• Supplementary File •

## Hybrid quantum particle swarm optimization algorithm and its application

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## Appendix A Generation method of Lévy vector

In the HQPSO algorithm, the  $L\acute{e}vy$  vector is generated using the Mantegna rule with  $L\acute{e}vy$  distribution characteristics. In the Mantegna rule, the step length s is designed as follows:

$$s = \frac{u}{|v|^{\frac{1}{\beta}}}.$$
(A1)

where,  $u \sim V(0, \sigma_u^2)$ ,  $v \sim N(0, \sigma_v^2)$ ,  $\sigma_u$  and  $\sigma_v$  are defined as follows:

$$\sigma_v = \left(\frac{\Gamma(1+\beta)\sin(\frac{\pi\beta}{2})}{\Gamma[(1+\beta)/2]\beta 2^{(\beta-1)/2}}\right)^{1/\beta}.$$
(A2)

where,  $\beta = 1.5$ . A three-dimensional (3D) figure of the Lévy flight process is shown in Figure A1.



Figure A1 3D figure of Lévy flight process.

The figure shows that frequently small steps and occasional large steps occur alternately during the process of *Lévy* flight, which helps the algorithm jump out of local minima.

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**Figure B1** Curve of  $\psi(t)$ .

# Appendix C Experimental results and statistical analysis of HQPSO algorithm and other comparison algorithms.

## Appendix C.1 Benchmark functions

To evaluate the performance of HQPSO and compare it with QPSO-based evolutionary (i.e., QPSO [1],DIR-QPSO [2],HC-QPSO [4],and ESH-CQPSO [5]) and other recently improved evolutionary algorithms(i.e., SLPSOA [9], LGWO [10], E-BA [11],and NoCuSa [12]), the benchmark functions listed in Table C1 were tested using the above algorithms. The functions are divided into three classes:  $f_1$  to  $f_7$  are unimodal functions,  $f_8$  to  $f_{13}$  are multimodal functions, and  $f_{14}$  to  $f_{18}$  are rotated and shifted functions. The corresponding dimensions D, range, global minimum values  $f_{opt}$ , and acceptance values of the functions are also listed in Table C1 as well.

 Table C1
 Benchmark functions

Name	Function	D	Range	$f_{opt}$	Acceptance
Shpere	$f_1(x) = \sum_{i=1}^D x_i^2$	30	$[-100, 100]^D$	0	$10^{-6}$
DeJongF4	$f_2(x) = \sum_{i=1}^D i x_i^4$	30	$[-10, 10]^D$	0	$10^{-6}$
Sum Square	$f_3(x) = \sum_{i=1}^D i x_i^2$	30	$[-100, 100]^D$	0	$10^{-6}$
Schwefel 2.21	$f_4(x) = \max(abs(x))$	30	$[-100, 100]^D$	0	$10^{-6}$
Schwefel 2.22	$f_5(x) = \sum_{i=1}^{D}  x_i  + \prod_{i=1}^{D}  x_i $	30	$[-10, 10]^D$	0	$10^{-10}$
Zakharov	$f_6(x) = \sum_{i=1}^{D} x_i^2 + \sum_{i=1}^{D} 0.5ix_i^2 + \sum_{i=1}^{D} 0.5ix_i^4$	30	$[-10, 10]^D$	0	$10^{-6}$
Rosenbrock	$f_7(x) = \sum_{i=1}^{D} [100(x_{i+1} - x_i)^2 + (x_i - 1)^2]$	30	$[-100, 100]^D$	0	28
Ackley	$f_8(x) = -20\exp(-\frac{1}{5}\sqrt{1/\sum_{i=1}^D x_i^2}) - \exp(\frac{1}{D}\sum_{i=1}^D \cos(2\pi x_i)) + 20 + e$	30	$[-32, 32]^D$	0	$10^{-6}$
Schwefel	$f_9(x) = 418.9829D - \sum_{i=1}^{D} x_i \sin( x_i ^{\frac{1}{2}})$	30	$[-500, 500]^D$	0	2500
Alpin	$f_{10}(x) = \sum_{i=1}^{D} abs(x_i \sin x_i + 0.1i)$	30	$[-50, 50]^D$	0	1
Rastrigin	$f_{11}(x) = \sum_{i=1}^{D} (x_i^2 - 10\cos(2\pi x_i) + 10)$	30	$[-5.12, 5.12]^D$	0	$10^{-6}$
Griewank	$f_{12}(x) = \frac{1}{4000} \sum_{i=1}^{D} x_i^2 + \prod_{i=1}^{D} \cos(x_i/\sqrt{i}) + 1$	30	$[-600, 600]^D$	0	$10^{-6}$
Michalewicz	$f_{13}(x) = \sum_{i=1}^{D} \sin(x_i) \sin(ix_i^2/\pi)^{20}$	30	$[0,\pi]^D$	-	-18
Shifted	$f_{i}(m) = \sum_{i=1}^{D} i(m - \sqrt{i})^2$	20	[100, 100]D	0	10-6
Sum Square	$\int 14(x) - \sum_{i=1} i(x_i - \sqrt{i})$	30	[-100, 100]	0	10
Shifted	$f_{15}(x) = \sum_{i=1}^{D} [100(y_{i+1} - y_i)^2 + (y_i - 1)^2] + 390,$	20	$[100, 100]^D$	200	400
Rosenbrock	$y_i = x_i - \sqrt{i}$	30	[-100, 100]	390	490
Shifted	$f_{16}(x) = \sum_{i=1}^{D} (y_i^2 - 10\cos(2\pi y_i) + 10),$	30	[512512]D	0	10 - 6
Rastrigin	$y_i = x_i - rac{i}{D}$	30	[-0.12, 0.12]	0	10
Rotated	$f_{17}(x) = \frac{1}{4000} \sum_{i=1}^{D} y_i^2 + \prod_{i=1}^{D} \cos(y_i/\sqrt{i}) + 1,$	20	[ 600 600]D	0	$10^{-6}$
Griewank	where $y = Mx, M$ is an orthogonal matrix	30	[-000,000]	0	10
Rotated	$f_{18}(x) = \sum_{i=1}^{D} (y_i^2 - 10\cos(2\pi y_i) + 10),$	20	[ 5 19 5 19] <i>D</i>	0	$10^{-6}$
Rastrigin	where $y = Mx, M$ is an orthogonal matrix	30	[-5.12, 5.12]	0	10

