Using Double Well Function as a Benchmark Function for Optimization Algorithm

IEEE Congress on Evolutionary Computation
28.06-1.07.2021 Kraków, Poland (VIRTUAL)

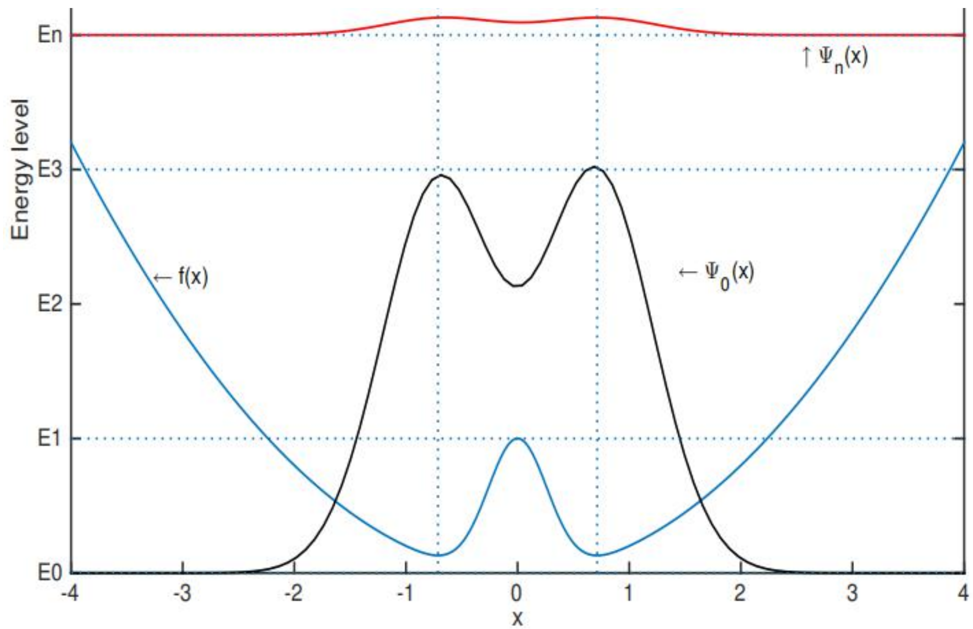
Peng Wang
School of Computer Science and Engineering
Southwest Minzu University
Chengdu, China
qhoalab@163.com

Guosong Yang
Chengdu Institute of computer application
Chinese Academy of Sciences
School of Computer Science and Engineering
Southwest Minzu University
Chengdu, China
University of Chinese Academy of Sciences
Beijing, China
yangguosong19@mails.ucas.ac.cn

Contents

History of double well function

- The double well function (DWF) is an important model originating from quantum physics and has been used as a model for decades to analyze energy, wave function, and tunnel effect [1].



The DWF f(x) used in quantum physics and it energy E_i and wave fuction $\Psi n(x)$

- Moreover, in structural chemistry, the interaction between molecules and atom clusters can often be described by the DWF (NH_3 and PH_3).

DWF and structural chemistry

- Generally, the lower the energy of the molecule system, the more stable the structure is.

- If we view the formation process of the molecular structure as an optimization problem that aims to seek the architecture with the lowest potential energy, it would then be quite natural that the DWF can be used as a benchmark function to test the performance of the optimization algorithm.

corresponding to

Global minimum of the DWF ⟷ Position of the given particle with minimum potential

Fitness of the objective function ⟷ Potential energy to be minimized

Study background

- The Lennard-Jones potential and optimization algorithms are widely used together to seek the structure of atom cluster with the lowest energy [5].
- Functions such as Ackley, Griewank, and Rosenbrock are all benchmark functions with many local minima[6].
- DWF has been applied to test quantum-inspired optimization algorithms [7, 8] and demonstrate the principle of quantum annealing [9] used for optimization problems without a thorough research.
- Therefore, it would be interesting and necessary to study the possibility of using a high-dimensional DWF as a benchmark function for the optimization algorithm.

II. DOUBLE WELL AND ITS MATHEMATICAL ANALYSIS

A. One-dimensional double well function

- A typical DWP can be determined through by:

$$f(x) = h\frac{\left(x^2 - l^2\right)^2}{l^4} + kx \tag{1}$$

where $h > 0$, $l > 0$, and $k \geq 0$. Evidently, the curve of $f(x)$ passes through the fixed point $(0, h)$.

