Decomposition of Spectral Contour into Gaussian Bands using Gender Genetic Algorithm

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One of the methods for analysis of complex spectral contours (especially for spectra of liquid objects) is their decomposition into a limited number of spectral bands with physically reasonable shapes (Gaussian, Lorentzian, Voigt etc.). The problem with the required decomposition is that such decomposition is an inverse problem that is often ill-conditioned or even incorrect, especially in presence of noise in spectra. Therefore, this problem is often solved by advanced optimization methods less subject to be stuck in local minima, such as genetic algorithms (GA). In the conventional version of GA, all individuals are similar regarding the probabilities and implementation of the main genetic operators (crossover and mutation) and the procedure of selection. In this study, we test a new version of GA – gender GA (GGA), where the individuals of the two genders differ by the probability of mutation (higher for the male gender) and by the procedures of selection for crossover. In this study, we compare the efficiency of gradient descent and conventional GA and GGA followed by gradient descent from the found point in solving the problems of decomposition of the Raman valence band of liquid water into Gaussian shaped components.

Keywords: spectrum decomposition, genetic algorithm, gender genetic algorithm

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1. Introduction

In modern physics, many problems are reduced to solving an optimization problem for a function of many variables. Gradient methods have gained the greatest prevalence due to their effectiveness in finding a solution. But in the case of the multidimensional search space, there is a large chance of premature convergence into a local minimum, which greatly hinders the search for a suitable solution. In this case, the alternative may be the use of population methods, in particular, genetic algorithms (GA). As opposed to gradient methods, these methods cover a vast search area in the solution process, as a result of which they are less prone to converging into local minima.

However, due to the lack of directional search, the solutions obtained using GA are often not optimal in some small neighborhood of the obtained solution. Therefore, in order to combine the advantages of both methods, one can use a tandem of these algorithms: first apply GA and then use the resulting solution as an initial approximation for gradient descent.

This article will investigate the behavior of genetic algorithms and their modifications in comparison with gradient method in solving the problem of decomposition of a spectrum of an aqueous-ethanol solution into Gaussian shaped components.

2. Description of the physical task

The decomposition of a spectrum of an aqueous-ethanol solution into a certain set of Gaussians was chosen as the problem to be solved. As the result of experiments described in [Plastinin et al., 2017], the spectra of an aqueous ethanol solution were obtained at different temperatures (-5, 0, 10, 20, 25, 35, 45, 55, 65, 75, 85, 92 ºC) in the range of the wave number k = [2400, 4000] cm^{-1} (Fig. 1). The decomposition of such a spectrum into Gaussians is not trivial, but it is extremely important to study vibrational processes in aqueous-ethanol solutions at different temperatures. Gradient methods are unproductive with problems of this type; however, evolutionary algorithms, due to their ability to avoid convergence into local minima, can be effective in solving them. Therefore, this task was chosen as a test for GA and its modifications

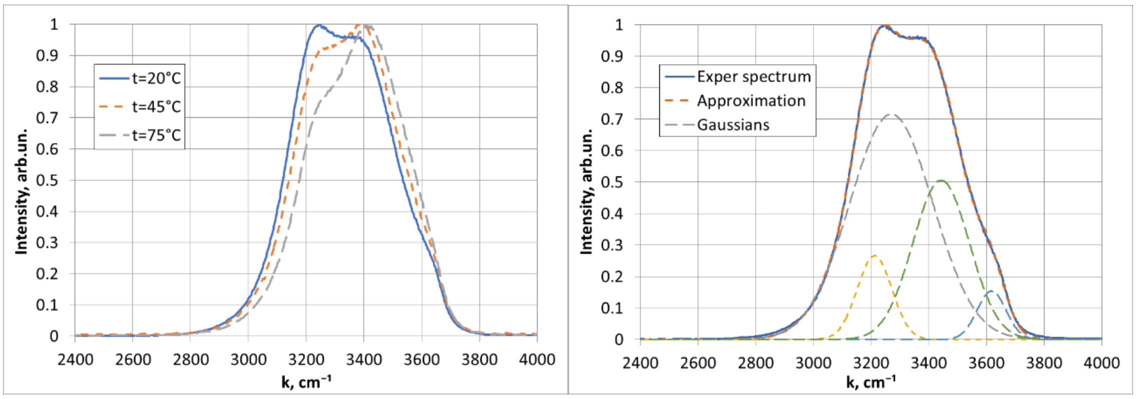

Fig. 1. Left – Examples of experimental spectra of aqueous-ethanol solutions at T = 20, 45, 75 ºC; Right – Example of decomposition of the spectrum of aqueous-ethanol solution at T = 20 ºC into four Gaussian shaped contours.