## Appendix C.2 Comparisons with other QPSOs

## Appendix C.2.1 Parameter settings of HQPSO and other QPSOs

The parameter settings of HQPSO and other QSPOs are given in Table C2, where the parameter settings of the comparison algorithms are based on the suggestions in the corresponding references.

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Algorithm	Reference	Parameters
QPSO	$\operatorname{Ref.}[1]$	$\alpha_{max} = 1, \alpha_{min} = 0.5$
DIR-QPSO	$\operatorname{Ref.}[2]$	$\alpha_{max} = 1, \alpha_{min} = 0.5, N_{s1} = N_{s2}$
HCQPSO	$\operatorname{Ref.}[4]$	$\alpha_{max} = 1, \alpha_{min} = 0.5$
ESH-CQPSO	$\operatorname{Ref.}[5]$	$\alpha_{max} = 1, \alpha_{min} = 0.5$
HQPSO	Present	$\lambda = 3, L = 10$

Table C2	Parameters	settings of	of algorithms	used in	the comparisons
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## Appendix C.2.2 Population diversity analysis of HQPSO and QPSO

To illustrate the details of the population diversity in QPSO and HQPSO, we take two two-dimensional(2D) test functions as an example. One is the unimodal Sphere function  $(f_2)$ , and the other is the multimodal Griewank function  $(f_{12})$ , where the space range is [-10, 10]). Firstly, we obverse the population diversity of QPSO and HQPSO through the distributions of the points during the search process. For the two minimization problems, the population size is 30 and the number of maximum iterations is 1000 for both algorithms. The distributions of the points during the search process are observed and shown in Figure C1.



Figure C1 Comparison of distributions between QPSO and HQPSO algorithms.

It can be seen from Figure C1 that HDPSO produces a wider range of points than that of QPSO. Therefore, HQPSO has stronger abilities to lead the swarm escape from local minima.

Second, we use a diversity measure [8] to analyze the changes in diversity during the QPSO and HPSO search process. In this letter, the diversity measure is a new distance to best point measure defined as follows:

$$divs = \frac{1}{M(X_{max} - X_{min})^2} \sum_{i=1}^{N} \sqrt{\sum_{j=1}^{D} (x_{ij} - x_j^*)^2}$$
(C1)

where M denotes population size;  $X_{max}$  and  $X_{min}$  the are upper and lower limits of the search spaces, respectively; D denotes problem dimension;  $x_{ij}$  is the value of the *j*th dimension of the *i*th individual, and  $x_j^*$  is the value of the *j*th dimension of the current best point. A low divs value indicates that the swarm has clustered in a small region. Conversely, a high divs value indicates that the swarm has scattered over in a wide region. Hence, the diversity could be considered together with the problem and the search process of the algorithm. In this test, for the QPSO and HQPSO algorithms, the population size N is 50, problem dimension is 30 and the number of maximum iterations is 1000. The change in diversity during the search process is recorded in Figure C2.



Figure C2 Diversity comparison between QPSO and HQPSO algorithms.

Figure C2 shows that the diversity of QPSO decreases rapidly with increasing iteration number, so the algorithm can very easily fall into local minima. The diversity of HQPSO can be maintained at a certain level, except in the later stages of the search process, and it has stronger abilities to lead swarm escape from local minima. In the later stages, the rapidly decreasing diversity beneficial for enhancing the convergence precision of HQPSO.

