroz, 2013).

The use of methods of multi-parameter data visualization by transformation of multidimensional space into two-dimensional space makes it possible to show multi-parameter data on computer screen. This allows to conduct a qualitative data analysis in the most natural way for human with a sense of sight. One of such methods is the Principal Component Analysis (PCA). It was used in the work 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 coals). It was decided to check whether this method allows to state that an amount of information contained in seven coal features is sufficient for the proper classification of coal types. The application of various methods for analyzing possibilities of recognition of various coal properties is becoming an increasingly interesting issue. Earlier, other visualization methods were applied, including the observational tunnels method (Jamroz and Niedoba, 2013; 2014). An application of the PCA method for this purpose is a new way of approaching the subject.

Material 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 (Olejnik et al., 2010). The classification of coal types can be found in (Drzymala, 2009). The coals originated from three various Polish 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. Subsequently, 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 framework for further consideration and additional coal features were determined by means of chemical analysis. For each density-size fraction the following parameters were determined: combustion heat, ash contents, sulfur contents, volatile parts contents and analytical moisture, making up, together with the mass of these fractions, seven various features for each coal. The examples of such data were presented in Table 1 containing the data for size fractions of 14.00-12.50 mm for each type of coal. The complete data can be found in Niedoba (2013a).

Principal Component Analysis

Method description

The PCA method is one of statistical methods of factor analysis. It consists of perpendicular projection of multi-parameter 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 greatest number of data changes whose mutual distance is the biggest (Li et al., 2000).

Algorithm

A set of input data consists of parts described by n of features. It can be then treated as a set of n-dimensional vectors. Let us mark the vector of input data as $x_k=(x_{k,1}, x_{k,2}, \ldots x_{k,n})$. The algorithm performing visualization by means of PCA consists of several steps:

- scaling of initial data. Individual features represented by individual data dimensions are scaled in the way ensuring their compliance with the same selected range. In this paper, the individual coordinates (features) of data set vectors were scaled to the range (0, 1),

Table 1. Data for size fractions of 14.00-12.50 mm for all three types of coal

Coal type 31						
Density [Mg/m^3]	Mass [g]	Combustion heat [kJ]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	308.6	29.51	6.41	0.72	34.32	3.23
1.3–1.4	292.5	24.53	19.61	0.7	29.22	3.36
1.4–1.5	36.1	12.34	16.55	0.76	28.92	3.87
1.5–1.6	10.7	21.42	26.10	1.55	31.08	3.40
1.6–1.7	25.6	18.70	35.78	2.28	26.71	2.40
1.7–1.8	139	16.41	37.20	1.23	29.24	2.19
1.8–1.9	12.7	12.89	48.20	1.13	24.05	2.23
>1.9	601.2	1.91	86.53	0.40	9.30	0.91
Coal type 34.2						
Density [Mg/m^3]	Mass [g]	Combustion heat [kJ]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	360.5	34.44	2	0.32	28.96	1.04
1.3–1.4	57	32.02	7.67	0.71	24.16	1.87
1.4–1.5	25.5	28.89	15.33	0.83	24.58	1.34
1.5–1.6	12.2	24.27	33.73	0.17	27.85	0.95
1.6–1.7	3.2	20.22	34.3	0.34	no data	no data
1.7–1.8	15	17.38	36.15	0.34	27.93	0.37
1.8–1.9	3.6	18.48	27	0.05	31.75	1.01
>1.9	68.9	2.90	79.33	0.91	12.08	0.52
Coal type 35						
Density [Mg/m^3]	Mass [g]	Combustion heat [kJ]	Ash contents [%]	Sulfur contents [%]	Volatile parts contents V^a	Analytical moisture W_a
<1.3	268.7	34.86	2.38	0.28	20.28	1.45
1.3–1.4	89.3	31.86	8.97	0.36	20.10	1.21
1.4–1.5	39.8	27.49	19.61	0.56	18.83	1.28
1.5–1.6	22.0	21.06	35.68	0.39	16.22	1.32
1.6–1.7	25.7	20.88	34.62	1.26	19.42	1.47
1.7–1.8	29.0	19.21	40.60	0.38	18.86	1.61
1.8–1.9	28.1	13.76	52.24	1.14	17.95	1.51
>1.9	589.5	2.94	80.57	0.20	10.84	1.37

