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# PCA multivariate analysis for concentration in anions and cations of mineral water samples collected from the western, central and northern Romania

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***Abstract***

In the present paper were statistically analyzed by PCA method the concentration values of anions and cations from nine mineral water samples collected from western, central and northern Romania. In case of principal component analysis using anion concentration data present in mineral waters not found a clear grouping of samples, which is distributed relatively evenly scoring chart. In case of PCA analysis for the cation concentration data obtain a good group of samples B and C, the explained variance of the data of 54%, 41% and 4% for the first three principal components.

***Keywords***: mineral water, anions, cations, Principal Component Analysis – PCA

## 1. Introduction

Natural mineral water springs from an aquifer or underground layer protected against any pollution risk. It comes from an unused source through one or several natural emergences or drills and is bottled close to its source, under special hygienic precautions. The cations found in natural mineral water have special importance, given the role they play in the processes in the organism and its structure. [1]

The natural mineral water is clearly different from the spring water, due it's specific natural content in dissolved mineral salts, characteristic relative proportions, oligoelements presence or other constituents and native microbiological purity, which could give some health favorable properties. [2, 3]

Ionic chromatography (ionic exchange), is an analysis method that depends on a porous stationary solid phase formed from specific materials – ions exchangers – substances with a solid loosened network, organic or anorganic, on which are found grafted, by obtaining process, some ionic exchange centers. [4, 5]

HPIC is suited to the analysis of either anions or cations (depending on whether an anion-exchange or cation-exchange resin is used) and both inorganic and organic ions can be separated using this technique. In this experiment an anion-exchange column will be used. In HPIC, the separation of analytic ions involves the electrostatic interaction between solute anions and the positively charges sites on the stationary phase (the greater the degree of electrostatic attraction, the stronger the anion is retained on the column). [6, 7]

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PCA is a mathematical tool which performs a reduction in data dimensionality and allows the visualisation of underlying structure in experimental data and relationships between data and samples. [8]

In some cases, when the data set contains a large number of dependent variables, it may prove useful to reduce the data set into smaller segments to provide a clearer and more interpretable result. Principal component analysis (PCA) is an ideal tool for such tasks, in that a data set can be described by principal components according to the degree of variance within the data. Components with little explained variance can be left out of the analysis, thus reducing the amount of data and still keeping most of the information. PCA may also be used in exploratory analysis, where plots of the principal component loadings can be used to identify variables that are similar to each other. [9]

## 2. Material and methods

For principal component analysis (PCA) was used program The Unscrambler 9, trial version.
Principal components analysis (PCA) was performed in two steps as follows:

- in the first stage have been used as input data the anions concentrations determined from mineral water samples by means of high-performance ion chromatography (HPIC);

- in the second stage as input data were used cation concentration values determined from mineral water samples by the same method. [9, 10]

## 3. Results and discussion

***3.1. PCA data analysis to determine the concentration of anions in the mineral waters studied.*** If principal component analysis using anion concentration data present in mineral waters there was an obvious group of samples, which are relatively uniformly distributed on scores graphic (Figure 1), however, seemed to have influence on the distribution of chloride ions and nitrate in particular (Figure 2).

**3.2. PCA analysis of data obtained by determining the concentration cations from mineral waters studied.** If we consider the PCA analysis for the cation concentration data to obtain a good group of samples B and C (except B3) on the right side of the graph scores (Figure 3) with the variance of the data explained 54%, 41% and 4 % for the first three principal components. From the records graphic (Figure 4) it is noted the importance of this classification variables: the concentration of $Ca^{2+}$ to first principal component and $Na^{+}$ for the second. Even and $Mg^{2+}$ appears to play a role in this classification. Also, there is a good correlation between the residual variance tests (black in Figure 5) and variable (in gray in Figure 5).

***Table. 1.*** The input data for the multivariate analysis PCA for anions concentration (mg / L) [10]

| Sample | $F^-$ | $NO_3^-$ | $Cl^-$ | $SO_4^{2-}$ |
|---|---|---|---|---|
| A1 | 0.000 | 0.000 | 126.659 | 22.823 |
| B1 | 0.099 | 0.000 | 34.454 | 43.803 |
| C1 | 0.000 | 3,511 | 0,450 | 24.111 |
| A2 | 2.140 | 0.000 | 13.953 | 25.435 |
| B2 | 0.490 | 0.000 | 0.272 | 16.280 |
| C2 | 0.126 | 1,328 | 14.439 | 0.000 |
| A3 | 0.556 | 0.000 | 5.175 | 44.468 |
| B3 | 0.000 | 5.167 | 104.943 | 32.700 |
| C3 | 0.377 | 1.629. | 4.397 | 13.754 |

