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A hybrid particle swarm optimization and genetic algorithm with population partitioning for large scale optimization problems

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Abstract In this paper, a new hybrid particle swarm optimization and genetic algorithm is proposed to minimize a simplified model of the energy function of the molecule. The proposed algorithm is called Hybrid Particle Swarm Optimization and Genetic Algorithm (HPSOGA). The HPSOGA is based on three mechanisms. The first mechanism is applying the particle swarm optimization to balance between the exploration and the exploitation process in the proposed algorithm. The second mechanism is the dimensionality reduction process and the population partitioning process by dividing the population into sub-populations and applying the arithmetical crossover operator in each sub-population in order to increase the diversity of the search in the algorithm. The last mechanism is applied in order to avoid the premature convergence and avoid trapping in local minima by using the genetic mutation operator in the whole population. Before applying the proposed HPSOGA to minimize the potential energy function of the molecule size, we test it on 13 unconstrained large scale global optimization problems with size up to 1000 dimensions in order to investigate the general performance of the proposed algorithm for solving large scale global optimization problems then we test the proposed algorithm with different molecule sizes with up to 200 dimensions. The proposed algorithm is compared against the standard particle swarm optimization to solve large scale global optimization problems and 9 benchmark algorithms, in order to verify the efficiency of the proposed algorithm for solving molecules potential energy function. The numerical experiment results show that the proposed algorithm is a promising and

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efficient algorithm and can obtain the global minimum or near global minimum of the molecular energy function faster than the other comparative algorithms.

1. Introduction

The potential energy of a molecule is derived from molecular mechanics, which describes molecular interactions based on the principles of Newtonian physics. An empirically derived set of potential energy contributions is used for approximating these molecular interactions. The minimization of the potential energy function is a difficult problem to solve since the number of the local minima increases exponentially with the molecular size [1]. The minimization of the potential energy function problem can be formulated as a global optimization problem. Finding the steady state (ground) of the molecules in the protein can help to predict the 3D structure of the protein, which helps to know the function of the protein.

Several optimization algorithms have been suggested to solve this problem, for example, the random method [1–4], branch and bound method [5], simulated annealing [6], genetic algorithm [7–9] and variable neighborhood search [10,11]. A stochastic swarm intelligence algorithm, known as Particle Swarm Optimization (PSO) [12], and PSO and the Fletcher–Reeves algorithm [13], have been applied to solve the energy minimization problem. PSO is simple, easy to implement, and requires only a small number of user-defined parameters, but it also suffers from premature convergence.

In this paper, new hybrid particle swarm optimization algorithm and genetic algorithm is proposed in order to minimize the molecular potential energy function. The proposed algorithm is called Hybrid Particle Swarm Optimization and Genetic Algorithm (HPSOGA). The proposed HPSOGA algorithm is based on three mechanisms. In the first mechanism, the particle swarm optimization algorithm is applied with its powerful performance with the exploration and the exploitation processes. The second mechanism is based on the dimensionality reduction and the population partitioning processes by dividing the population into sub-population and applying the arithmetical crossover operator on each sub-population. The partitioning idea can improve the diversity search of the proposed algorithm. The last mechanism is to avoid the premature convergence by applying the genetic algorithm mutation operator in the whole population. The combination between these three mechanisms accelerates the search and helps the algorithm to reach to the optimal or near optimal solution in reasonable time.

In order to investigate the general performance of the proposed algorithm, it has been tested on a scalable simplified molecular potential energy function with well-known properties established in [5].

This paper is organized as follows: Section 2 presents the definitions of the molecular energy function and the unconstrained optimization problem. Section 3 overviews the standard particle swarm optimization and genetic algorithms. Section 4 describes in detail the proposed algorithm. Section 5 demonstrates the numerical experimental results. Section 6 summarizes the contribution of this paper along with some future research directions.

2. Description of the problems

2.1. Minimizing the molecular potential energy function

The minimization of the potential energy function problem considered here is taken from [7]. The molecular model considered here consists of a chain of m atoms centered at $x_1, \ldots, x_m$, in a 3-dimensional space. For every pair of consecutive atoms x_i and x_{i+1}, let $r_{i,i+1}$ be the bond length which is the Euclidean distance between them as seen in Fig. 1(a). For every three consecutive atoms x_i, x_{i+1}, x_{i+2}, let $\theta_{i,i+2}$ be the bond angle corresponding to the relative position of the third atom with respect to the line containing the previous two as seen in Fig. 1(b). Likewise, for every four consecutive atoms x_i, x_{i+1}, x_{i+2}, x_{i+3}, let $\omega_{i,i+3}$ be the torsion angle, between the normal through the planes determined by the atoms x_i, x_{i+1}, x_{i+2} and x_{i+1}, x_{i+2}, x_{i+3} as seen in Fig. 1(c).

The force field potentials correspond to bond lengths, bond angles, and torsion angles are defined respectively [11] as

$$\begin{aligned} E_1 &= \sum_{(i,j)\in M_1} c_{ij}^1 \left(r_{ij} - r_{ij}^0\right)^2, \\ E_2 &= \sum_{(i,j)\in M_2} c_{ij}^2 \left(\theta_{ij} - \theta_{ij}^0\right)^2, \\ E_3 &= \sum_{(i,j)\in M_3} c_{ij}^3 \left(1 + \cos\left(3\omega_{ij} - \omega_{ij}^0\right)\right), \end{aligned} \tag{1}$$

where c_{ij}^1 is the bond stretching force constant, c_{ij}^2 is the angle bending force constant, and c_{ij}^3 is the torsion force constant. The constants r_{ij}^0 and θ_{ij}^0 represent the preferred bond length and bond angle, respectively. The constant ω_{ij}^0 is the phase angle that defines the position of the minima. The set of pairs of atoms separated by k covalent bond is denoted by M_k for $k = 1, 2, 3$.

Also, there is a potential E_4 which characterizes the 2-body interaction between every pair of atoms separated by more than two covalent bonds along the chain. We use the following function to represent E_4:

$$E_4 = \sum_{(i,j)\in M_3} \left(\frac{(-1)^i}{r_{ij}}\right), \tag{2}$$

where r_{ij} is the Euclidean distance between atoms x_i and x_j.

The general problem is the minimization of the total molecular potential energy function, $E_1 + E_2 + E_3 + E_4$, leading to the optimal spatial positions of the atoms. To reduce the number of parameters involved in the potentials above, we simplify the problem by considering a chain of carbon atoms.

In most molecular conformational predictions, all covalent bond lengths and covalent bond angles are assumed to be fixed at their equilibrium values r_{ij}^0 and θ_{ij}^0, respectively. Thus, the molecular potential energy function reduces to $E_3 + E_4$ and

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