GENETIC-ALGORITHM OPTIMIZATION OF THE ANALYSIS OF ELASTIC SCATTERING OF LIGHT NUCLEI BASED ON THE S-MATRIX MODEL

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A genetic algorithm for an optimization problem in nuclear physics is discussed.
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INTRODUCTION

Analysis of elastic scattering of ^{4}He-nuclei by 120 MeV ^{92}Zr-nuclei [1] has been performed in [2] with the use of the scattering matrix having the form:

$S(L)=\eta(L)\exp\{2i[\delta(L)+\sigma_C(L)]\}$,

$\eta(L)=\exp[\ln\varepsilon\cdot g(L,L_0,\Delta_0)]$, $2\delta(L)=\delta_0 g^2(L,L_1,\Delta_1)$,

$g(x,x_0,\Delta)=\{1+\exp[(x-x_0)/\Delta]\}^{-1}$, $L=l+1/2$,

where $\sigma_C(L)$ is the phase of point-charge scattering by the uniformly charged sphere having the radius $R_C=1.3\cdot 92^{1/3}$; $\varepsilon<<1$ determines the nucleus transparency in the small moment region; δ_0 characterizes the nucleus refraction. It is noted that the parameter space of the problem is highly dimensional (six parameters should be varied), highly nonlinear (parameters are strongly coupled) and has an unknown and unpredictable topography (χ^2 surface is very complicated). Hence, to find S-matrix parameters we need the appropriate search method.

The grid methods can explore an arbitrary search space with evidently arbitrary precision but take for that eventually infinite time. The gradient methods are much quicker than the grid ones but often become stuck in a local minimum. Besides, such methods can accumulate the errors of function evaluations because each the new test point in the parameter space depends on the previous one. The random search methods are stable against the mentioned disadvantage and can "hop" from one minimum to another but are time intensive.

The approach which is proven to perform efficiently on such complicated problem spaces is a genetic algorithm (GA) [3-5]. GA treats an optimization problem as a selection of the fittest set of parameters under optimization. But GA does not simply use the Darwinian idea of biological evolution by the selection of the fittest, it even mimics the details of mechanisms via which that evolution occurs: mutation and heredity. From the evolutionary point of view, the gradient methods of optimization are totally hereditive because each the new function evaluation is fully determined by the previous one. The random search approaches are absolutely mutative because any consequent function evaluations are totally independent. Following the biological example, GA mutation and heredity the way, which can be easily tuned to fit almost any optimization problem [6, 7].

Dealing with real problems GAs usually face two general problems: (i) a perfect solution cannot be obtained while a "good" one can be found quite quickly (the inherent nondeterminism of GA itself); (ii) GAs are also time-consuming when performed on a single sequential processor.

The situation can be partially improved by performing a set of optimization runs with different initial populations and different population sizes, but it is difficult to predict how many runs, generations and individuals would be needed. Besides, one can combine GAs with gradient and other deterministic methods, but these hybrids are still more of an art than a science. So, we need to refine GA with respect to these problems.

TRADITIONAL GENETIC ALGORITHM

The essentials of a traditional GA are as follows. Every parameter under optimization is represented by the 16-bit string called a gene, so the parameter range is divided on 2^{16} parts, which is usually sufficiently precise. A set of genes representing optimization parameters is called a genome (an individual). Selective quality of an individual is called a fitness. Population consists of a fixed number of individuals. Evolution begins from the initial population filled with randomly chosen genomes. For each individual the function under optimization is evaluated and the fitness is attached. Two individuals (parents) are chosen randomly according to their fitnesses to produce offsprings. Mating of parents uses two key GA operators: mutation and crossover. Mutation means the inversion of gene's bits while crossover is the exchange of portions of bits between offsprings. After the replication offsprings are tested to acquire fitness. If the given offspring has a better fitness than the worst individual in the population then the latter is substituted by the former to keep the population size. Next pair of parents is chosen and so forth. Algorithm terminates when the best fitness of the population is found equal to the worst one so that no further improvement should be expected.

REFINED GENETIC ALGORITHM

To handle the problem (i) we tested the traditional GA on minimizing the simplest one-dimensional functions having the only one minimum and allowing the algorithm to reach it exactly. We discovered that GA often stopped in the several points of the space of optimization parameters, pointing out the existence of a

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number of local minima. But neither the functions were so complicated to have local minima in these points nor the population size was too small to take into consideration the random deviations from the true minimum due to the inherent nondeterminism of GA. Our efforts to change the situation by varying the population size, the mutation probability and the crossover rate failed. So we were forced to treat the genes corresponding to these unexisting minima as "magic".