3. Mathematical formulation of the problem

In the mathematical formulation, the problem of spectrum approximation is reduced to the problem of minimizing the error function. In our case, the adjusted parameters are real numbers describing the Gaussians: the position of the center, the amplitude and the halfwidth of each of the Gaussians. The error function is the square of the deviation of the experimental and decomposition spectra.

3.1 Description of the genetic algorithm

Genetic Algorithm (GA) is an iterative process, at each iteration of which the individuals are selected based on their target (fitness) function, and are subject to crossover (exchange of certain parts of the solutions of two individuals) and mutation. The mutation operator changes a part of an individual randomly with a small probability. Also, the elitism operator is often used – copies of several individuals with the best fitness function are transferred to the next generation without change.

In this paper, we used a binary representation of the solutions, a single-point crossover operator, and a single-bit mutation operator, and roulette wheel selection of the individuals. The stopping criterion was chosen as follows: the algorithm stops working if after the last N generations there has not been a decrease in the best fitness function value in the population by more than Δ.

3.2 Description of the gender modification of GA

One of the modifications of GA is its gender modification (GGA) [Drezner, Drezner, 2006; Drezner, Drezner, 2020; Holzinger et al., 2014; Kowalczuk, Białaszewski, 2018; Shukla et al., 2013; Sizov, Simovici, 2020]. In GGA, each individual is assigned an additional characteristic – gender. The selection of individuals takes place within the same gender; the crossing of individuals of the same gender is prohibited.

In most cases, two genders are used – male and female [Drezner, Drezner, 2006; Drezner, Drezner, 2020; Holzinger et al., 2014; Kowalczuk, Białaszewski, 2018; Shukla et al., 2013; Sizov, Simovici, 2020]. The probability of mutation in females is less than in males. In addition, we introduced a new GGA parameter – a restrictive parameter (RP) for the permissible number of times of one female individual to be selected within one generation. The ratio of male and female individuals in the population in this study was fixed at 1:1.

4. Computational experiments

Each configuration of algorithms solving the problem was run 10 times for a set of statistics, so for all the obtained results we provide average values and variances.

4.1 Determination of the number of Gaussians sufficient to decompose the spectrum

In the first experiment, sufficient number of Gaussians to approximate the experimental spectrum was determined. To do this, a combination of GA and gradient descent (GD) was used (GA+GD): the solution obtained as a result of the GA operation was used as an initial decomposition for gradient descent.

The spectra for three temperatures (20, 45, 75 °C) were approximated. The results are shown in Fig. 2.

The setting of the GA parameters was the result of a limited grid search around reasonable values. However, it is possible that some parameter combinations providing better optimization results may exist. At the same time, the main purpose of this study was comparison of different GA modifications for the same parameter values rather that search for the best result.

GA parameters were set to be the following:

- Population size – 106 individuals;
- Number of elite individuals – 6;
- Probability of mutation – 1%;
- In the stopping criterion, N = 50, $\Delta = 1\times10^{-9}$;
- The l-BFGS-r algorithm was used as the gradient method [Zhu et al., 1997; SciPy].