### Appendix C.2.3 Experimental results and discussion

In this subsection, the proposed HQPSO is compared with QPSO, DIR-QPSO, HCQPSO, and ESH-CQPSO. For fair comparison, all algorithms were tested using the same population size M = 50 and the same maximum number of iterations T = 1000. In each trial, each algorithm was run 30 times independently on each test function.

#### 1. Comparisons of convergence precision

The comparison results of convergence precision between HQPSO and other QPSOs are listed in Table C3, where "Mean" indicates the average of best fitness values averaged over 30 runs. "Std. Dev" denotes the standard deviation. The best values are highlighted in bold font. From the results in Table C3, we can draw the following conclusions:

(1) In the case of the unimodal functions, HQPSO and ESH-CQPSO could obtain the global best solution of  $f_2$  in each trial. On functions other than  $f_2$ , HQPSO outperformed the other algorithms. QPSO performed badly on all unimodal functions, and loses in  $f_6$  and  $f_7$ . As for  $f_7$ , only HQPSO achieved satisfactory performance. To sum up, HQPSO performed better than the other algorithms on the selected unimodal functions.

(2) As for multimodal functions, HQPSO, HCQPSO, and ESH-CPQSO can obtain the global best solution on  $f_{11}$ . DIR-QPSO, HQPSO, HCQPSO, and ESH-CPQSO can obtain the global best solution on  $f_{12}$ . As for  $f_7$ ,  $f_{10}$ , and  $f_{13}$ , the best performance was achieved by HQPSO. As for  $f_8$ , the best performance was achieved by DIR-QPSO, ESH-CQPSO, and HQPSO, and their best values, worst values, mean values, and standard deviations reached 8.8817e-016, 8.8817e-016, 8.8817e-016, and 0, respectively. As for  $f_9$ , HQPSO lost only to DIR-QPSO in terms of Best and mean values, and its performance was considerably better than that of the other algorithms. Therefore, we can conclude that HQPSO has better performance than the other algorithms on the selected multimodal functions.

(3) On the rotated and shifted functions, HQPSO performed satisfactorily on  $f_{14}$  to  $f_{18}$  and lost out only to ESH-CQPSO on  $f_{17}$ . From Table C3, the best Std.Dev was achieved by HQPSO on all test functions except  $f_{17}$ . The lower Std.Dev illustrates that HQPSO has better stability. Meanwhile, convergence comparisons of all the algorithms are shown graphically in Figure C3. These comparisons confirm the results presented in Table C3.

From Table C3, the best Std.Dev is achieved by HQPSO on all test functions except  $f_{17}$ . The lower Std.Dev illustrates that HQPSO is of better stability. Meanwhile, the convergence comparisons of all algorithms are graphically shown in Figure C3. It confirms the results in Table C3.

## 2. Comparisons on convergence speed

In solving real-world problems, fitness evaluation (FE) time overwhelms the algorithm overhead. Hence, for comparing convergence speed, the mean FE(FEs) required to reach an acceptable accuracy level would be considerably more interesting than CPU time [6]. In this letter, the FEs required to arrive at acceptable solutions in the successful runs are listed in Table C4. The best result is shown in bold font. If an algorithm can not reach its acceptable value in the search process, its FEs is denoted by " $\times$ ".

