SCIENCE CHINA
Information Sciences

• LETTER •

May 2020, Vol. 63 159201:1–159201:3
https://doi.org/10.1007/s11432-018-9618-2

# Hybrid quantum particle swarm optimization algorithm and its application

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Received 11 May 2018/Revised 2 August 2018/Accepted 5 September 2018/Published online 10 September 2019

**Citation** Wang Y K, Chen X B. Hybrid quantum particle swarm optimization algorithm and its application. Sci China Inf Sci, 2020, 63(5): 159201, https://doi.org/10.1007/s11432-018-9618-2

Dear editor,

Quantum-behaved particle swarm optimization (QPSO) is an evolutionary algorithm with quantum behavior. It can be used to solve optimization problems by establishing a potential well at the local attraction point to influence the location of particles [1, 2]. The algorithm offers many advantages, such as the requirement of a few parameters, simple operation, and strong convergence ability. It has been applied successfully in many engineering fields. However, for complex multi-modal optimization problems, similar to other algorithms, the QPSO algorithm suffers from premature and poor precision [3]. To enhance population diversity, balance exploration and exploitation abilities, and improve precision of the QPSO algorithm, a hybrid quantum particle swarm optimization (HQPSO) algorithm is proposed in this study. A new global, local, and enhanced search strategy, lévy flight [4] and hopping operation technology, and new convergence speed control method are incorporated into HQPSO. The numerical test results demonstrate that the proposed HQPSO algorithm offers better performance than the other comparison algorithms. This algorithm is applied to the optimization of cluster ground state structure in chemistry (a typical NP problem). The ground state structures of Au($n$) ($n = 12, \ldots, 30$) clusters could be determined successfully.

*Methodology.* In QPSO, it is easy to become trapped into local minimum points owing to poor population diversity. Meanwhile, there are no effective measures to enhance the precision of QPSO in local search [5]. We propose the following improvements to enhance the population diversity, increase convergence speed, and improve convergence precision of the proposed HQPSO algorithm.

(1) A new local attraction point for HQPSO is designed as

$$p_{ij}(t) = \cos(2\pi r_1 C_j(t)) - \sin(2\pi r_2 \mathrm{Pb}_{ij}(t)), \quad (1)$$

where $p_{ij}(t)$ is the local attraction point of the $j$-th dimension of the $i$-th particle; $i = 1, 2, \ldots, M$, $M$ is the population size; $j = 1, 2, \ldots, D$, $D$ is the dimension of the search space; $r_1$ and $r_2$ are uniformly distributed random numbers between 0.0 and 1.0; $\mathrm{Pb}_{ij}(t)$ is the personal best solution of the $j$-th dimension of the $i$-th particle in iteration $t$, and $C_j(t)$ is the $j$-th dimension of the average value of $\mathrm{Pb}_{ij}(t)$.

(2) New global and local search equations are designed. This ensures that HQPSO can execute independent global and local search. If the location of the $i$-th particle is updated using the global search strategy, the new location of the $j$-th dimension of the particle in iteration $t+1$ can be calculated using the following global search equation:

$$X_{ij}(t+1) = X_{ij}(t) + 2\gamma_i |p_{ij}(t) - \mathrm{Pb}_{ij}(t)| \ln\left(\frac{1}{v_i(t)}\right), \quad (2)$$

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where $X_{ij}(t)$ is the location of the $j$-th dimension of the $i$-th particle in iteration $t$; $\gamma_i$ and $v_i$ are uniformly distributed random numbers between 0.0 and 1.0. If the location of the $i$-th particle is updated using the local search strategy, the new particle location in iteration $t+1$ can be calculated using the following local search equation:

$$X_i(t+1) = \mathrm{Pb}_i(t),$$

$$l = \mathrm{fix}(\omega \times D + 1),$$

$$k = \mathrm{fix}(\mu \times M + 1), \quad k \neq i,$$

$$X_{il}(t+1) = \mathrm{Pb}_{il}(t) + (X_{il}(t) - X_{kl}(t))\text{lévy}, \quad (3)$$

where $\mathrm{fix}(\cdot)$ is a function of rounding towards zero; $\omega$ and $\mu$ are uniformly distributed random number between 0.0 and 1.0; lévy is a random vector that obeys Lévy distribution (method for generating lévy vector is shown in Appendix A).

