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Editor
Komarytskyy M.L.
Ph.D. in Economics, Associate Professor

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APPLICATION OF THE PRINCIPAL COMPONENT METHOD TO VISUALIZE STUDIES OF EXHALED BREATH CONDENSATE

Komlevoi Oleksandr
PhD
Odessa National Medical University
Odessa, Ukraine

Introductions. A variety of research approaches are used to obtain information about metabolic processes occurring in the human respiratory system. Functional study of the lungs and broncho-alveolar system is an important area in pathological physiology and can be studied on the basis of analysis of exhaled breath condensate (EBC) [1]. The spectrum of substances found in exhaled air ranges from diatomic molecules such as hydrogen (H2), oxides of carbon (CO) and nitrogen (NO) to polyhydric aliphatic and aromatic hydrocarbons. The study of gas exchange of biological objects and analysis of the composition of exhaled air (biological particles suspended in it) is a large area of research with different instrumental approaches and a wide range of analytical characteristics [2, 3].

Aim. The aim of this work is to study the possibility of applying the method of principal components to simplify the visualization of the spectral distribution of exhaled breath condensate.

Materials and methods. To study the spectral composition of the EBC, it is convenient to use the method of laser correlation spectroscopy, which provides fast and accurate results. It is possible to determine the concentration of particles ranging in size from 1 to 18500 nanometers (nm). Since the size range of the histogram with the distribution spectrum is very wide, the particle size distribution function is depicted on a logarithmic scale for convenience.

Traditionally, histograms are used to visually represent the spectral distribution of condensate particles. In order to show the spectral distribution of condensate particles in a group of people, the arithmetic mean and standard deviation are indicated on the histogram (Fig. 1). In addition, the error of the mean value, the coefficient of variation and the confidence intervals of the arithmetic mean values in the general set of features for each studied indicator are calculated.

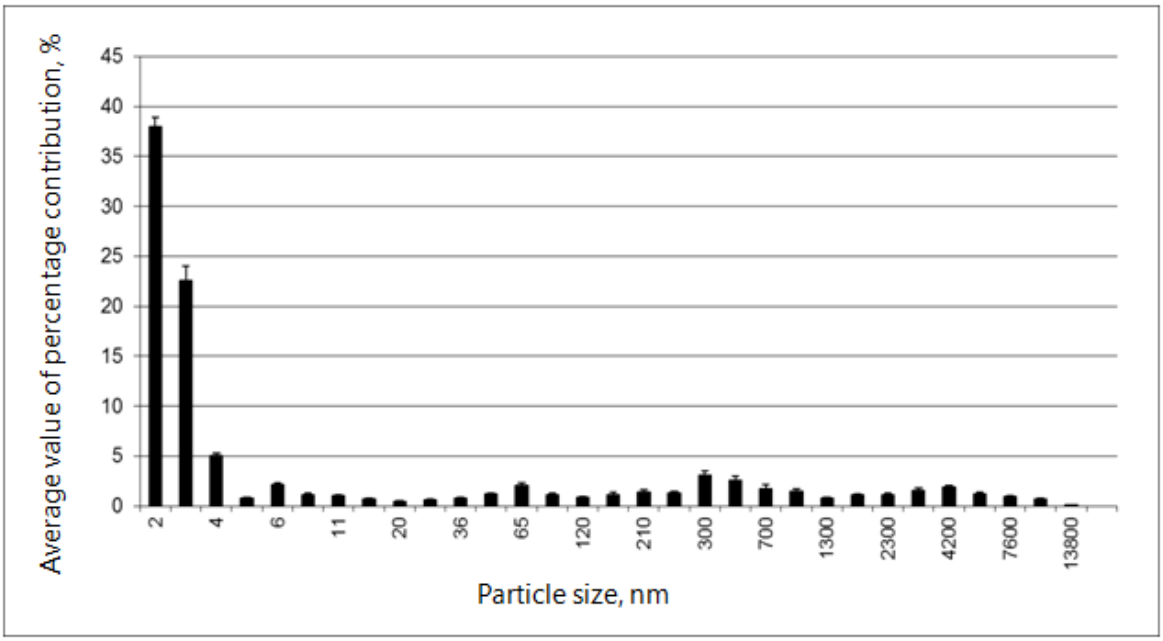

Fig. 1. Example of the averaged spectrum of moisture of exhaled air

Previously, studies were carried out, which showed that for groups of people with different diseases, the types of spectra differ [1 – 3]. But it is not convenient to compare histograms by 32 indicators with each other. Therefore, research to reduce the number of indicators while minimizing the loss of information is relevant.