 ${\bf Table \ C3} \quad {\rm Statistical \ results \ on \ test \ functions}$ 

Algorithm	Statistics	$f_1$	$f_2$	$f_3$	$f_4$	$f_5$	$f_6$
	Best	7.8660e-069	9.2646e-115	3.4242e-068	5.7739e-022	8.3403e-040	6.7463e-010
	Worst	8.6563e-065	6.0899e-107	5.2459e-060	2.5132e-019	3.2618e-038	9.2301e-006
QPSO	Mean	4.4739e-065	9.1765e-108	4.7531e-063	3.7184e-020	7.7575e-039	1.8392e-006
	Std.Dev	5.0442e-130	4.2097e-214	6.4574e-126	5.4133e-039	1.2058e-076	6.4335e-012
	Best	3.6258e-162	1.4535e-323	8.2134e-196	1.6902e-086	7.1579e-100	1.4245e-161
	Worst	1.1534e-121	7.0284e-258	7.4245e-104	1.9809e-070	2.2965e-078	4.2981e-125
DIR-QPSO	Mean	1.1543e-122	6.0315e-259	6.3532e-132	2.0627e-071	2.0917e-079	5.7302e-132
	Std.Dev	5.8404e-243	0	7.3760e-238	3.5387e-141	4.7929e-157	3.2421e-261
	Best	1.2953e-184	1.5363e-311	3.3224e-183	1.1059e-146	7.1333e-082	3.4294e-301
	Worst	6.4249e-156	1.7571e-309	4.5324e-150	5.4612e-093	7.1482e-072	4.5204e-202
HCQPSO	Mean	6 4249e-157	1.0123e-310	3 5356e-151	4 9697e-094	6 5098e-073	3 5294e-203
	Std Dev	4 1279e-312	0	2.5363e-300	2 7108e-186	4 6436e-144	0
	Best	$3.7912e_{-216}$	0	4 2243e-207	1.4883e-105	2.0712e-120	2 3572e-218
	Worst	3.8951 - 178	0	3 67430-168	1.40000-100	$1.1572e_{-101}$	1 1/350-168
ESH-CQPSO	Moon	3.8951e-178	0	3 63520 160	4.01826-082	1.13726-101	2.34520.160
	Std Dov	0	0	0	4.13326-082	1.07516-102	2.3452e-109 $2.0471e^{-317}$
	Boot	1 20250 200	0	0	7 02800 150	1.2127e-203	2.04716-317
	Worst	1.30336-309	0	9 56490 997	1.0380e-150	3.4242e-227	U 9 56910 915
HQPSO	Moon	4.89526-230	0	3.30430-237	4.84416-100	4.2342e-103	3.5051e-215 4 5674o 241
	Std Dev	4.5001e-251	0	0	2 1331 <sub>0-</sub> 212	2 917/e-336	4.00746-241
	Dtd.Dev	f <sub>7</sub>	f <sub>o</sub>	fo	f10	2.3174e-330	f10
	Bost	28.08669	J8 8 85470-016		5 97397	5 4352	9.31960-006
	Worst	28.00003	4 44080 015	$0.30760 \pm 003$	73 2201	$1.3246_{0} \pm 0.02$	0.0221
QPSO	Moon	28.3092	4.4408e-015	$9.30700\pm003$	18 2014	20 0202	0.0251
	Std Dov	28.1014	4.1179e-015	$5.90350\pm003$	16.3914	$1.6426_{0} \pm 0.02$	2.65700.004
	Dest	0.0038	1.1474e-030	3.2043e+004	$5.50200\pm002$	2 4225	2.03796-004
	Wanat	27.2340	8.8817e-010	3.8182e-004	0.7000	2.4220	0
DIR-QPSO	Worst	27.0334	8.8817e-010	3.7949e + 003	0.7000	9.55540+001	0
	Mean	27.4395	8.8817e-016	1.1686e+003	0.1083	21.0890	0
	Std.Dev	0.0168	0	2.0859e + 006	0.0644	1.9342e+003	0
	Best	20.5518	4.4408-015	$7.4034e \pm 003$	0.3000	0	0
HCQPSO	Worst	26.8177	7.9936e-015	8.5963e+003	11.3000	0	0
	Mean	26.6965	6.0557e-015	8.1559e+003	3.7916	0	0
	Std.Dev	0.0077	3.4423e-030	1.2726e + 005	8.9990	0	0
	Best	9.9025e-014	8.8817e-016	3.9583e+003	0.2000	0	0
ESH-CQPSO	Worst	22.86823	8.8817e-016	5.2797e+003	4.7000	0	0
	Mean	2.0789	8.8817e-016	4.5014e + 003	1.8833	0	0
	Std.Dev	47.5413	0	2.0521e + 005	1.8815	0	0
	Best	4.4674e-018	8.8817e-016	1.6367e + 003	4.7220e-006	0	0
HQPSO	Worst	2.0489e-009	8.8817e-016	2.3065e+003	4.5278e-004	0	0
	Mean	2.5250e-010	8.8817e-016	1.9470e+003	1.4736e-004	0	0
	Std.Dev	4.0164e-019	0	4.0381e+004	1.3962e-008	0	0
		<i>f</i> 13	<i>f</i> 14	<i>f</i> 15	<i>f</i> <sub>16</sub>	<i>f</i> 17	<i>f</i> 18
	Best	-20.6514	1.5538e-008	4.1480e + 002	9.5448	2.0144e-011	16.1655
QPSO	Worst	-12.5972	3.2287e-006	1.1922e + 003	41.2121	0.0467	32.9471
	Mean	-15.0762	4.6135e-007	6.4062e+002	26.3916	0.0139	23.9673
	Std.Dev	7.9384	8.7674e-013	1.1197e + 005	73.6934	2.9293e-004	21.0433
	Best	-20.9575	1.7543e-007	4.0439e+002	19.8995	5.5178e-014	3.1942e-004
DIR-QPSO	Worst	-13.5859	9.2656e-006	4.1726e+002	43.7786	2.0838e-013	0.0011
-	Mean	-18.5097	1.4439e-006	4.0714e + 002	26.7981	1.1562e-013	5.9164e-004
	Std.Dev	4.3585	6.8737e-012	13.1782	36.8351	2.0960e-027	5.4644e-008
HCQPSO	Best	-15.3225	4.3099e-008	4.1982e + 002	0.0353	1.2741e-009	0.0055
-	Worst	-9.5057	2.7781e-007	4.9759e + 002	3.01185	2.9893e-007	0.0195