- Linear transformation: let $k_1 = h/l^4$, $k_2 = l^4k/h$, and:

$$h(x) = (x^2 - l^2)^2 + k_2 x \tag{2}$$

- thus, $f(x) = k_1 h(x)$.

Mathematical analysis of one-dimensional DWF

- Considering the first derivative of h(x), and letting h'(x) = 0:

$$4x^3 - 4l^2 x + k_2 = 0 \qquad (3)$$

- According to Shen-jin's Formula [10], the discriminant of (3):

$$\Delta = 48(27k_2^2 - 64l^6) \qquad (4)$$

- where $A = b^2 - 3ac$, $B = bc - 9ad$, $C = c^2 - 3bd$, and $a = 4$, $b = 0$, $c = -4l^2$, and $d = k_2$ are the factors of (3).
- Moreover, the roots of Equation (3) can be discussed in four cases according to the Shen-jin Formula:

- **(1)** If A = B = 0, then equation (3) has a triple root. However, from A = B = 0, we obtain l = 0, and thus this case will not happen.

- (2) If $\Delta < 0$, then equation (3) has three unequal real roots:

$$\begin{cases} x_1 = -2l\cos(\theta/3)/\sqrt{3} \\ x_2 = l[\cos(\theta/3) - \sqrt{3}\sin(\theta/3)]/\sqrt{3} \\ x_3 = l[\cos(\theta/3) + \sqrt{3}\sin(\theta/3)]/\sqrt{3} \end{cases} \tag{6}$$

- and $\theta = \arccos(3\sqrt{3}k_2/(8l^3))$, $A > 0$, $0 \le T < 1$.

- Monotonicity: because $x_1 < 0 \le x_2 < x_3$ and the cubic factor of h(x) is positive, h(x) strictly and monotonically decreases in $(-\infty, x_1) \cup (x_2, x_3)$ and monotonically increases in $(x_1, x_2) \cup (x_3, +\infty)$.

- If $k_2 = 0$ then h(x) is symmetric about $x = 0$, and $x_3 = -x_1 = l$.
- If $k_2 > 0$, then h(x) becomes an asymmetric DWF:

$$\begin{cases} h(x)_{gmin} = h(x_1) \\ h(x)_{lmax} = h(x_2) \\ h(x)_{lmin} = h(x_3) \end{cases} \tag{7}$$

Mathematical analysis of one-dimensional DWF

- **(3) If $\Delta = 0$**, then $3\sqrt{3}k_2 = 8l^3$, and (3) has three real roots, including a double root, namely $x_1 = -b/a + K$, $x_2 = x_3 = -K/2$ where $K = B/A$ and $A \neq 0$. By combining the factors in (3), we obtain:

$$\begin{cases} x_1 = -3k_2/(4l^2) \\ x_2 = x_3 = 3k_2/(8l^2) \end{cases} \tag{8}$$

- **Monotonicity**: h(x) strictly and monotonically decreases in $(-\infty, x_1)$ and monotonically increases in $(x_1, +\infty)$; thus, **x_1 is the only global minimum:**

$$h(x)_{gmin} = h(x_1) \tag{9}$$

- and **h(x) becomes a single well function with a special stagnation point** at $(x_2, h(x_2))$.

Mathematical analysis of one-dimensional DWF

- **(4) If $\Delta > 0$**, then (3) has a real root and a pair of conjugate complex roots, and the real root is $x_1 = [-b-(3\sqrt{Y_1} + 3\sqrt{Y_2})]/(3a)$, where $Y_{1,2} = Ab + 3a[-B \pm \sqrt{(B_2 - 4AC)}]/2$. By replacing the aforementioned factors, we obtain:

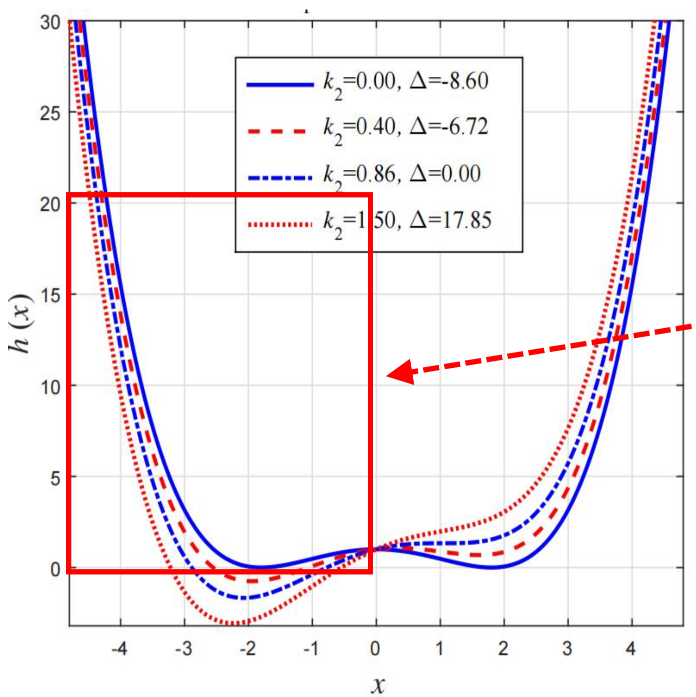
$$x_1 = -\frac{\sqrt[3]{3[9k_2+\sqrt{3(27k_2^2-64l^6)}]}}{6} - \frac{\sqrt[3]{3[9k_2-\sqrt{3(27k_2^2-64l^6)}]}}{6} \quad (10)$$

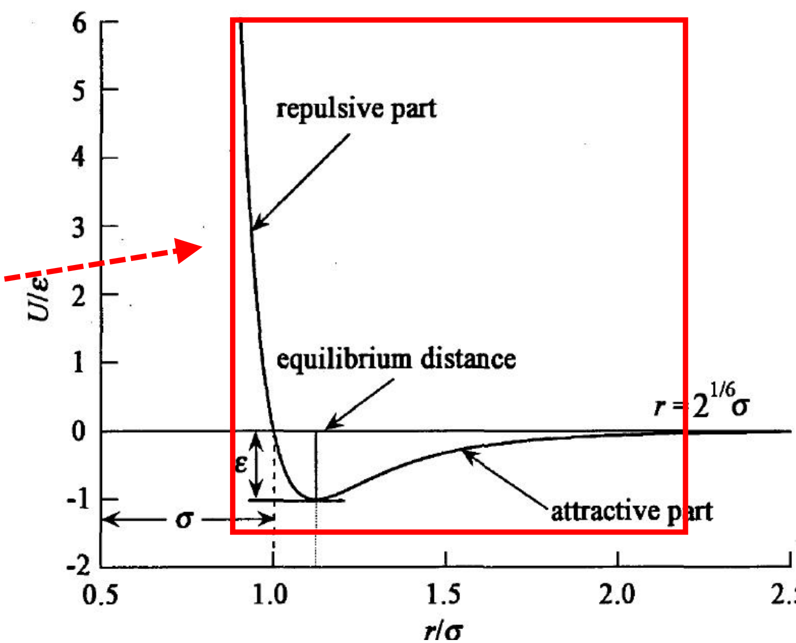
- **Monotonicity**: the complex roots do not affect the monotonicity of h(x) in R. As a result, h(x) monotonically decreases in $(-\infty, x_1)$ and monotonically increases in $(x_1, +\infty)$
- **h(x) turns out to be a single well with the only minimum** at $(x_1, h(x_1))$, as described in (9).

Mathematical analysis of one-dimensional DWF

- In conclusion, h(x) is not a real DWF if $\Delta \geq 0$; however, in this case, h(x) is also useful for creating benchmark functions with different features in high-dimensional cases.

- It is very interesting to note that the curve of h(x) in interval $(-2l, x_2)$ is quite similar to the potential curves of the Morse potential and the Lennard–Jones potential.





The curves of Lennard-Jones potential

Fig. 1. The curves of h(x), where k_1 = 1.00 and l = 1.80, and k_2 and Δ are different.

- Consider the second-order differentials of h(x):

$$\begin{cases} h''(x) = 12x^2 - 4l^2 \\ \frac{\partial^2 h(x)}{\partial x \partial l} = -8lx \\ \frac{\partial^2 h(x)}{\partial x \partial k_2} = 1 \end{cases} \tag{11}$$

- Let $h''(x) = 0$, we obtain $x = \pm l/\sqrt{3}$. In addition, at these two points, $h'''(x) \neq 0$. Thus, h(x) always has two fixed inflection points at $(\pm l/\sqrt{3}, 4l^4/9 \pm k_2 l\sqrt{3})$ despite the value of Δ.
- Moreover, in $(-\infty, -2l)$, h(x) drops quickly, whereas in $(2l, \infty)$, it increases dramatically. Thus, it is advisable to set an optimization interval containing $(-2l, 2l)$ if the DWF is used as a benchmark function considering the change rate and the distribution of local minima.
- $\partial^2 h(x)/(\partial x \partial l) = -8lx$ is the partial differential function of h(x) and has a stagnation point $x = 0$, and as $l > 0$, it is positive when $x < 0$ and negative when $x > 0$, and $h'(x)$ changes more rapidly as l increases.
- $\partial^2 h(x)/(\partial x \partial k_2) = 1$ shows that the effect of k_2 on the changing rate is linear and constant, and k_2 always drives $h'(x)$ to increase in R, and the rate of change increases as k_2 increases.