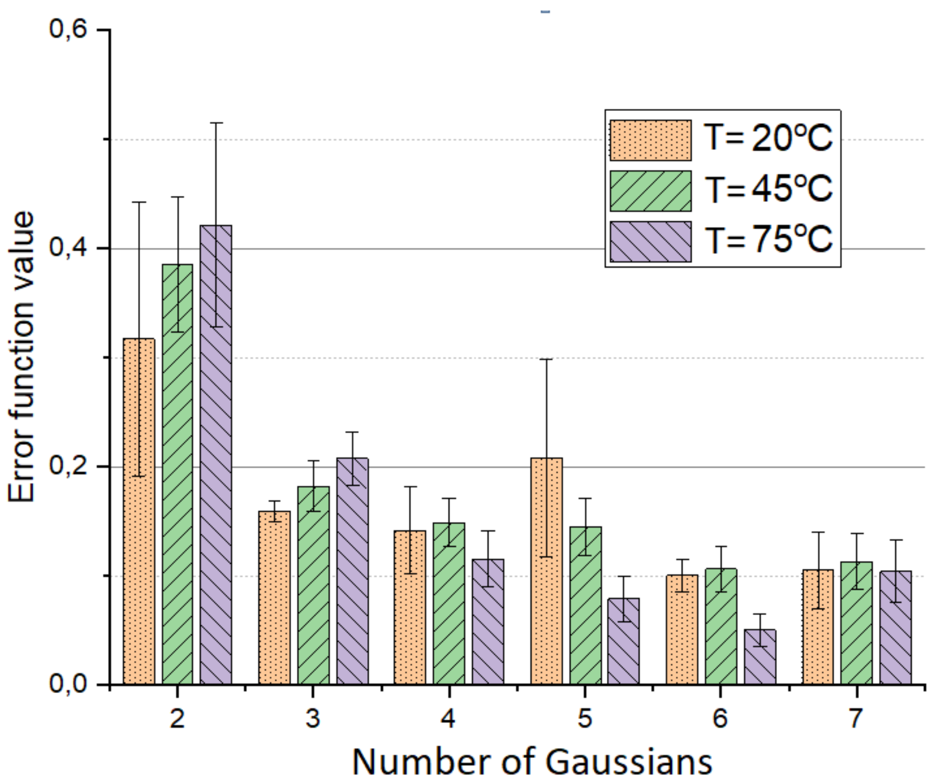

Fig. 2. The error function of the solutions obtained as a result of GA+GD approximating the spectra with a different number of Gaussians for the three specified temperatures.

From Fig. 2, it can be concluded that 4 Gaussians are sufficient to approximate the studied spectra, which is consistent with the conclusions made in the article [Plastinin et al., 2017]. The improvement of the fitness function obtained at further increase in the number of Gaussians, if any, is not statistically significant, taking into account the variance of the obtained fitness function values. Also, while 6 Gaussians seem to provide somewhat better results than 4, this can hardly be explained from the physical point of view, and the positions and halfwidths of extra two Gaussians turn out to be close to those already taken into account. That is why it was decided to limit the number of Gaussians in the considered decomposition to 4.

4.2 Application of GA with different values of the restrictive parameter

In the second experiment, the effectiveness of GGA was investigated at different values of the restrictive parameter (RP). The spectra for the three temperatures were decomposed by GGA with different RP values. The results are shown in Fig. 3.

The GGA parameters were set the same as for GA, except for the probability of mutation which had to be set different for different genders.

GGA parameters were set to be the following:

- Approximation of the spectrum by 4 Gaussian shaped components;
- Population size – 106 individuals;
- Number of elite individuals – 6;
- Probability of mutation – 5 % and 0.5% for male and female individuals, respectively;
- In the stopping criterion, N = 50, $\Delta = 1\times10^{-9}$.

There is no obvious dependence of the fitness of the solutions obtained on the RP used. Therefore, in further experiments, RP=3 was used as the one most successful in approximating the selected three spectra.