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Algorithm	Statistics	$f_{13}$	$f_{14}$	$f_{15}$	$f_{16}$	$f_{17}$	$f_{18}$
	Mean	-11.4797	1.0232e-007	4.4284e + 002	1.3936	4.2209e-008	0.0106
	$\operatorname{Std.Dev}$	2.6859	4.7773e-015	4.8276e + 002	0.8775	6.7702 e- 015	9.7929e-006
	Best	-20.5971	5.0467 e-004	4.0242e + 002	0.0188	0	0.0112
ESH-CQPSO	Worst	-18.0571	0.0033	5.2325e + 002	0.0648	0	0.0556
	Mean	-19.0912	0.0015	4.2604e + 002	0.0383	0	0.0321
	$\operatorname{Std.Dev}$	0.8222	5.6207 e-0076	1.3187e + 003	1.6321e-004	0	1.6129e-004
	Best	-21.5724	1.8009e-011	$4.0038\mathrm{e}{+002}$	2.1232 e-013	0	$4.5474 \mathrm{e}{-013}$
HOPSO	Worst	-18.6207	1.1681e-009	$4.1159\mathrm{e}{+002}$	4.6361e-010	2.2204e-016	$6.7643 \mathrm{e}{\textbf{-}} 012$
HQPSO	Mean	-20.5760	2.6934 e - 010	$4.0652\mathrm{e}{+002}$	7.6537 e-011	3.7007 e-017	1.6029 e-012
	$\operatorname{Std.Dev}$	0.6765	1.6578 e - 019	8.2104	2.3526e-022	5.2291e-033	2.7202e-024











Figure C3 Comparisons of convergence speed.

From the results in Table C4, the convergence speed of the improved QPSO algorithms is significantly better than that of QPSO. DIR-QPSO has the best convergence speed on  $f_1, f_2, f_3, f_4, f_5, f_8, f_9$ , and  $f_{12}$ . HQPSO has the best convergence speed on  $f_7$ ,  $f_{10}$ ,  $f_{11}$ ,  $f_{13}$ ,  $f_{14}$ ,  $f_{15}$ ,  $f_{16}$ ,  $f_{17}$ , and  $f_{18}$ . HCQPSO has the best convergence speed only on  $f_6$ . HQPSO successfully reached the acceptance value on all test functions, DIR-QPSO lost in  $f_1, f_{12}, f_{16}$ , and  $f_{18}$ , and HCQPSO lost in  $f_{11}, f_{12}, f_{16}$ , and  $f_{18}$ . QPSO had the worst performance in the comparison algorithms, and its success rate on all test functions was only 67%. The most interesting result was that HQPSO converged faster on multimodal, shifted, and rotated functions; thus, DIR-QPSO has better convergence speed on unimodal functions. In real-world problems, multimodal, shifted, and rotated functions are more common, so HQPSO is more suitable for solving real-world optimization problems.

Table C4 Statistical results of FEs on test functions

Algorithm	$f_1$	$f_2$	$f_3$	$f_4$	$f_5$	$f_6$	$f_7$	$f_8$	$f_9$
QPSO	25246	22811	25413	25004	26334	31647	×	29524	×
DIR-QPSO	3414	2263	3645	3424	3346	9147	48051	3435	6061
HCQPSO	3607	3341	4157	3864	4327	4645	47775	16566	×
ESH-CQPSO	8352	4342	8962	10057	4711	11611	19534	9252	×
HQPSO	7643	4118	8014	8433	4432	10323	14439	8948	39547
	$f_{10}$	$f_{11}$	$f_{12}$	$f_{13}$	$f_{14}$	$f_{15}$	$f_{16}$	$f_{17}$	$f_{18}$
QPSO	×	×	×	×	×	47109	×	×	×
DIR-QPSO	21824	×	4213	29613	×	34333	×	44102	×
HCQPSO	×	8322	4542	×	48217	43404	×	37632	×
ESH-CQPSO	×	3314	10150	29441	×	46301	×	31229	×
HQPSO	10137	3071	9264	26642	42338	33639	260570	10233	20341

### 3. Comparison on other indicators

To further illustrate the superiority of the proposed HQPSO algorithm, comparison results of success rate (SR, the percentage of successful runs in which acceptable solutions are obtained), "w/t/l" and ranking performances (ranking by mean value listed in table C3) among HQPSO and the other compared algorithms are listed in Table C5. Here, SR stands for the probability that the tested algorithm has successfully reached the acceptance value for each tested function, and

"w/t/" means that the HQPSO wins against w algorithms, ties with t algorithms, and loses against l algorithms, compared to other QPSO algorithms.