B. High-dimensional Double Well Function

- **Extending the dimension of f(x):**

$$F_n(\boldsymbol{x}) = \sum_{i=1}^{n} f_i(x) = \sum_{i=1}^{n} h_i \frac{\left(x^2 - l_i^2\right)^2}{l_i^4} + k_i x \qquad (12)$$

- **where n∈N and n ≥ 2.**
- **Corresponding to the one dimensional case, H_n(x) can be obtained through the transformation H_n(x) = F_n(x)/k_1:**

$$H_n(\boldsymbol{x}) = \sum_{i=1}^{n} h_i(x) = \sum_{i=1}^{n} \left(x^2 - l_i^2\right)^2 + k_{i2} x \qquad (13)$$

- **Definition: we use Δ_i, x_{i1}, x_{i2}, x_{i3}, h_i, l_i, k_i, k_{i1}, and k_{i2} to denote the factors in the i-th dimension corresponding to their counterparts in one dimension; thus, $\mathbf{x}_1 = (x_{11}, \ldots, x_{n1}) \in R^n$, Δ, k_1, l_2, k_2, etc.**

Mathematical analysis of high-dimensional DWF

Similarly, we discuss $H_n(x)$ instead of $F_n(x)$ for simplicity as follows:

- **(1)** If $\Delta_i < 0$ for $i = 1, \ldots, n$, then $H_n(x)$ has 2^n local minima and the only global minimum is:

$$H_n(\boldsymbol{x})_{gmin} = H_n(\boldsymbol{x}_1) = H_n(x_{11}, \ldots, x_{n1}) = \sum_{i=1}^{n} h_i(x_{i1}) \tag{14}$$

- In addition, $H_n(\mathbf{x})$ also has $3^n - 2^n$ unstable points.

- **(2)** If $\Delta_i = 0$ for $i = 1, \ldots, n$, then $H_n(\mathbf{x})$ has only one local minimum with the same expression as in (14). Besides, $H_n(\mathbf{x})$ also has $2^n - 1$ special stagnation points. Thus, $H_n(\mathbf{x})$ is a single well function with numerous unstable points.

Mathematical analysis of high-dimensional DWF

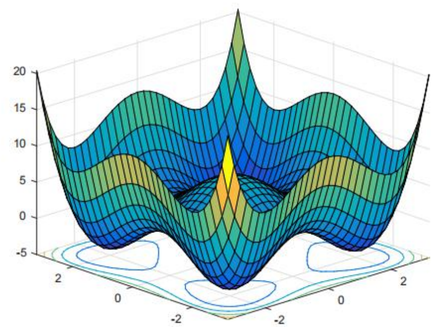
- **(3)If $\Delta_i > 0$ for i = 1, ..., n,** then $H_n(\mathbf{x})$ has a unique stagnation point and global minimum as expressed in (14); thus, it is a single well function.

$$H_n(\boldsymbol{x})_{gmin} = H_n(\boldsymbol{x}_1) = H_n(x_{11}, ..., x_{n1}) = \sum_{i=1}^{n} h_i(x_{i1}) \tag{14}$$

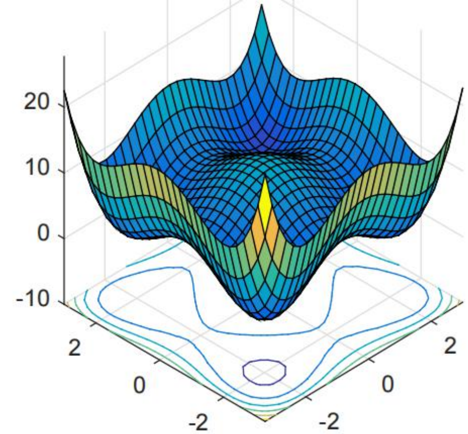
- **(4)If the situation is a mixture of the above cases**, then $H_n(x)$ can be discussed according to the value of Δ_i in each dimension.