Having analyzed the binary configurations of "magic" genes we found that a binary representation of genes itself caused the anomaly. For instance, the binary representation of the integer number 0 has all 16 bits zeros while its nearest neighbor -1 has all 16 bits units (for 16-bit strings). So, if we want to transform the gene g=-1 into the gene g=0 via the traditional mutation operation (gene's bit inversion) we must invert all 16 bits. As far as the probability of such a mutation event is vanishingly small GA can stop at these "magic" genes without any motivation from the function under optimization or the details of GA implementation. Note that the neighbor gene pairs (-2, -1) and (0, 1) are separated by the only one bit inversion each. To fix the problem, before the conventional inversion of bits it is worthwhile randomly shifting the value of gene by -1, 0, +1. Repeating the simple function minimization experiments with application of the corrected mutation procedure, we found it demonstrating excellent performance in dramatic increase of the successive runs percentage.

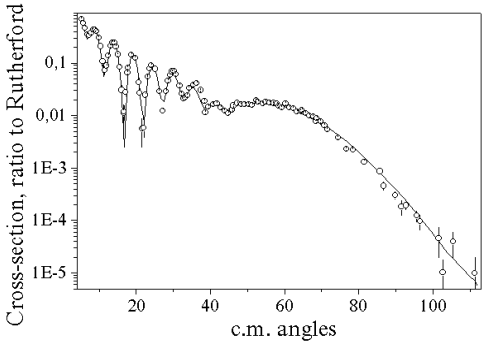
To deal with the problem (ii) we should optimize basic GA parameters and operators in respect to the number of function evaluations, keeping the quality of optimization along with that. Mutation is a major GA operator making the evolution possible. Frequency of mutation determines the degree of inheritance: if it is too high the heredity is almost absent and GA becomes one of the stochastic methods; if it is too low the heredity is almost total and GA appears one of the deterministic approaches. Maximum speed of evolution occurs when the frequency of mutation acquires some optimum value at the middle and cannot be estimated in general.

In our approach the frequency of mutation is implemented as a number of replicated bits one of which is flipped. That number has the initial value of 1 (every bit in a gene will be inverted). During replication the mutation genes of the parent and its offspring are randomly changed by -1, 0, +1. This mechanism was found accelerating the evolution at the initial stage and keeping the optimum genetic diversity rate in the population.

To minimize harmful consequences of highly inexact replication we have modified the bit inversion procedure itself. Traditional mutation operation assumes that the probability of inversion of a bit in a gene is distributed uniformly, so that the probability of a drastic change is equal to the probability of a slight one. Altering the shape of that distribution we can, in principle, decrease the probability of lethal changes even if the mutation rate in genome is very high. In biological genetics the similar alteration is called the degeneracy of genetic code and leads to the similar result [8]. It is impossible to calculate or predict the distribution in closed form. So, we introduce 16 bit-inversion-weight-genes (one gene for every bit in a 16-bit string). The initial values of the weight-genes provide uniform distribution of mutation probability in a gene. Our experiments show that under the high frequency of mutation the weight-genes rapidly adopt and the final number of function evaluations substantially reduces.

APPLICATION EXAMPLE

Figure shows the results of optimization of S-matrix parameters obtained with the help of our GA software package created for the single sequential processor. The values of parameters found and the quality of the fit are in good agreement [2]. We emphasize that the only input data required for GA is the range of parameters and the optimization itself is performed automatically.



The cross-section of the 120 MeV α-particle elastic scattering by ^{92}Zr: L_0=29.13, L_1=24.78, Δ_0= 3.26, Δ_1=5.99, ε=0.0115, δ_0=29.20, χ^2=4.48. Experimental data are from [1].

REFERENCES

1. L.W. Put, A.M.J. Paans. The form factor of the real part of the α-nucleus potential studied over a wide energy range // *Nucl. Phys*. 1977, v. A291, p. 93-105.

2. Yu.A. Berezhnoy, V.V. Pilipenko. Analysis of refraction effects in nuclear scattering on the basis of the S-matrix approach//*Mod. Phys. Let.* 1995, v. A10, p. 2305-2312.

3. J.H. Holland. *Adaptation in Natural and Artificial Systems.* Univ. of Michigan, Ann Arbor, 1975, 265 p.

4. D.E. Goldberg. *Genetic Algorithms in Search, Optimization and Machine Learning.* Addison-Wesley, 1989, 351 p.

5. Z. Michalewicz. *Genetic Algorithms+Data Structures=Evolution Programs.* Springer-Verlag, Berlin, 1994, 284 p.

6. K. Michaelian. Evolving an energy dependent optical model description of heavy-ion elastic scattering//*Revista Mexicana de Fisica.* 1996, v. 42 (s.1), p. 203-218.

7. C. Winkler, H.M. Hofmann. Determination of bound-state wave functions by a genetic algorithm // *Phys. Rev.* 1997, v. C55, p.684-690.

8. M. Ycas. *The Biological Code.* North-Holland Publishing Co., Amsterdam, London, 1969, 512 p.