Results and discussion. The convenience of comparing groups among themselves could be improved by reducing the dimension of the data. To reduce the dimensionality of the data, the principal component method is traditionally used. We will apply the method of principal components to 32 indicators of EBC and explore its possibilities of visualizing such data.

In the Fig. 1 shows the orthogonal projection onto the plane of the first two main components for visualizing a set of EBC data for groups of healthy people (group «norm»), as well as with the following diseases: asthma, pneumonia and bronchitis.

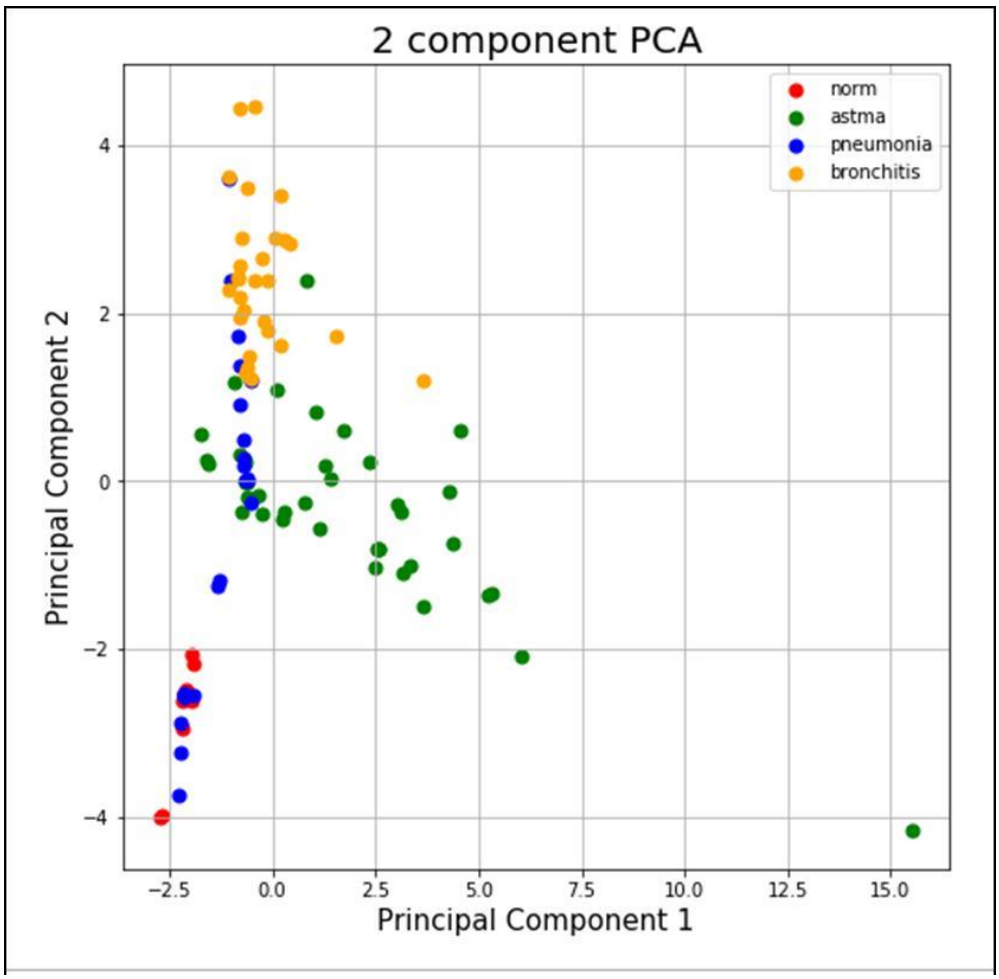

Fig. 2. Visualization by the method of 2 component PCA the EBC data of 4 examined people groups

The efficiency of the method is based on the following requirements: the minimum sum of the squares of the distances from the EBC data points to their projections onto the plane of the first two principal components; the minimum of the sum of distortions of the squared distances between all pairs of projections of the EBC data on the plane of the principal components.