- By employing different parameters in case (4), we can create a more complicated benchmark function, and an even more irregular distribution of local minima can be realized by introducing negative k_{i2} in some dimensions instead of non-negative k_{i2} in all dimensions. Furthermore, the rotation matrix and linear shift can be used to make it more general [6].

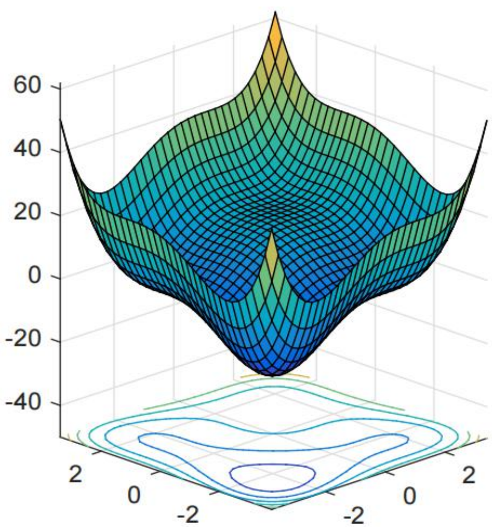
- **In the two-dimensional case, $F_2(\mathbf{x})$ for different basic cases is shown in Fig. 2.**



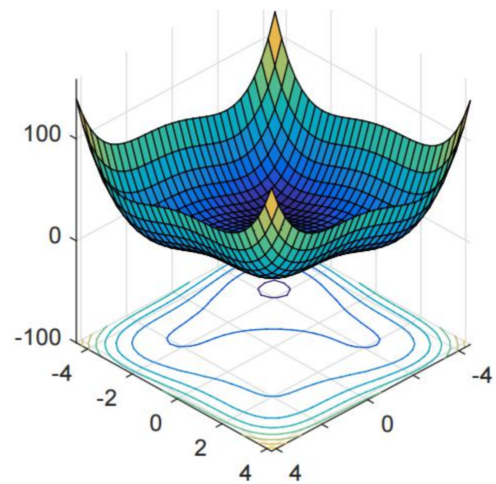
(a) $k_i = 0.00$ and $\Delta_i = -1875.00$



(b) $k_i = 0.30$ and $\Delta_i = -1863.60$



(c) $k_i = 3.84$ and $\Delta_i = 0.00$



(d) $k_i = 5.00$ and $\Delta_i = 1289.06$

Fig. 2. The three-dimensional surface of $F_2(x)$, where $h_i = 5.00$ and $l_i = 2.00$, and where k_i and Δ_i differ in each case ($i = 1, 2$).

III. EXPERIMENT AND ANALYSIS

- **Experiment Environment**: All of these experiments were conducted using MATLAB R2015a with a 3.4-GHz i7 CPU and 8 GB of memory, running on Windows 10.
- **Setting**: the optimization interval was $(-2l, 2l)$ for each dimension, the maximum function evaluations was 10^4*dimension. An optimization was considered successful if the error between the optimization output and the theoretical minimum was less than 10^{-6}. k_{i1}, l_i, and k_{i2} were set to the same values for each dimension for convenience in experiment.
- **Indicators**: the success rate (SR) was introduced to describe the overall effect of 100 independent runs. Similarly, the mean function evaluations (MeanFEs) , mean optimization time (MeanOT), mean error (MeanErr), and standard deviation of error (StdErr) were calculated for all of these repeats.

Algorithms used in experiment

Five algorithms with different features were introduced:

- The multi-scale quantum harmonic oscillator algorithm (MQHOA) [11] was employed for its balanced performance between unimodal optimization and multimodal optimization.
- The δ-well model, a variety **of** MQHOA, was used for its improved efficiency in locating global minimum among massive local minima since the δ-well potential it used has higher resolution than the harmonic oscillator potential used in MQHOA.
- Quantum behaved particle swarm optimization (QPSO) is chosed [12] because of its high accuracy.
- The covariance matrix adaptation evolution strategy (CMAES) [13] is chosed for its good ability for unimodal optimization.
- The bare bones fireworks algorithm (BBFWA) was introduced for its simple and limited operations in optimization process.

A. Optimization under different values of discriminant and dimensions

- In the first experiment, different values of Δ and n are tested. As discussed in Section II, $H_n(x)$ and $F_n(x)$ are unimodal when $\Delta_i \geq 0$ and turn out to be multimodal when $\Delta_i < 0$, so we set a series of Δ_i values ranging from -0.3 to 0.1. Besides, different values of n were also tested.