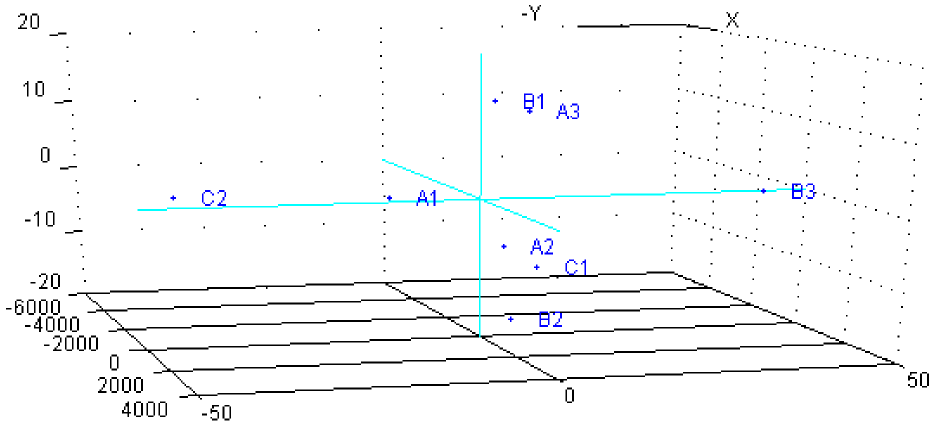


***Figure 1.*** $PC_3$ vs. $PC_1$, $PC_2$ scores graphic for PCA analysis using as input data the anions concentration in mineral water samples analyzed

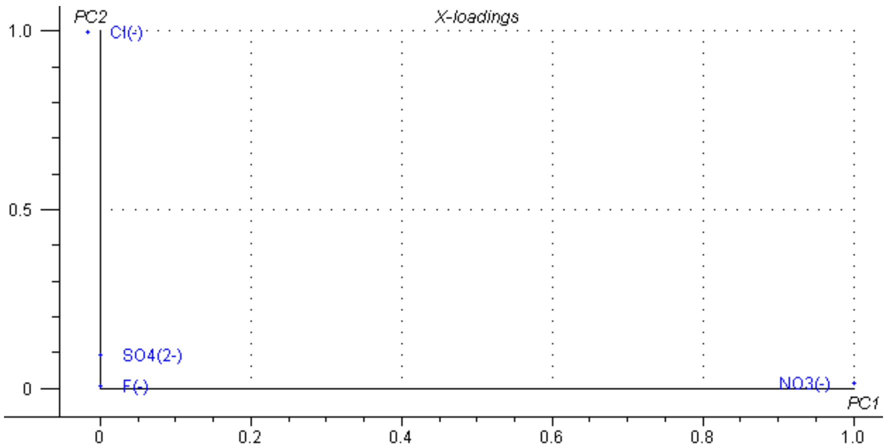


***Figure 2.*** $PC_3$ vs. $PC_1$ , $PC_2$ records graphic for PCA analysis using as input data the anions concentration in mineral water samples analyzed

***Table 2.*** The input data for the multivariate analysis PCA cation concentration (mg / L) [10]

| **Sample** | **$Li^+$** | **$Na^+$** | **$NH_4^+$** | **$K^+$** | **$Mg^{2+}$** | **$Ca^{2+}$** |
|---|---|---|---|---|---|---|
| A1 | 0.097 | 235.849 | 0.000 | 11.199 | 33.125 | 118.214 |
| B1 | 0.019 | 118.86 | 1.628 | 4.051 | 40.681 | 106.076 |
| C1 | 0.000 | 0.95 | 0.035 | 0.437 | 3.087 | 60.003 |
| A2 | 0.213 | 86.269 | 0.000 | 18.445 | 101.723 | 349.629 |
| B2 | 0.000 | 30.02 | 0.000 | 1.377 | 45.798 | 97.994 |
| C2 | 0.084. | 70.549 | 0.000 | 43.289 | 43.289 | 107.104 |
| A3 | 0.033 | 19.639 | 0.23 | 2.877 | 9.776 | 376.095 |
| B3 | 0.719 | 236.881 | 12.108 | 39.48 | 94.802 | 268.946 |
| C3 | 0.029 | 20.866 | 0.000 | 3.552 | 50.22 | 140.939 |