(3) Hopping operation is introduced into HQPSO. This helps HQPSO to be able to jump out of local minima. If the fitness value of $\mathrm{Pb}_i(t)$ is not updated in recent $L$ iterations ($L$ is a positive integer, and it is also an initial parameter set by the algorithm), the $i$-th particle is considered trapped into a local minimum. Then $\mathrm{Pb}_i(t)$ is updated using Eq. (4). Meanwhile, the fitness value $\mathrm{Fb}_i(t)$ of $\mathrm{Pb}_i(t)$ is updated as well.

$$\mathrm{Pb}_i(t+1) = \mathrm{Pb}_i(t) + 0.1(X_{\max} - X_{\min})\theta, \quad (4)$$

where $\theta$ is a $D$-dimensional uniformly distributed random vector between $-1.0$ and 1.0; $X_{\max}$ and $X_{\min}$ are the upper and lower limits of the search range, respectively.

(4) An enhanced search equation for searching the neighborhood of the current best solution is designed as follows:

$$X_i(t+1) = G(t),$$

$$s = \mathrm{fix}(\alpha \times D + 1),$$

$$X_{is}(t+1) = G_s(t) + ((M-i)/M)^5 \lambda(0.5 - \eta), \quad (5)$$

where $\lambda$ is the step length factor; $\alpha$ and $\eta$ are uniformly distributed random numbers between 0.0 and 1.0; $G_s(t)$ is the $s$-th dimension of the globe best solution in iteration $t$. If the location of the $i$-th particle is updated using the enhanced search strategy, the new location of the particle in iteration $t+1$ can be calculated using Eq. (5).

(5) A convergence control parameter $\psi$ is defined. $\psi$ is an iteration dependent parameter and it is calculated as follows:

$$\psi = -0.5\tanh(0.02 \times (t - 0.8T)) + 0.5, \quad (6)$$

where $t$ and $T$ are the number of current iteration and maximum iteration, respectively. $\psi$ is used to control the convergence speed, and avoid premature convergence of HQPSO. The curve of $\psi$ with increasing number of iterations is shown in Appendix B. The proposed HQPSO algorithm is introduced in Algorithm 1.

**Algorithm 1** HQPSO

**Require:** The population size $M$, maximum iteration number $T$, search range $[X_{\min}, X_{\max}]$, step length factors $\lambda$ and parameter $L$;
**Ensure:** Obtain the best solution $G$ and best fitness value Fg of the problem;
$t = 1$; initialize the population, calculate the fitness value of each particle, and record the personal best solution $\mathrm{Pb}_i$ and its fitness $\mathrm{Fb}_i$, the globe best solution $G$ and its fitness Fg;
**while** $t < T$ **do**
  **for** $i$ to $M$ **do**
    **if** rand $< \psi$ ($\psi$ is calculated using Eq. (6)) **then**
      **if** rand $< 0.5$ **then**
        Execute global search strategy using Eq. (2);
      **else**
        Execute local search strategy using Eq. (3);
      **end if**
    **else**
      Execute enhanced search strategy using Eq. (5);
    **end if**
    Calculate the fitness of each new particle; update $\mathrm{Pb}_i$ and $\mathrm{Fb}_i$, $G$ and Fg by using greedy selection method;
    **if** fitness of $\mathrm{Pb}_i$ has not updated in recent $L$ iterations **then**
      Execute hopping operation using Eq. (4);
    **end if**
  **end for**
  $t = t + 1$;
**end while**