TABLE I

SUCCESS RATE/MEAN ERROR/MEAN FUNCTION EVALUATIONS/MEAN OPTIMIZATION TIME(/s) FOR $H_n(x)$ UNDER DIFFERENT VALUES OF DISCRIMINANT AND DIMENSION

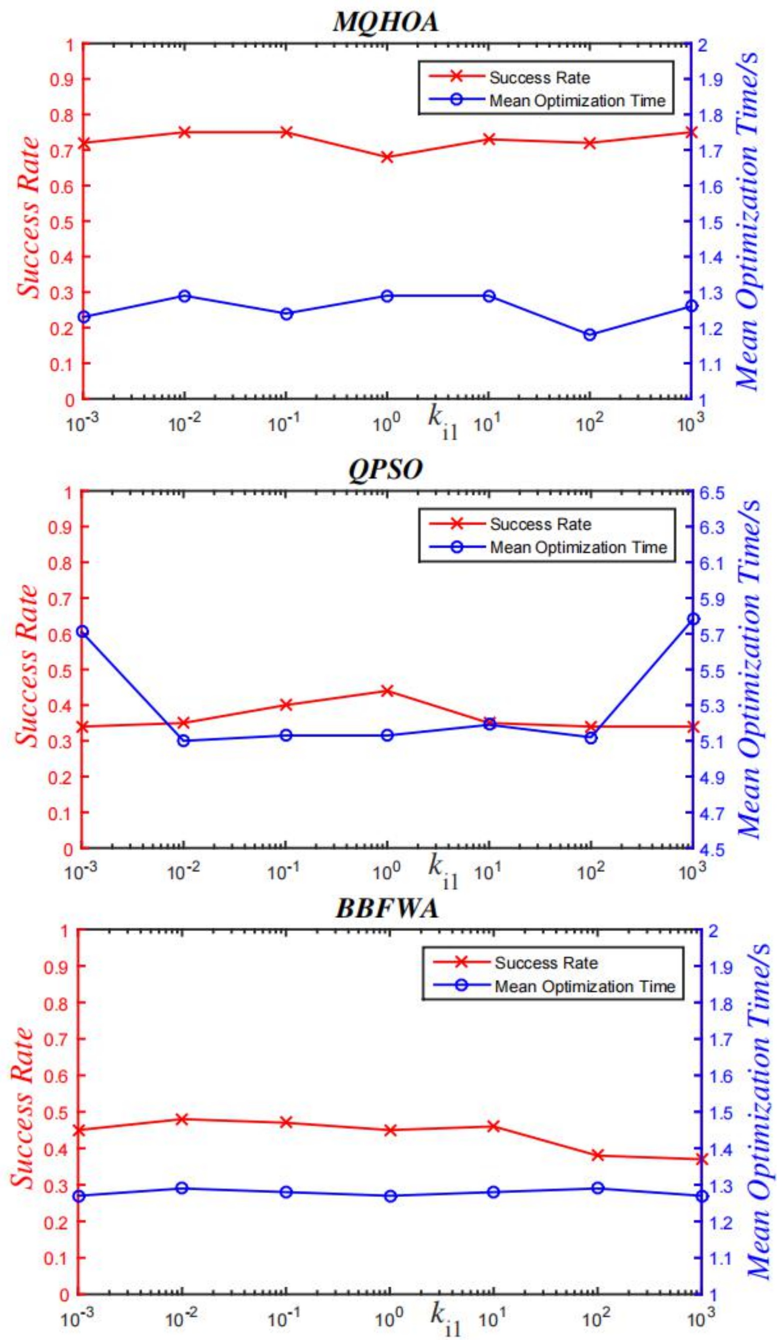
	dim	$\Delta_i = -0.30$	$\Delta_i = -0.20$	$\Delta_i = -0.10$	$\Delta_i = 0.00$	$\Delta_i = 0.10$
	5	**1.00/0.00E+00**/6.24E+03/**1.15E-03**	**1.00/0.00E+00**/5.95E+03/**1.14E-03**	**1.00/0.00E+00**/5.48E+03/**1.11E-01**	**1.00/0.00E+00**/5.65E+03/**1.06E-01**	**1.00/0.00E+00**/5.62E+03/**9.68E-02**
M	10	**1.00/1.86E-12**/1.01E+04/**2.29E-01**	**1.00**/1.97E-12/8.80E+03/**1.77E-01**	**1.00**/2.30E-12/8.65E+03/**1.74E-01**	**1.00**/2.19E-12/8.50E+03/**1.76E-01**	**1.00**/2.38E-12/7.91E+03/**1.63E-01**
Q	15	0.92/5.11E-02/1.31E+04/4.52E-01	0.99/1.88E-02/1.19E+04/**2.56E-01**	**1.00**/7.63E-12/1.25E+04/**2.60E-01**	**1.00**/7.75E-12/1.10E+04/**2.50E-01**	**1.00**/8.28E-12/1.09E+04/**2.29E-01**
H	20	0.72/2.58E-01/1.65E+04/**5.35E-01**	0.98/3.76E-02/1.39E+04/**3.61E-01**	**1.00**/1.78E-11/1.37E+04/**3.51E-01**	**1.00**/1.93E-11/1.36E+04/**3.41E-01**	**1.00**/1.81E-11/1.37E+04/**3.07E-01**
O	25	0.63/3.87E-01/3.12E+04/7.99E-01	0.90/1.88E-01/1.60E+04/**4.66E-01**	0.98/5.04E-02/1.63E+04/**4.58E-01**	**1.00**/3.13E-11/1.64E+04/**4.30E-01**	**1.00**/3.32E-11/1.59E+04/**4.00E-01**
A	30	0.38/7.42E-01/2.80E+04/1.20E+00	0.82/3.95E-01/2.92E+04/**6.20E-01**	0.98/5.04E-02/1.92E+04/**5.70E-01**	**1.00**/5.42E-11/1.82E+04/**5.87E-01**	**1.00**/5.40E-11/1.84E+04/**4.99E-01**
	35	0.20/1.23E+00/3.40E+04/**1.04E+00**	0.74/6.02E-01/2.23E+04/**8.18E-01**	0.94/1.51E-01/2.23E+04/**8.29E-01**	**1.00**/8.02E-11/2.11E+04/**6.65E-01**	**1.00**/8.22E-11/2.10E+04/**6.08E-01**
	40	0.13/1.65E+00/5.43E+04/**1.28E+00**	0.69/7.53E-01/2.99E+04/**9.48E-01**	0.90/2.46E-01/2.30E+04/**1.04E+00**	0.98/6.00E-02/2.26E+04/**1.04E+00**	**1.00**/1.13E-10/2.27E+04/**7.37E-01**