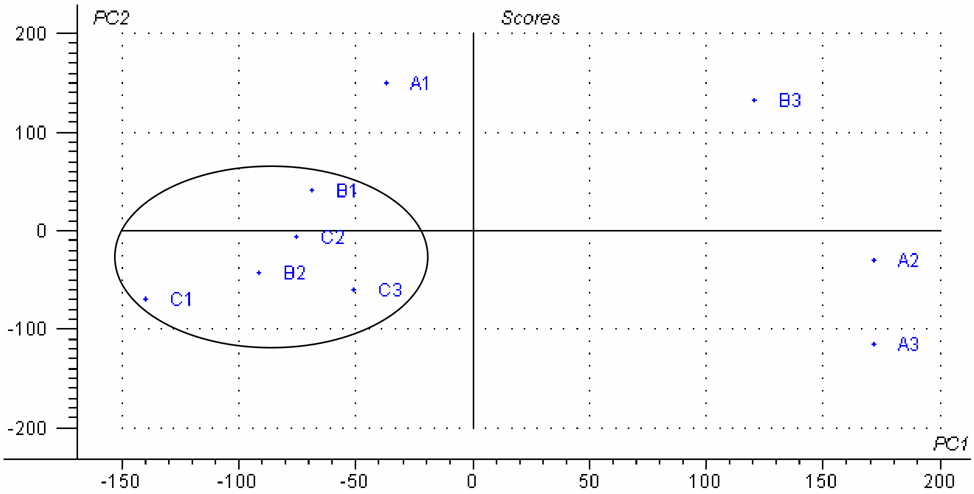


***Figure 3.*** $PC_3$ vs. $PC_1$, $PC_2$ scores graphic for PCA analysis using as input data the cations content in mineral water samples analyzed

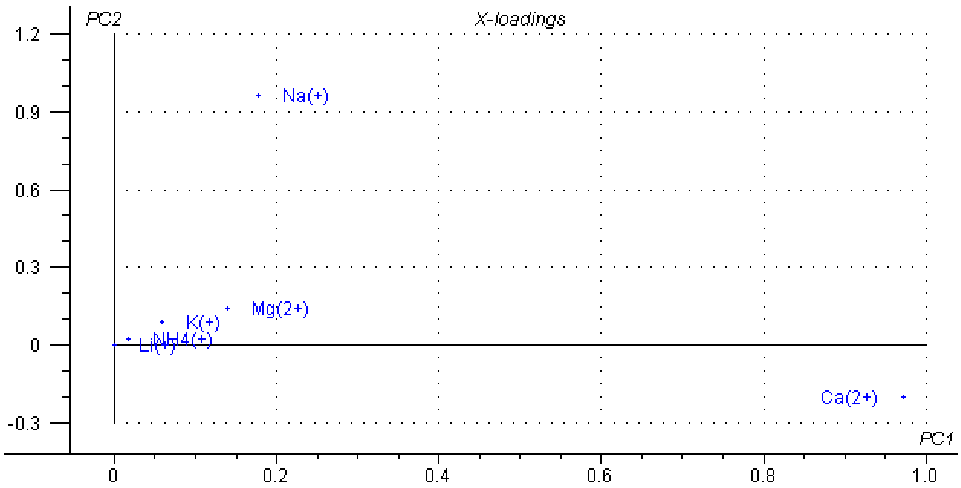


***Figure 4***. $PC_3$ vs. $PC_1$, $PC_2$ records graphic for PCA analysis using as input data the cations content in mineral water samples analyzed

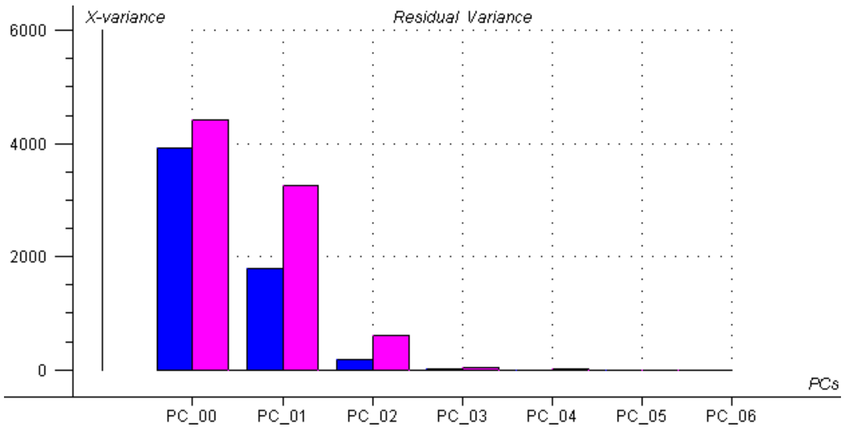


***Figure 5.*** Residual variance for PCA analysis using as input data the cations content in mineral water samples analyzed

## 4.Conclusions

Principal components analysis (PCA) using as input the concentrations of anions: fluorides, chlorides, nitrates and sulfates obtained by high performance ion chromatography (HPIC) allowed an obvious group of samples, which are relatively evenly distributed. Responsible for this classification as chloride ions and nitrate.

Principal components analysis (PCA) using as input data the concentrations of cations: lithium, sodium, potassium, magnesium, calcium, ammonium, obtained by high-performance ion chromatography (HPIC) allowed a clear group of samples B and C except for the sample B3. Responsible for this classification are the calcium and sodium, the magnesium element present the importance even in this classification.

**Compliance with Ethics Requirements.** Authors declare that they respect the journal's ethics requirements. Authors declare that they have no conflict of interest and all procedures involving human / or animal subjects (if exist) respect the specific regulation and standards.

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