- calculation of covariance matrix. The general formula for covariance was used:

$$\mathrm{cov}(X,Y) = E(X \cdot Y) - E(X) \cdot E(Y) \tag{1}$$

where E is the expected value. First, the expected values are calculated:

$$E_i = \frac{\sum_{k=1}^{m} x_{k,i}}{m} \tag{2}$$

and

$$E_{i,j} = \frac{\sum_{k=1}^{m} x_{k,i} x_{k,j}}{m} \tag{3}$$

where, E_i – expected value of i^{th} coordinate of input data, $E_{i,j}$ – expected value of product of i^{th} and j^{th} coordinate of input data, m – number of vectors of input data, $x_{k,i}$ – i^{th} coordinate of k^{th} vector of input data. If the covariance matrix is marked as A, then each element of the matrix a_{ij} is calculated as:

$$a_{ij} = E_{i,j} - E_i E_j \,. \tag{4}$$

In this way, the symmetrical covariance matrix of input data set is obtained,

- calculation of eigenvalues and eigenvectors of covariance matrix. For numerical calculations the Jacobi method was selected. It draws upon the fact that orthogonal transformation does not change own values and vectors of matrix. Consequently, it is possible to perform a set of orthogonal transformations on matrix A to conduct it to diagonal form D:

$$A = W \cdot D \cdot W^T \,. \tag{5}$$

In the diagonal matrix the eigenvalues are located on the main diagonal while the related eigenvectors are located in columns of matrix W. Matrices D and W which fulfill Eq. 5 by means of the Jacobi method can be achieved in the following steps:

1. as matrix W the identity matrix of dimension nxn is accepted,
2. as matrix A covariance matrix of dimension nxn is accepted, calculated according to equation (4),
3. the main element is selected apart from the main diagonal of matrix A, which is the element of the highest module value not located on the main diagonal. The location of this element in the matrix is searched, so coordinates p and q must be found fulfilling the condition:

$$\forall i, j = 1,\ldots,n \text{ and } i \neq j \text{ is} : \left|a_{pq}\right| \geq \left|a_{ij}\right|, \tag{6}$$

4. the values *c* and *s* are calculated using the following formulas:

$$r = \frac{a_{qq} - a_{pp}}{2a_{pq}} \tag{7}$$

$$t = \frac{\operatorname{sgn}(r)}{|r| + \sqrt{r^2 + 1}} \tag{8}$$

where: a_{ij} is an element of the matrix from i^{th} line and j^{th} column, sgn(r) = 1 for r>=0 and sgn(r) = –1 for $r < 0$. Next, the calculations are performed according to formulas (9) and (10):

$$c = \frac{1}{\sqrt{t^2 + 1}} \tag{9}$$

and

$$s = tc \tag{10}$$

1. having applied calculated values *c* and *s*, matrix *B* is created ensuring identity matrix of dimension *nxn* in which four elements are changed: $b_{pp} = c$, $b_{qq} = c$, $b_{pq} = s$ and $b_{qp} = -s$,
2. the new value of matrix *A* is assigned by application of previous value of matrix *A*, matrix *B* created in the previous step and transposition matrix *B*:

$$A := B^T \cdot A \cdot B, \tag{11}$$

3. the new value of matrix *W* is assigned by application of previous value of matrix *W* and matrix *B* created in step 5.

$$W := W \cdot B, \tag{12}$$

4. it is checked whether the matrix *A*, obtained as a result of transformations, is a diagonal matrix according to previously accepted preciseness of calculations ε, so:

$$\frac{\max\limits_{i,j=1,\ldots,n \wedge i \neq j} \left|a_{ij}\right|}{\max\limits_{i=1,\ldots,n} \left|a_{ii}\right|} < \varepsilon. \tag{13}$$

For experiments described in section 3, $\varepsilon = 0.000001$ was accepted. If inequality (13) is not fulfilled, a return to step 3 is required and calculations are continued. In

other case, the obtained matrix A is diagonal. The situation described by Eq. 5 is achieved in this way. That means that the eigenvalues of output matrix are located on the main diagonal of obtained matrix A and the eigenvectors related to these values occur in columns of obtained matrix W,