	5	**1.00/0.00E+00**/7.62E+03/1.91E-01	**1.00**/2.55E-13/7.60E+03/1.87E-01	**1.00/0.00E+00**/7.72E+03/1.99E-01	**1.00/0.00E+00**/7.34E+03/1.97E-01	**1.00/0.00E+00**/7.25E+03/1.86E-01
δ	10	**1.00**/1.98E-12/1.25E+04/3.42E-01	**1.00**/2.16E-12/1.20E+04/3.25E-01	**1.00**/2.23E-12/1.15E+04/3.21E-01	**1.00**/2.32E-12/1.17E+04/3.47E-01	**1.00**/2.45E-12/1.11E+04/3.17E-01
ı	15	**1.00**/6.76E-12/1.56E+04/4.87E-01	**1.00**/7.39E-12/1.59E+04/4.62E-01	**1.00**/7.62E-12/1.56E+04/4.52E-01	**1.00**/9.08E-12/1.57E+04/4.83E-01	**1.00**/8.69E-12/1.59E+04/4.52E-01
w	20	**1.00/1.50E-11**/1.99E+04/6.17E-01	**1.00**/1.56E-11/2.04E+04/6.54E-01	**1.00**/1.86E-11/1.98E+04/6.34E-01	**1.00**/1.97E-11/1.91E+04/6.38E-01	**1.00**/1.96E-11/1.95E+04/5.80E-01
e	25	**1.00**/2.58E-11/2.43E+04/**7.70E-01**	**1.00**/3.03E-11/2.48E+04/7.61E-01	**1.00**/3.08E-11/2.35E+04/8.05E-01	**1.00**/3.22E-11/2.36E+04/7.78E-01	**1.00**/3.64E-11/2.33E+04/7.34E-01
l	30	**1.00**/3.86E-11/2.82E+04/**9.96E-01**	**1.00**/4.36E-11/2.62E+04/9.72E-01	**1.00**/4.98E-11/2.76E+04/9.18E-01	**1.00**/5.34E-11/2.70E+04/1.01E+00	**1.00**/5.35E-11/2.73E+04/8.90E-01
l	35	**1.00**/5.73E-11/3.17E+04/1.19E+00	**1.00**/6.64E-11/3.12E+04/1.10E+00	**1.00**/7.39E-11/3.20E+04/1.11E+00	**1.00**/7.91E-11/3.21E+04/1.19E+00	**1.00**/7.91E-11/3.20E+04/1.07E+00
	40	**1.00/7.76E-11**/3.50E+04/1.34E+00	**1.00**/8.83E-11/3.50E+04/1.29E+00	**1.00**/1.03E-10/3.66E+04/1.34E+00	**1.00**/1.01E-10/3.45E+04/1.32E+00	**1.00**/1.06E-10/3.56E+04/1.27E+00
	5	0.98/1.61E-02/5.00E+04/1.19E+00	**1.00/0.00E+00**/5.00E+04/1.40E+00	**1.00/0.00E+00**/5.00E+04/1.20E+00	**1.00/0.00E+00**/5.00E+04/1.11E+00	**1.00/0.00E+00**/5.00E+04/1.09E+00