The following conclusions can be drawn:

– the groups «norm» and «pneumonia» overlap strongly, their separation is impossible;

– the «asthma» group has a partial overlap with the «pneumonia» group;

– the «bronchitis» group has a slight overlap with the «asthma» group and partial overlap with the «pneumonia» group.

Let's try to apply the PCA method for the same 4 groups using 3 components. The projection on 1 and 2 principal components is the same as in the Fig. 1. The

results of the projection of 2 and 3 main components are shown in the Fig. 2. As you can see, the «pneumonia» group also overlaps with the «norm», «astma» and «bronchitis» groups.

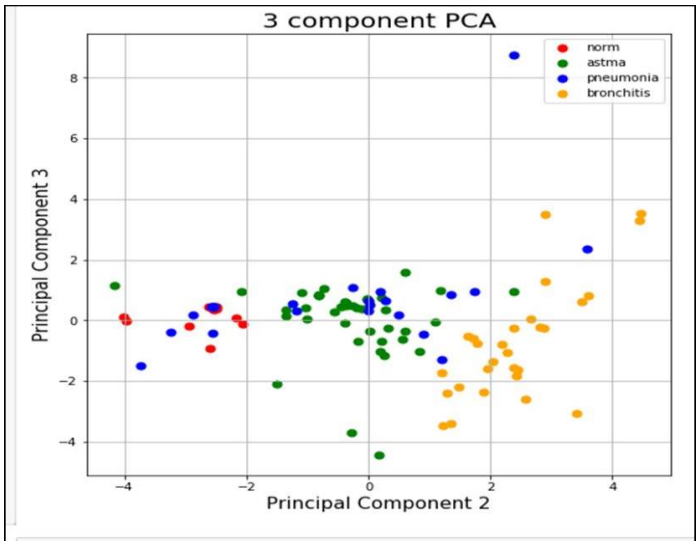

Fig. 3. Visualization by the method of 3 component PCA the EBC data of 4 examined people groups

Experiments have shown that an increase in the number of components of the PCA method does not lead to an increase in the quality of visualization. It was decided to exclude the "pneumonia" group from the list of groups that are visualized using the PCA method.

In Fig. 3 shows a two-component PCA method for visualizing EBC data for the «norm», «asthma» and «bronchitis» groups.

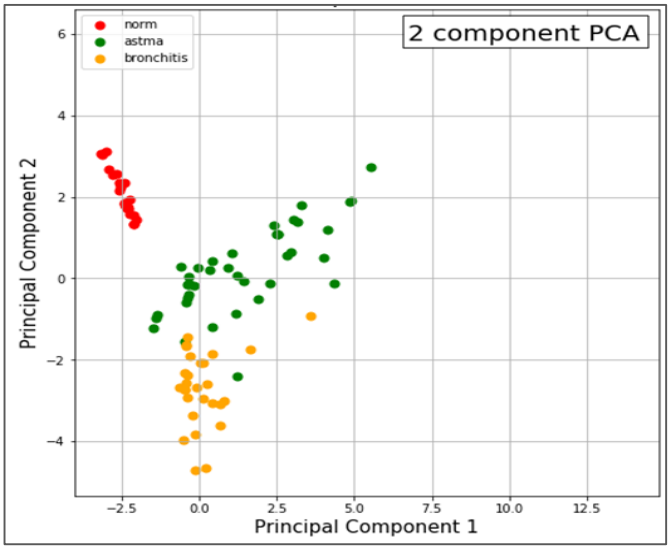

Fig. 4. Visualization by the method of 2 component PCA the EBC data of 3 examined people groups

Как видно, ЕАС данные для всех групп хорошо визуально разделяются. Следовательно метод PCA можно эффективно использовать для визуализации ЕВС данных for the «norm», «asthma» and «bronchitis» groups, obtained using the method of laser correlation spectroscopy.

Conclusions. The article explored the possibilities of using the principal component method to simplify the visualization of the spectral distribution of the exhaled air condensate. 4 groups of examined people were considered: group «norm», as well as with the diseases «asthma», «pneumonia» and «bronchitis». The results showed that the exclusion of the «pneumonia» group makes it possible to visually differentiate the EAC data of the groups «norm», «asthma» and «bronchitis» using the EAC method.

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