- the determination of two coordinate axes. Two eigenvectors related to two biggest module eigenvalues of covariance matrix are selected from vectors calculated in stage C. Let us mark them as $V_1 = (v_{1,1}, v_{1,2}, \ldots v_{1,n})$, $V_2 = (v_{2,1}, v_{2,2}, \ldots v_{2,n})$. In this way two coordinates axes are obtained on which all data will be projected,
- drawing the set of points on screen. For each point x_k two coordinates are calculated $(\tilde{x}_{k,1}, \tilde{x}_{k,2})$ preceded by their projection on axes V_1 and V_2, which means:

$$\tilde{x}_{k,1} = \sum_{i=1}^{n} v_{1,i} x_{k,i} \tag{14}$$

$$\tilde{x}_{k,2} = \sum_{i=1}^{n} v_{2,i} x_{k,i} \ . \tag{15}$$

As a result, the image of each vector can be presented on computer screen. It is achieved by drawing on the screen a symbol, in place of coordinates $(\tilde{x}_{k,1}, \tilde{x}_{k,2})$, representing fraction to which the related data vector x_k belongs. In this way the image of multidimensional points representing various coal types is created on the computer screen.

Results of experiment

As part of the investigation, for the purpose of visualizing seven-parameter data describing various coal types, a computer program was created based on assumptions presented in the previous chapter. The obtained results were presented in Figs 1-4. The views show a transformation of seven-parameter data by means of PCA into two dimensions. The visualization algorithm in PCA, despite reduction to only two dimensions, has been organized to ensure the view representing the biggest number of data changes whose mutual distance is the biggest. In this way it is possible to see significant features of seven-parameter data on the computer screen.

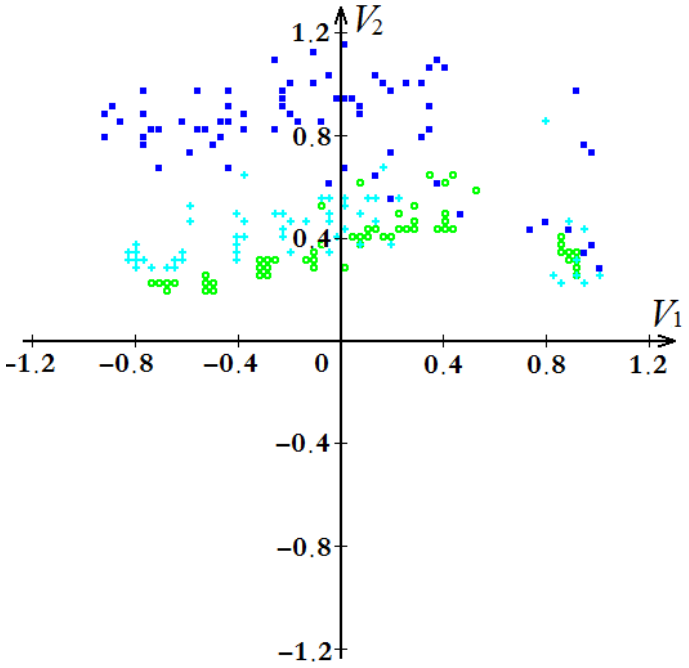

Fig. 1. View of seven-parameter data representing three various types of coal. Images of points representing coal, type 31 were marked with (■), (+) – samples of coal type 34.2, (o) – samples of coal type 35.

Figure 1 presents obtained view of points representing seven-parameter data vectors that describe three various coal types: 31, 34.2 and 35. In order to obtain it, the system calculated the covariance matrix:

$$\mathrm{cov} = \begin{bmatrix} 0.0834 & -0.0101 & -0.0773 & 0.0751 & 0.0162 & -0.0419 & -0.0151 \\ -0.0101 & 0.0241 & 0.0057 & -0.0056 & -0.0049 & 0.0049 & 0.0062 \\ -0.0773 & 0.0057 & 0.0810 & -0.0771 & -0.0135 & 0.0418 & 0.0079 \\ 0.0751 & -0.0056 & -0.0771 & 0.0770 & 0.0097 & -0.0473 & -0.0148 \\ 0.0162 & -0.0049 & -0.0135 & 0.0097 & 0.0438 & 0.0074 & 0.0150 \\ -0.0419 & 0.0049 & 0.0418 & -0.0473 & 0.0074 & 0.0545 & 0.0245 \\ -0.0151 & 0.0062 & 0.0079 & -0.0148 & 0.0150 & 0.0245 & 0.0396 \end{bmatrix}.$$

