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To cite this article: D I Galiakhmetova et al 2017 J. Phys.: Conf. Ser. 917 042007

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The deconvolution of complex spectra by artificial immune system

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Abstract. An application of the artificial immune system method for decomposition of complex spectra is presented. The results of decomposition of the model contour consisting of three components, Gaussian contours, are demonstrated. The method of artificial immune system is an optimization method, which is based on the behaviour of the immune system and refers to modern methods of search for the engine optimization.

1. Introduction
The problem of separating complex spectral contours into components is important in the study of optical spectra in spectral analysis. The decomposition of a complex spectral contour into components can be reduced to finding the optimal values of the parameters of the elementary components, with which the reconstructed total contour will have minimum deviation from the experimentally obtained one.

Currently, one of the directions for the solution of the optimization problem is the so-called Natural Computing [1-3], which represents dynamic models containing the laws and processes of nature. Natural Computing is divided into several types, namely, Artificial Neural Network, Autonomic Computing, Membrane Computing, Artificial Life, Amorphous Computing. One of the classes of Autonomic Computing is Artificial Immune System. This approach is based on the processes and principles of the vertebrate immune system.

In this work, the optimization method was used, which is based on the behavior of an artificial immune system, in order to solve the problem of decomposition of a complex spectral contour into elementary components. The biological prototype of the artificial immune system is the human immune system, the information inside which is processed by protein molecules (peptides). This system is a complex adaptive structure using a combination of different mechanisms for protection against external pathogens, which can be any microorganisms (including viruses and bacteria) that can cause a human pathological condition (disease). The protective system has a hierarchical multilevel structure. Each successive level increases the specificity of protection. The congenital and acquired immune systems are the protection methods.

2. Results and Discussion
Biological immune system solves the problems of searching and classification. It is able to learn, and it possesses memory. The immune system processes huge amounts of information, producing complex parallel computations, so the algorithms using it as a basis have proved to be effective in mathematical problems of search, recognition and optimization.

An artificial immune network is a set of B-lymphocytes, which are interconnected and are subject to certain operations of cloning and mutation. When a foreign agent enters the body, molecules called
antigens are formed, in response to their appearance, antibodies reacting with them are formed. Antibodies are the molecules of B-lymphocytes that circulate in the blood circulatory and lymphatic systems and wait for collision and neutralization of antigens. If, by the recognition of antigens, the degree of closeness (similarity) of genetic sets of antigen and antibodies (R^ab - affinity) is small, mutation of antibodies occurs. Then, for the protection of the body, the best antibodies are cloned with the highest possible affinity. If contact with a foreign agent occurs not for the first time, the immune memory of the system, that is, the best antibodies produced earlier by the first contact with these pathogens, is used.

In the artificial immune system, affinity measures are used for the description of the interaction of the components of the system (antibodies), and immune algorithms are used as adaptation mechanisms [4]. To build such a system, the knowledge of the application area or objective function is required [5]. The following biological concepts and corresponding mathematical definitions are used in this work:

- antigen – the initial spectral contour obtained experimentally;
- antibody – the decision x∈D (D is the tolerance range), which is a sum of spectral components, each of which depends on three parameters (frequency, intensity and half-width);
- affinity – the measure of the usefulness of antibodies, it determines the difference between the experimental contour and the solution x;
- population – the set of antibodies;
- clone – the antibody formed from another antibody by cloning (copying);
- mutation – the change in antibody corresponding to a random alteration in the components of the vector x.

The following notation is used:

- b – antibody;
- f(b) – the value of the objective function corresponding to the antibody;
- B={b_i, i∈[1: n_b]} – population of antibodies;
- b_i,1, b_i,2,..., b_i,n – components of antibodies b_i∈B;
- q_i = -f(b) – the affinity of the antibody b_i;
- M – population of memory cells (antibodies that are not part of the population B);
- C_i – set of antibody clones b_i;
- C={C_i, i∈[1: n_C]} – set of all antibody clones;
- b^{C_i}_j – j-th clone of antibody b_i;
- b^{C_i}_{best} – the best clone antibodies b_i (the clone corresponds to the minimum value of the objective function);
- n_c – the number of clones generated by each antibody in the population B;
- α – step of mutation.