Algorithm		$f_1$	$f_2$	$f_3$	$f_4$	$f_5$	$f_6$	$f_7$	$f_8$	$f_9$
	SR(%)	100	100	100	100	100	63	0	100	0
QPSO	w/t/l	0/0/4	0/0/4	0/0/4	0/0/4	0/0/4	0/0/4	0/0/4	1/0/3	0/0/4
	Rank	5	5	5	5	5	5	5	4	5
	$\mathrm{SR}(\%)$	100	100	100	100	100	100	100	100	80
DIR-QPSO	w/t/l	2/0/1	1/0/3	3/0/1	3/0/1	2/0/2	3/0/1	1/0/3	2/0/2	4/0/0
	Rank	4	4	2	2	3	2	4	3	1
	$\mathrm{SR}(\%)$	100	100	100	100	100	100	100	0	0
HCQPSO	w/t/l	0/0/3	2/0/2	2/0/2	1/0/3	1/0/3	1/0/3	2/0/2	0/0/4	1/0/3
	Rank	3	3	3	4	4	4	3	5	4
	$\mathrm{SR}(\%)$	100	100	100	100	100	100	100	100	0
ESH-CQPSO	w/t/l	1/0/2	3/1/0	1/0/3	2/0/2	3/0/1	2/0/2	3/0/1	3/1/0	2/0/2
	Rank	2	1	4	3	2	3	2	1	3
	$\mathrm{SR}(\%)$	100	100	100	100	100	100	100	100	100
HQPSO	w/t/l	4/0/0	3/1/0	4/0/0	4/0/0	4/0/0	4/0/0	4/0/0	3/1/0	3/0/1
	Rank	1	1	1	1	1	1	1	1	2
		$f_{10}$	$f_{11}$	$f_{12}$	$f_{13}$	$f_{14}$	$f_{15}$	$f_{16}$	$f_{17}$	$f_{18}$
	SR(%)	0	43	0	0	73	40	0	80	0
QPSO	w/t/l	0/0/4	0/0/4	0/0/4	0/4/0	2/0/2	0/0/4	1/0/3	0/0/4	0/0/4
	Rank	5	5	5	4	3	5	4	5	5
	$\mathrm{SR}(\%)$	100	83	100	50	53	100	0	100	0
DIR-QPSO	w/t/l	3/0/1	1/0/3	1/3/0	2/0/2	1/0/3	3/0/1	0/0/4	2/0/2	3/0/1
	Rank	2	4	1	3	4	2	5	3	2
	$\mathrm{SR}(\%)$	0	100	100	0	100	93	0	100	0
HCQPSO	w/t/l	1/0/3	2/2/0	1/3/0	0/0/4	3/0/1	1/0/3	2/2/0	1/0/3	2/0/2
	Rank	4	1	1	5	2	4	3	4	3
	$\mathrm{SR}(\%)$	0	100	100	100	0	77	0	100	0
ESH-CQPSO	w/t/l	2/0/2	2/2/0	1/3/0	3/0/1	0/0/4	2/0/2	3/1/0	4/0/0	1/0/3
	Rank	3	1	1	2	5	3	2	1	4
	$\mathrm{SR}(\%)$	100	100	100	100	100	100	100	100	100
HQPSO	w/t/l	4/0/0	2/2/0	1/3/0	4/0/0	4/0/0	4/0/0	4/0/0	3/0/1	4/0/0
	Rank	1	1	1	1	1	1	1	1	2

**Table C5** Statistical results of SR, "w/t/l" and ranking performance

Form table C5, HQPSO has a 100% success rate on all test functions. HQPSO has rank "1" on all test functions, except  $f_9$  and  $f_{917}$ . As for  $f_9$  and  $f_{917}$ , HQPSO lost only against DIR-QPSO and ESH-CQPSO, respectively. TableC6 provides an overall comparison among all QPSOs. The total rank and final rank of each comparison algorithm are listed in TableC6.

Table C6 Total and final rank of each comparison algorithm

Rank –			Algoritm		
	QPSO	DIR-QPSO	HCQPSO	ESH-CQPSO	HQPSO
Total rank	85	51	60	42	20
Final rank	5	3	4	2	1

From the results presented in Table C6, HQBPSO achieved the lowest total rank, that is, "20", and the best final rank, that is, "1". This indicates that HQPSO is superior in terms of overall performance on all test functions than the other algorithms. We can obviously observe that the total rank value of HQPSO is considerably less than that of the other algorithms. This indicates that the overall performance of HQPSO is considerably better than that of the other algorithms.

## Appendix C.3 Comparisons with other recently improved evolutionary algorithms

To further illustrate the superiority of the proposed HQPSO algorithm, we compare it with the other recently improved evolutionary algorithms listed in Table C7.

Table C7 Comparison algorithms and their parameters settings

Algorithm	Reference	year	parameters
SLPSOA	Ref.[9]	2017	$M=10, \alpha=0.1, G=5$
LGWO	Ref.[10]	2017	$\alpha_0 = 2, \beta \sim U(0, 1), p \sim U(0, 1),$
$\operatorname{EBA}$	Ref.[11]	2017	$r_0 = 0.1, A_0 = 0.95, f_{min} = 0, f_{max} = 2, Limit1 = 0.8, Limit2 = 0.5$
NoCuSa	Ref.[12]	2017	$pa = 0.3, \alpha = 1.1, \beta = 1.7, \delta = 1.6$
HQPSO	Present	_	$\lambda = 3, L = 10$
SLPSOA LGWO EBA NoCuSa HQPSO	Ref.[9] Ref.[10] Ref.[11] Ref.[12] Present	2017 2017 2017 2017 	$\begin{split} M &= 10, \alpha = 0.1, G = 5\\ \alpha_0 &= 2, \beta \sim U(0,1), p \sim U(0,1),\\ r_0 &= 0.1, A_0 = 0.95, f_{min} = 0, f_{max} = 2, Limit1 = 0.8, Limit2 = 0.5\\ pa &= 0.3, \alpha = 1.1, \beta = 1.7, \delta = 1.6\\ \lambda &= 3, L = 10 \end{split}$