Furthermore, eigenvectors were calculated:

$$V_1 = (0.5401, -0.0589, -0.5340, 0.5307, 0.0763, -0.3425, -0.1225),$$

$$V_2 = (0.1289, 0.0025, -0.1631, 0.0202, 0.6594, 0.4273, 0.5822).$$

In the above Figure, it is clearly visible that images of data points representing coal samples of a certain type gather in separated subareas and create clusters. It can be noticed that almost on the whole area of the Figure these clusters can be separated. In some parts of the space, however, the images of points representing various coal types overlap. Therefore, according to Figure 1, it is impossible to state that the analyzed data allow to classify coal types properly.

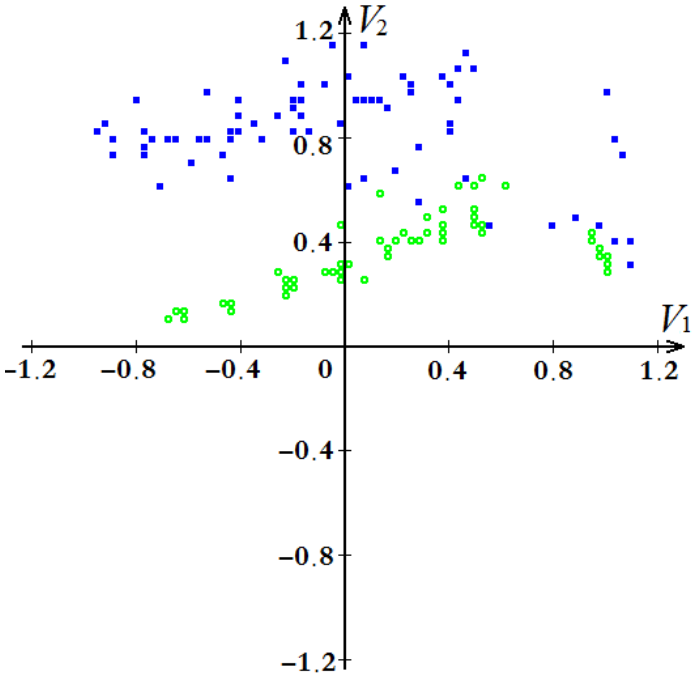

Fig. 2. View of seven-parameter data representing two various types of coal. Images of points representing coal type 31 were marked with (■), (o) – samples of coal type 35.

With a view to achieving clearer results, it was decided to present this data by means of the PCA method in some other way. A decision was made to analyze the data representing various types of coal in pairs. Figure 2 shows the view obtained for data representing coal types 31 and 35. In order to obtain this view, the system calculated the covariance matrix:

$$\mathrm{cov} = \begin{bmatrix} 0.1071 & -0.0115 & -0.0827 & 0.0842 & 0.0214 & -0.0466 & -0.0261 \\ -0.0115 & 0.0305 & 0.0053 & -0.0056 & -0.0077 & 0.0068 & 0.0056 \\ -0.0827 & 0.0053 & 0.0731 & -0.0719 & -0.0144 & 0.0351 & 0.0149 \\ 0.0842 & -0.0056 & -0.0719 & 0.0746 & 0.0095 & -0.0445 & -0.0251 \\ 0.0214 & -0.0077 & -0.0144 & 0.0095 & 0.0508 & 0.0159 & 0.0152 \\ -0.0466 & 0.0068 & 0.0351 & -0.0445 & 0.0159 & 0.0564 & 0.0453 \\ -0.0261 & 0.0056 & 0.0149 & -0.0251 & 0.0152 & 0.0453 & 0.0498 \end{bmatrix}.$$

Furthermore, eigenvectors were calculated:

V_1 = (0.5936, -0.0637, -0.4798, 0.5031, 0.0701, -0.3325, -0.2116),

V_2 = (0.1948, -0.0316, -0.1952, 0.0507, 0.6128, 0.4902, 0.5519).