From Algorithm 1, we can see that HQPSO has the same probability of global search and local search around $\mathrm{Pb}_i$. It has stronger ability to balance the global and local search than that of QPSO. In the later stage of the search process, the probability of enhanced search around the best solution $G$ will increase rapidly, which is helpful for enhancing the precision and speed of convergence. The proposed HQPSO is evaluated using 18 benchmark functions. It compared with several QPSO-based algorithms (i.e., QPSO, DIR-QPSO [2], HCQPSO [5], and ESH-CQPSO [6]) and a few other recently improved evolutionary algorithms (i.e., SLPSOA, LGWO, EBA, and NoCuSa). The comparison results and statistical analysis are presented in Appendix C. The comparative experimental results demonstrate that HQPSO performs better than the other algorithms in solving major nonlinear functions.

*Application.* A cluster is a micro-structure composed of $2 - 10^4$ atoms or molecules held to-

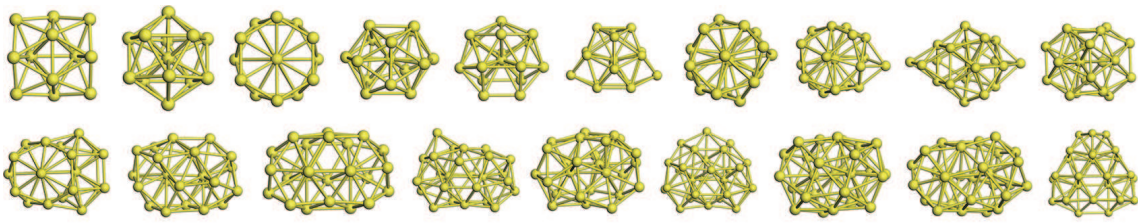

**Figure 1** (Color online) GSTs of Au($n$) ($n = 12, \ldots, 30$) clusters achieved by HQPSO.

gether under physical or chemical forces. Clusters have attracted considerable attention from scientific communities owing to their practical and theoretical applications. In cluster science, searching the ground state structure (GSS) of a cluster is an important and fundamental topic. Mathematically, the GSS is related to the lowest energy structure on the atomic or molecular potential energy surface (PES). Searching for the GSS of a cluster is a typical global optimization problem. The variables to be optimized are coordinates $X \equiv (v_1, \ldots, v_N) \equiv (x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$ of the cluster. The objective function is the potential energy function $E(X)$. The PES of a cluster containing $N$ atoms or molecules has $3N$ degrees of freedom, and the number of local minima points increases exponentially with $N$. GSS search is usually a rather difficult task [7]. In this study, HQPSO is applied to the optimization of an Au cluster formed by the Gupta potential energy function (parameters settings of HQPSO, Gupta function and its parameters for the Au cluster are shown in Appendix D). For each cluster, HQPSO was run 10 times independently, and the best solution was recorded as the GSS coordinates. The GSS of Au($n$) ($n = 12, \ldots, 30$) clusters are obtained successfully by HQPSO and are shown graphically in Figure 1. The energies achieved by HQPSO and the current lowest energies recorded in the literature [8] are presented in Appendix E. It can be seen from the comparison results that the energies achieved by HQPSO are more precise.

*Conclusion.* We introduce a hybrid operation strategy into QPSO, which is called HQPSO, to balance the exploration and exploitation abilities of QPSO and improve search precision. Plots of the distribution figures (Appendix C) show that HQPSO has better population diversity than QPSO. This improves the chances of the algorithm to jump out of local minima and obtain better solutions. By adjusting the control parameter $\psi$, the intensity with which the neighborhood of the current best solution is searched is increased rapidly in the later stages of HQPSO search, thus improving the convergence precision. The lowest energies of Au($n$) ($n = 12, \ldots, 30$) clusters achieved using HQPSO proved that the algorithm can be applied to complex optimization problems. In the future, we will focus on applying the proposed HQPSO algorithm to other real-world optimization problems.

**Acknowledgements** This work was supported by National Natural Science Foundation of China (Grant Nos. 71571091, 71771112, 61473054).

**Supporting information** Appendixes A–E. The supporting information is available online at info.scichina.com and link.springer.com. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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