These algorithms include scatter learning particle swarm optimization algorithm (SLPSOA) [9], grey wolf optimization algorithm with Lvy flight (LGWO) [10], enhanced bat algorithm with mutation operator (EBA) [11], and nonhomogeneous cuckoo search algorithm based on quantum Mechanism (NoCuSa) [12]. For a fair comparison, all algorithms were tested using the same population size M = 50, except NoCuSa (NoCuSa evaluates fitness twice per iteration, and the population size M = 25), and the same maximum number of iterations T = 1000. In each trial, each algorithm was run 30 times independently, and the dimension of each selected function was 40. The acceptance value of  $f_{13}$  was -24, and the other selected functions are listed based on their acceptance values in TableC1.

Table C8 Comparison results with other evolutionary algorithms

Algorithm	Statistics	$f_1$	$f_3$	$f_5$	$f_7$	$f_9$	$f_{11}$
	Mean	3.4524e-036	1.5309e-041	1.0391e-63	0.8371	21.4562	7.3928e-06
SLPSOA	$\operatorname{Std}$ .Dev	1.4292e-071	3.3940e-080	3.8374e-122	0.2109	4.2983	4.5729e-10
	FEs	21409	23502	11093	15072	27832	10352
	Mean	2.3442e-028	5.3492e-032	5.4534e-e41	12.3343	2.9203e + 003	0.1235
LGWO	$\operatorname{Std}$ .Dev	1.3424e-41	3.4933e-056	3.2040e-78	3.2349	4.4245e + 005	1.0134
	FEs	9327	8429	12764	15357	×	×
	Mean	2.3031e-201	5.3924e-223	0	6.3456	2.6434e + 003	0
EBA	$\operatorname{Std}$ .Dev	0	0	0	1.4029	$1.4535e{+}005$	0
	FEs	8164	8915	4319	13641	×	4165
	Mean	3.0931e-136	3.0493e-153	3.9284e-114	4.2134	3.3294e + 003	4.5920e-006
NoCuSa	$\operatorname{Std}$ .Dev	1.3423e-270	5.3824e-301	1.9238e-225	1.2904	6.3123e + 005	1.3947 e-011
	FEs	9103	8130	8279	16837	×	9712
	Mean	2.4713e-227	7.5374 e - 261	3.9204e-151	1.7886e-08	$2.2465e{+}003$	0
HQPSO	$\operatorname{Std}$ .Dev	0	0	1.1037e-300	8.6573 e - 017	$4.0483e{+}004$	0
	FEs	8148	8313	4764	14952	41546	4354
		$f_{13}$	$f_{14}$	$f_{15}$	$f_{16}$	$f_{17}$	$f_{18}$
	Mean	-24.2943	1.4829e-007	4.1984e + 002	1.2938e-007	3.4342e-007	1.6464 e-010
SLPSOA	$\operatorname{Std}$ .Dev	1.2901	2.1947e-013	17.3903	3.2298e-011	1.3985e-014	6.3019e-020
	FEs	41094	48293	34013	27439	15432	23410
	Mean	-17.4452	4.5367 e-007	4.3436e + 002	4.4214	2.3552e-011	0.1343
LGWO	$\operatorname{Std}$ .Dev	4.2983	1.3940e-012	17.4354	2.4512	1.3435e-010	1.1372
	FEs	$\times$ 45354	37548	×	13563	×	
	Mean	-9.3247	4.9204 e - 008	4.6453e + 002	9.3942	1.3944e-014	3.4920e-009
EBA	$\operatorname{Std}$ .Dev	0.9345	7.3534e-015	15.7453	4.6361	2.3492e-027	1.0293e-015
	FEs	×	45635	35245	×	11204	23532
	Mean	-25.4521	2.3903e-007	4.8214e + 002	5.2942	7.3054e-08	1.3948e-007
NoCuSa	$\operatorname{Std}$ .Dev	2.4124	1.4920e-014	23.4209	2.2391	1.3428e-015	5.2304 e-013
	FEs	43357	47292	41045	×	13871	23492
	Mean	-25.6128	4.3491e-09	$4.1703 \mathrm{e}{+002}$	7.2014e-010	1.5829e-016	9.4903e-012
HQPSO	$\operatorname{Std}$ . $\operatorname{Dev}$	2.3620	6.4920 e - 017	12.9203	1.4830e-020	3.5929e-031	1.0949 e- 023
	FEs	39463	45564	33902	26305	10552	20737

Form Table C8, HQPSO and SLPSOA have 100% success rate on all selected functions. LGWO loses on  $f_9$ ,  $f_{11}$ ,  $f_{13}$ ,  $f_{16}$ , and  $f_{18}$ ; EBA loses on  $f_9$ ,  $f_{13}$ , and  $f_{16}$ ; And NoCuSa loses on  $f_9$  and  $f_{16}$ . HQPSO achieved the best performance of convergence precision on  $f_1$ ,  $f_2$ ,  $f_7$ , and  $f_{13}$  to  $f_{18}$ , and achieved the best convergence speed on all test functions except  $f_3$ ,  $f_5$ ,  $f_9$ , and  $f_{11}$ . HQPSO has the most promising performance among these algorithms on the selected functions.