In Figure 2 it is clearly visible that images of points representing samples of coal type 31 gather in clusters, which can be easily separated from clusters of points representing coal type 35. In Figure 3 the view obtained for data representing coal types 34.2 and 35 is presented. Also, in this case it is clearly visible that images of points representing samples of coal type 34.2 gather in clusters, which can be easily separated from clusters of points representing samples of coal type 35. The covariance matrix obtained from the creation of this Figure is as follows:

$$\mathrm{cov} = \begin{bmatrix} 0.0840 & -0.0101 & -0.0851 & 0.0811 & 0.0111 & -0.0440 & -0.0021 \\ -0.0101 & 0.0222 & 0.0059 & -0.0046 & -0.0083 & -0.0007 & 0.0007 \\ -0.0851 & 0.0059 & 0.0922 & -0.0886 & -0.0059 & 0.0523 & 0.0028 \\ 0.0811 & -0.0046 & -0.0886 & 0.0868 & 0.0055 & -0.0542 & -0.0005 \\ 0.0111 & -0.0083 & -0.0059 & 0.0055 & 0.0278 & -0.0010 & 0.0015 \\ -0.0440 & -0.0007 & 0.0523 & -0.0542 & -0.0010 & 0.0650 & -0.0143 \\ -0.0021 & 0.0007 & 0.0028 & -0.0005 & 0.0015 & -0.0143 & 0.0374 \end{bmatrix}.$$

Its eigenvectors are as following:

V_1 = (-0.5174, 0.0414, 0.5554, -0.5404, -0.0480, 0.3575, -0.0090),

V_2 = (-0.2219, 0.1868, 0.1310, -0.0412, -0.1434, -0.6099, 0.7102).

Furthermore, Fig. 4 shows the view obtained for data representing coal types 31 and 34.2. It can be easily noticed that images of points representing samples of coal type 31 gather in clusters which can be easily separated from clusters of points representing samples of coal type 34.2. In this case the covariance matrix is as follows:

$$\mathrm{cov} = \begin{bmatrix} 0.0840 & -0.0121 & -0.0763 & 0.0745 & 0.0208 & -0.0494 & -0.0246 \\ -0.0121 & 0.0256 & 0.0080 & -0.0081 & -0.0037 & 0.0080 & 0.0103 \\ -0.0763 & 0.0080 & 0.0805 & -0.0770 & -0.0178 & 0.0518 & 0.0149 \\ 0.0745 & -0.0081 & -0.0770 & 0.0778 & 0.0149 & -0.0551 & -0.0227 \\ 0.0208 & -0.0037 & -0.0178 & 0.0149 & 0.0536 & -0.0020 & 0.0161 \\ -0.0494 & 0.0080 & 0.0518 & -0.0551 & -0.0020 & 0.0513 & 0.0254 \\ -0.0246 & 0.0103 & 0.0149 & -0.0227 & 0.0161 & 0.0254 & 0.0543 \end{bmatrix}.$$

The eigenvectors are:

V_1 = (-0.5243, 0.0776, 0.5169, -0.5167, -0.1134, 0.3743, 0.1788),

V_2 = (0.0762, 0.0760, -0.1317, 0.0184, 0.7040, 0.1959, 0.6608).

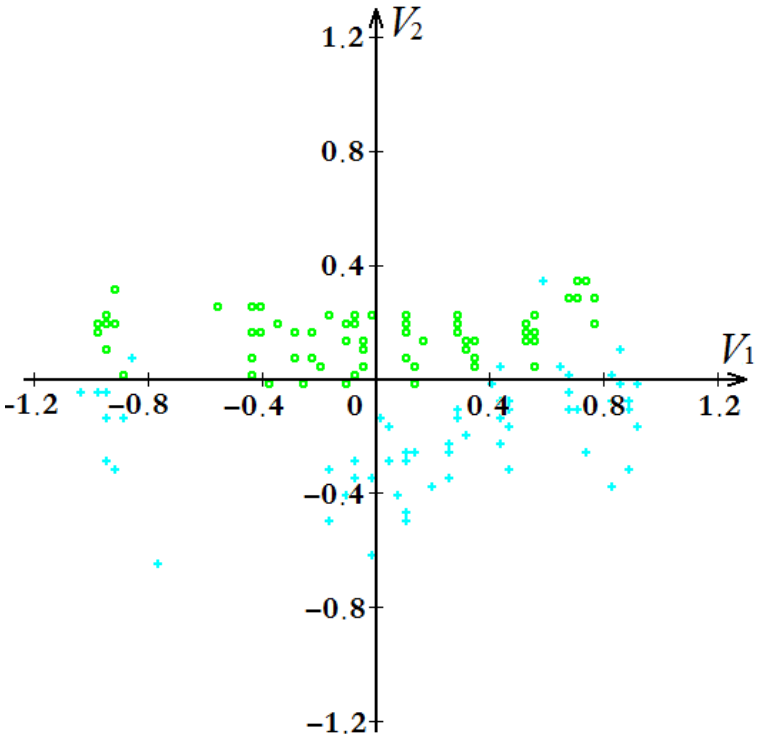

Fig. 3. View of seven-parameter data representing three various types of coal. Images of points representing coal type 34.2 were marked with (+), (o) – samples of coal type 35.