The main steps of the artificial immune system method are following:

1) Initializing the antibody population B, where the antibody b_i = (b_i,1, b_i,2,..., b_i,n) is a vector in the space of variates.
2) Determining the usefulness q_i of each antibody b_i in the population B.
3) Performing the cloning operation on the antibody with the greatest usefulness. A lot of antibodies C_i are created, which are identical to the original one C_i={b^{C_i}_j: b^{C_i}_j=b_i, j∈[1: n_c]}.
4) Performing the mutation b^{C_i}_j=b^{C_i}_j+α on the set of clones C, where α is determined by the formula
   \[ \alpha = 10^{-3}b^{C_i}_j. \]
5) Calculating the usefulness of all the cloned antibodies from the set C and finding the antibody b^{C_i}_{best} with the highest affinity.
6) Performing the clonal selection. The best of the antibodies’ descendants replace the parents in accordance with the formula

$$b_i = \begin{cases} 
 b_i, & \text{if } f(b_{\text{best}}^c) > f(b_i), \\
 b_{\text{best}}^c, & \text{if } f(b_{\text{best}}^c) \leq f(b_i).
\end{cases}$$

If the usefulness of the best antibody is higher than that of the corresponding memory cells, then the latter is replaced by the above mutated clone.

7) Replacing the worst solution $b_j, b_k$ by the new antibodies provided that

$$\|b_j - b_k\| < \beta, j \neq k,$$

where $\|b_j - b_k\|$ is a measure of the closeness of the cells (root-mean-square deviation); $\beta$ is the compression threshold.

8) The set of memory cells $M$ stores the best solutions found during the work of the method.

To study the effectiveness of the optimization method based on the algorithm of the artificial immune system in solving problems of complex spectral contour decomposition, the model spectra obtained by summing elementary contours were used [6]. The solid curve in figure 1 shows the model spectrum, the dotted lines show the components of the total contour calculated with the artificial immune system method. For the reconstruction of the elementary components, the number of components in the model contour and the frequency values corresponding to them were set [7]. The values of intensity and half-width of the reconstructed components were obtained. For comparison, table 1 represents the results of the initial parameter of the elementary components of the model contour consisting of two Gaussian contours and the parameters of the reconstructed elementary components. The following designations for the contours’ parameters are used in table 1: $\delta$ is the half-width, $\Delta$ is frequency, $I$ is intensity.

| Table 1. The parameters of the initial and reconstructed two-component contour. |
|--------------------------------|----------------------------|
| **Initial contour**          | **Reconstructed contour**  |
| $\delta$         | $\Delta$ | $I$ | $\delta$ | $\Delta$ | $I$ |
| 1st Gaussian contour | 70.0 | 20.0 | 5.0 | 71.6 | 20.0 | 5.2 |
| Gaussian contour    | 120.0 | 200.0 | 3.0 | 115.3 | 200.0 | 2.9 |

The error of half-width reconstruction is 2.28% and 3.92% for the 1st and 2nd contours, respectively. The error of reconstructing the intensity of the first contour is 4.00%, and for the second one it is 3.33%.

In this work, the decomposition of a three-component contour was carried out. Table 2 shows the parameters of the initial and reconstructed elementary components used by the separation of a three-component spectral contour. When the three-component contour was reconstructed, the error of intensity reconstruction did not exceed 1.43%.

| Table 2. Parameters of the initial and reconstructed three-component contour. |
|--------------------------------|----------------------------|
| **Initial contour**          | **Reconstructed contour**  |
| $\delta$         | $\Delta$ | $I$ | $\delta$ | $\Delta$ | $I$ |
| 1st Gaussian contour | 70.0 | 10.0 | 7.0 | 70.0 | 10.0 | 7.1 |
| Gaussian contour    | 120.0 | 630.0 | 4.0 | 120.0 | 630.0 | 4.0 |
| Gaussian contour    | 220.0 | 190.0 | 5.0 | 220.0 | 190.0 | 5.0 |

In addition, the decomposition of a three-component contour with closely spaced components was carried out. Figure 1 shows the result of this decomposition using the artificial immune system.
method. The values of the parameters of the model and reconstructed elementary components in the case of closely spaced components are indicated in table 3.

![Figure 1](image_url)

**Figure 1.** Deconvolution of a three-component model contour consisting of closely spaced Gaussian components.

| Initial contour     | Reconstructed contour |
|---------------------|-----------------------|
| δ                   | Δ                     | I       | δ       | Δ       | I       |
| 1st Gaussian contour| 59.0                  | 350.0   | 5.8     | 60.9    | 350.0   | 6.0     |
| Gaussian contour     | 83.0                  | 410.0   | 3.8     | 79.1    | 410.0   | 4.1     |
| Gaussian contour     | 96.0                  | 550.0   | 8.2     | 95.6    | 550.0   | 7.9     |

When the parameters of three elementary components of the initial contour were reconstructed in the case of closely spaced components, the half-width reconstruction error did not exceed 4.70%, the intensity reconstruction error was 7.89% of the set values of the model loop parameters.

In this work, an optimization method based on the artificial immune system algorithm was adapted to decomposition of complex spectra into elementary components. The basic elements and rules of the model were compared to mathematical concepts. The algorithm was tested on model two- and three-component contours.

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