Figure C4 Statistical results of HQPSO on high-dimensional functions.

### Appendix C.3.1 Adaptability of HQPSO to high-dimensional functions

In this subsection, the adaptability of HQPSO to high-dimensional functions is shown in Figure C4. In Figure C4, all selected functions were tested using the same population size M = 50 and the same maximum number of iterations T = 2000. For all selected functions,  $f_2$ ,  $f_4$ , and  $f_6$  are unimodal functions;  $f_8$ ,  $f_{10}$ , and  $f_{12}$  are multimodal functions; and  $f_{14}$ ,  $f_{16}$ , and  $f_{18}$  are rotated and shifted functions. To better illustrate the adaptability of HQPSO to high-dimensional functions, five different dimensions (i.e., 50, 60, 70, 80, and 100) are considered for each test function. In each trial, HQPSO was run 30 times independently on each dimension of the test functions. Each boxplot in Figure C4 shows the statistical results of the best fitness values achieved by HQPSO.

Figure C4 shows that HQPSO successfully achieves the acceptance value listed in Table C1 on all selected test functions, except  $f_{10}$ ,  $f_{14}$  and  $f_{16}$ . The most interesting result is that the statistical results of each test function worsen with increasing dimensions, except  $f_8$ . For the maximum number of iteration T = 5000, the statistical results of  $f_{10}$ ,  $f_{14}$ , and  $f_{16}$  are shown in Figure C5. Figure C5 shows that HQPSO successfully achieves the acceptance value on  $f_{10}$ ,  $f_{14}$ , and  $f_{16}$ when T = 5000. Therefore, we can conclude that it will become increasingly difficult for HQPSO to obtain the optimal solution with increasing dimensions, and the problem can be solved by increasing the number of iterations.

From the comparison results of all test algorithms and the adaptability of the HQPO algorithm on high-dimensional functions, we can conclude that the proposed HQPO performed better than the other algorithms. It had better convergence precision, speed and stability, and could complete the optimization of complex high-dimensional functions.



**Figure C5** Statistical results of  $f_{10}$ ,  $f_{14}$ , and  $f_{16}(T = 5000)$ .

# Appendix D Parameters settings of HQPSO, Gupta function and its parameters for Au cluster.

The parameters of the HQPSO algorithm were set as follows: search range [-5, 5], population size M = 100, max iteration number  $T = 10^5$ ,  $\lambda = 0.001$ , and L = 30.

The equation of the Gupta potential function is as follows:

$$V = \sum_{i} \left( \sum_{j(\neq i)} A \exp(-p(\frac{r_{ij}}{r_0} - 1)) - \sqrt{\sum_{j(\neq i)} \xi^2 \exp(-2q(\frac{r_{ij}}{r_0} - 1))} \right)$$
(D1)

where,  $r_{ij}$  is the distance of the *i*th and *j*th atoms; For Au cluster, A = 0.1156eV, p = 16.980, q = 2.691,  $\xi = 2.289eV$  and  $r_0 = 2.71 \text{ Å}[8]$ .

# Appendix E Energy comparison results achieved using HQPSO and the current best value [8].

		00 1 1		
No.	n	Ea	Eb	
1	12	-38.92256917465254	-38.92256917	
2	13	-42.55493083681036	-42.55493084	
3	14	-45.95827566086828	-45.95827566	
4	15	-49.50545131022577	-49.50545129	
5	16	-53.05765637989333	-53.05765637	
6	17	-56.54939854621972	-56.54939854	
7	18	-60.01051500664349	-60.01051500	
8	19	-63.43510905636050	-63.43510905	
9	20	-66.86962079634721	-66.86962080	
10	21	-70.35745012379466	-70.35745012	
11	22	-73.92076803655492	-73.92076803	
12	23	-77.47804456077746	-77.47804456	
13	24	-81.00593616084861	-81.00593615	
14	25	-84.43636253003858	-84.43636252	
15	26	-87.93389515032121	-87.93389515	
16	27	-91.50188836846107	-91.50188836	
17	28	-95.03354850404784	-95.03354849	
18	29	-98.62039883108864	-98.62039882	
19	30	-102.2182980311356	-102.21829802	

**Table E1** Energy comparisons of Au (n = 12 - 30) clusters

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