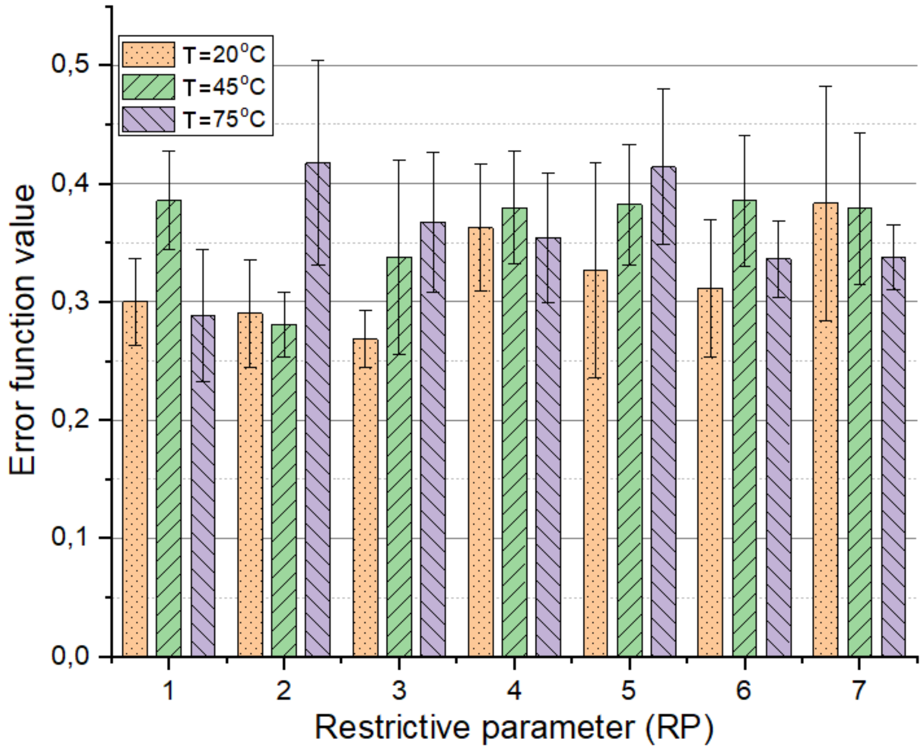

Fig. 3. The error function of the solutions obtained as a result of GGA+GD approximating the spectra with various RP values for the three specified temperatures.

4.3 Application of GA+GD and GGA+GD to the spectra for all temperatures.

In the third experiment, the algorithms GA+GD, GGA+GD and gradient descent from a randomly generated solution (RGD) were compared. The algorithms were run on the spectra of all 12 temperatures in two configurations with two different sets of mutation probabilities (Table 1). To make the comparison adequate, RGD was run repeatedly from random initial points until the total number of fitness calculations exceeded the average number of fitness calculations when working with GA+GD and GGA+GD, and the best of the solutions obtained was chosen as the resulting solution.

Two series of launches were made with different parameters of GA and GGA, indicated in Table 1. The results are shown in Fig. 4.

