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Nested Genetic Algorithm for Resolving Overlapped Spectral Bands

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Abstract: A nested genetic algorithm, including genetic parameter level and genetic implemented level for peak parameters, was proposed and applied for resolving overlapped spectral bands. By the genetic parameter level, parameters of genetic algorithm were optimized; moreover, the number of overlapped peaks was determined simultaneously. Then parameters of individual peaks were computed with the genetic implemented level.

Keywords: Nested genetic algorithm, resolving overlapped bands, spectra.

Resolving overlapped peaks is a main problem encountered in analyzing spectra and data processing. Optimization methods have been used for resolving overlapped bands. Genetic algorithms (GAs) are numerical optimization methods based on the concepts of genetics and natural selection. Therefore, GAs possesse better nonlinear parallel and self-adaptive properties[1]. In this work, a nested genetic algorithm (NGA), including genetic parameter level and genetic implemented level, was described and applied for resolving simulated unresolved bands.

Figure 1 shows the logic framework of the nested genetic algorithm. The parameters of GA and the number of overlapped peaks can be computed with GA, namely, its individual w is the initialization of the parameters of GA and the number of overlapped peaks; its parameters A were chosen according to experimental range. This procedure is defined as genetic parameter level. To each individual a_i, it can exclusively determine one GA for resolving overlapped peaks, namely, genetic implement level for peak parameters. If the individual x_i^* is assumed to be the obtained solution, the fitness of x_i^* is regarded as the fitness of the individual a_i. If GA is performed on genetic parameter level and its individual is a_i^*, its corresponding value of $(x_i^*)^*$ is no other than parameters of overlapped peaks after resolving. Note that the fitness and mutation form in the NGA is described as follows. If the original data of overlapped peaks is assumed as $\{(t_i, y_i), i=1, NUM\}$ (if $y_i>0$) while the computing data under the peak parameter x is assumed as $\{(t_i, f(x_i, t_i), i=1, m, NUM\}$. Error E(x) is defined by

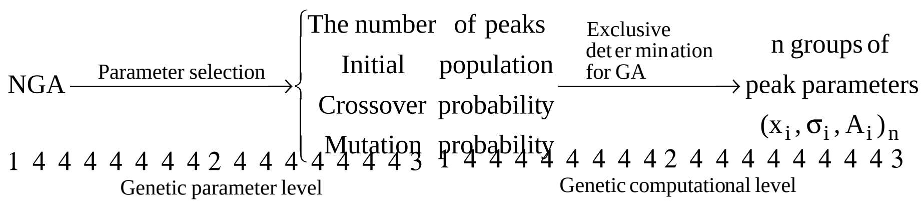
$$E(x) = \sum((1.0 + k_1 \cdot y_i) \cdot y_i - f(x, t_i) + k_2 \cdot y_i - f(x, t_i) / y_i)$$

where k_1 and k_2 are weighting coefficients of absolute and relative errors. So, fit(x)=1.0/E(x). NGA can yield better results with this fitness. To individual x, individualy can be created by mutation operator. To component i,

$$\bar{y}_i = x_i + s \cdot (\mu - 0.5) \cdot (0.2 \times (R[i] - L[i]))$$

here s is mutation step size and μ is chaos variable[2]. By substituting chaos variable for random in mutation process, the precision can be improved over the classical GA.

Figure 1 The logic framework of NGA



NGA was used for resolving simulated overlapped spectra and the computational results were shown in **Table 1**. It is clear that the deviation of peak position(d_p) and relative error of peak area(A %) decrease with the overlapped degree reduces and increase with the signal to noise ratio(SNR) decreases. But the errors are in the acceptable range even for the heavily overlapped bands.

Table1 The computational results of spectra comprising asymmetry peaks with NGA

spectra		resolu-tion	noise free		SNR=300		SNR=200		SNR=100	
			d_p (cm^{-1})	A%	d_p (cm^{-1})	A%	d_p (cm^{-1})	A%	d_p (cm^{-1})	A%
A	I	0.35	0.27	-0.8	0.12	0.8	0.34	6.8	0.54	6.0
	II		0.15	3.4	-0.23	3.1	-0.30	5.1	-0.35	1.1
B	I	0.50	0.96	1.2	0.76	6.4	0.98	6.0	0.83	0.0
	II		-0.23	-2.3	0.85	8.8	-0.36	5.7	0.21	13.3
	III		0.81	3.4	-0.24	-7.0	-0.26	-2.0	-0.55	-2.8

To summarize, with NGA, not only the parameters of GAs can be optimized but also the number of overlapped peaks can be determined simultaneously. In addition, a novel form of fitness and mutation are described in the NGA too. Consequently, NGA is superior to curve fitting technique in resolving overlapped peaks because it can detect the peak number by itself instead of by other techniques.

Acknowledgments

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