If we can state that the distinction of coal type 31 samples from coal type 35 samples is possible (Fig. 2) and we can state that the distinction of coal type 34.2

samples from coal type 35 samples is possible (Fig. 3), as well the distinction of coal type 31 samples from coal type 34.2 samples is possible (Fig. 4), then the possibility of distinction of samples of each of the three coal types is confirmed. Thanks to the visualization of multi-parameter data by means of PCA, it is possible to state that information covered in seven-parameter data describing samples of three types of coal is sufficient for its proper classification.

It is worth paying attention to the fact that the algorithm of visualization by means of PCA does not use the information of affiliation of points representing data to certain fractions. In this situation grouping of points representing certain fraction depends only on some properties of data noticed by the algorithm.

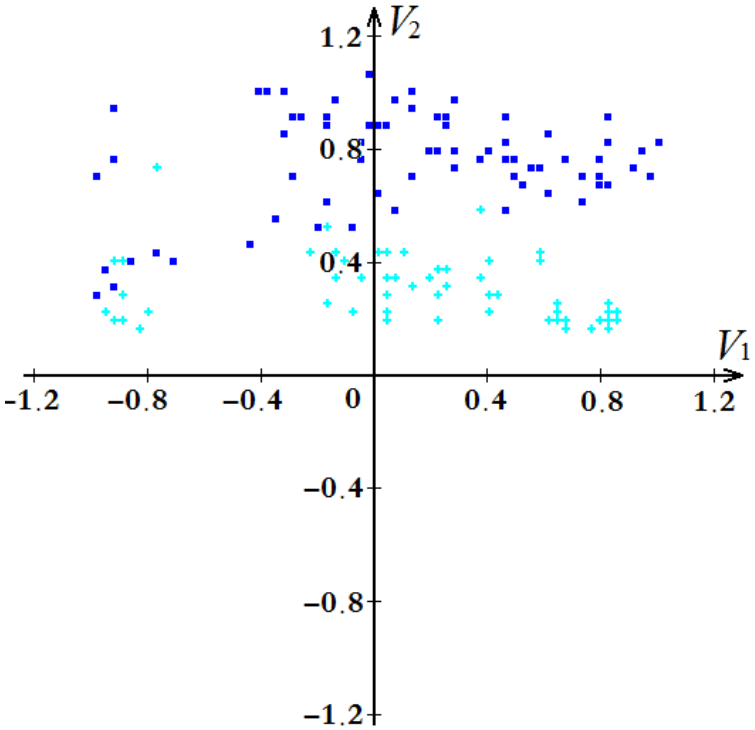

Fig. 4. View of seven-parameter data representing two various types of coal. Images of points representing coal type 31 were marked with (■), (+) – samples of coal type 34.2

Conclusions

The conducted experiments based on visualization of seven-parameter data by means of PCA allowed to arrive at the following conclusions.

1. Multi-parameter visualization by means of the PCA allows to state that information covered in analyzed seven-dimensional data is sufficient for a proper classification of coal types 31, 34.2 and 35.
2. The visualization of data concerning three types of coal within one figure allowed to state that images of data points representing coal samples of certain type gather in clusters which can be separated almost on the whole area of the figure. However, in some areas of the space, the images of points representing various coal types overlap. Therefore, based on such view it was impossible to state whether the analyzed data allows for a proper classification of coal types.
3. Only presentation of data representing three various types of coal in pairs allowed to obtain clear results. They allowed to conclude that images of points representing samples of coal of certain type gather in clusters which can be separated. It means that data contains a sufficient amount of information to classify coal types properly.
4. The advantage of the PCA method is the fact that during visualization it is not necessary to select any parameters in contrast to many other methods of multi-parameter data visualization.

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