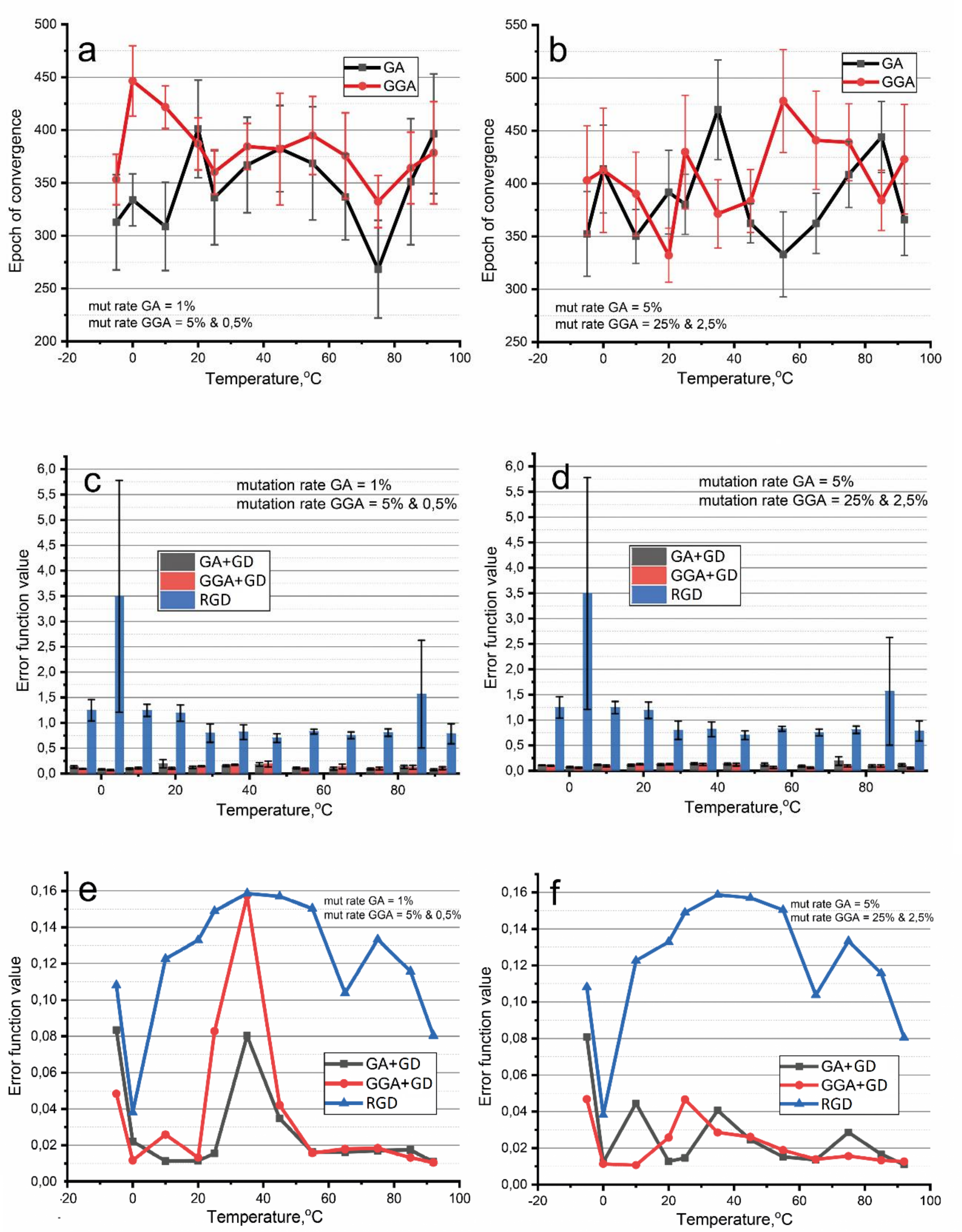

Fig. 4. a, b – epochs of convergence of GA and GGA in the approximation of spectra;
c, d – the values of the error function of solutions obtained by GA+GD, GGA+GD and RGD;
e, f – minimum values of the error function of solutions obtained by GA+GD, GGA+GD and RGD during all launches.

Table 1. Parameters of GA and GGA in the third experiment

Parameters	***GA***	***GGA***
Population size	106	
Number of elite individuals	6	
Stopping criteria	N = 50, $\Delta = 0$	
Gradient descend method	L-BFGS-B	
Probability of mutation	a) 5% b) 1%	a) 25% & 2.5% for male & female b) 5% & 0.5% for male & female

As can be seen, GA on the average converges faster than GGA, but at the same time the quality of solutions obtained using GA+GD and GGA+GD is on the average the same. In this case, the tandems GA+GD and GGA+GD are looking for solutions more efficiently than RGD.

5. Results and discussion

Let us briefly discuss the main results of this study.

Preliminary search for an initial decomposition for GD using GA/GGA significantly improves the quality of the solutions obtained compared to repeated use of RGD. This may be explained by the fact that for a multi-extremal optimization problem GA and its modifications have higher chance to find the area of the global extremum than RGD. RGD, in its turn, is much more efficient in converging into the point of the extremum itself starting from an initial approximation located in the “basin” of this extremum.

The efficiency of GA and GGA in solving the decomposition of the spectrum into Gaussians is approximately the same if they are used not by themselves but to find an initial point for GD. At the same time, previous results obtained by the authors on model problems, demonstrate that GA usually converges faster than GGA, but finds a worse solution; we explain this by a stronger tendency to degeneration for GA compared to GGA. Therefore, we can conclude that for the optimization problem investigated in this study, GA is as successful in finding the area of the global extremum as GGA is. This is possibly due to the fact that the number of different extremums for the investigated problem of spectra decomposition is relatively small.

The restrictive parameter introduced in the GGA does not significantly affect the efficiency of the algorithm. This may be possibly explained by a relatively small range of the fitness function values within the population. It this case, an individual is usually selected within one population only one or several times. If this is so, the RP exceeding 2 or 3 really should not affect the results much. However, this hypothesis should be checked in a special computational experiment.

6. Conclusion

In this paper, at the example of the real-world problem of decomposing a water-ethanol spectrum into a set of Gaussian shaped components, we compare the efficiency of genetic

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algorithm (GA) and its gender modification (GGA) combined with subsequent use of gradient descent starting from the point found by GA/GGA.

As a result of the computational experiments, it was found that:

1. It has been confirmed that use of GA/GGA to find a preliminary solution, to which gradient descent (GD) is subsequently applied, is an effective technique. The tandems GA+GD and GGA+GD gave better solutions than the gradient descent alone repeatedly started from random points, on spectra of all temperatures.
2. It has been found that GGA does not have an advantage over GA in solving this problem, and an explanation of this result has been suggested.

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