	10	0.99/8.06E-03/1.00E+05/2.49E+00	**1.00/0.00E+00**/1.00E+05/2.94E+00	**1.00/0.00E+00**/1.00E+05/2.49E+00	**1.00/0.00E+00**/1.00E+05/2.45E+00	**1.00/0.00E+00**/1.00E+05/2.33E+00
Q	15	**1.00/0.00E+00**/1.50E+05/4.01E+00	**1.00/0.00E+00**/1.50E+05/4.61E+00	**1.00/0.00E+00**/1.50E+05/4.04E+00	**1.00/0.00E+00**/1.50E+05/3.89E+00	**1.00/0.00E+00**/1.50E+05/3.77E+00
P	20	0.99/8.06E-03/2.00E+05/5.58E+00	**1.00/0.00E+00**/2.00E+05/6.48E+00	**1.00/0.00E+00**/2.00E+05/5.70E+00	**1.00/0.00E+00**/2.00E+05/5.48E+00	**1.00/0.00E+00**/2.00E+05/5.35E+00
S	25	**1.00/0.00E+00**/2.50E+05/7.64E+00	**1.00/0.00E+00**/2.50E+05/8.41E+00	**1.00/0.00E+00**/2.50E+05/7.59E+00	**1.00/0.00E+00**/2.50E+05/7.20E+00	**1.00/0.00E+00**/2.50E+05/7.00E+00
O	30	**1.00/0.00E+00**/3.00E+05/9.54E+00	**1.00/0.00E+00**/3.00E+05/1.07E+01	**1.00/0.00E+00**/3.00E+05/9.42E+00	**1.00/0.00E+00**/3.00E+05/9.36E+00	**1.00/0.00E+00**/3.00E+05/8.99E+00
	35	**1.00/0.00E+00**/3.50E+05/1.16E+01	**1.00/0.00E+00**/3.50E+05/1.31E+01	**1.00/0.00E+00**/3.50E+05/1.16E+01	**1.00/0.00E+00**/3.50E+05/1.17E+01	**1.00/0.00E+00**/3.50E+05/1.09E+01
	40	**1.00**/3.97E-09/4.00E+05/1.39E+01	**1.00/1.51E-11**/4.00E+05/1.53E+01	**1.00/7.24E-12**/4.00E+05/1.37E+01	**1.00/1.09E-11**/4.00E+05/1.45E+01	**1.00**/7.30E-12/4.00E+05/1.32E+01
	5	0.43/8.23E-01/**4.05E+03**/2.11E-01	**1.00/0.00E+00/4.01E+03**/2.06E-01	**1.00/0.00E+00/3.83E+03**/2.04E-01	**1.00/0.00E+00/4.01E+03**/2.04E-01	**1.00/0.00E+00/3.69E+03**/1.98E-01
C	10	0.38/9.68E-01/**9.27E+03**/5.12E-01	**1.00/0.00E+00/6.39E+03**/3.54E-01	**1.00/0.00E+00/6.30E+03**/3.50E-01	**1.00/0.00E+00/6.12E+03**/3.15E-01	**1.00/0.00E+00/6.39E+03**/3.45E-01
M	15	0.50/7.50E-01/**6.98E+03/3.72E-01**	0.99/1.88E-02/**8.64E+03**/4.94E-01	**1.00/0.00E+00/8.55E+03**/4.85E-01	**1.00/0.00E+00/8.69E+03**/4.37E-01	**1.00/0.00E+00/8.87E+03**/4.74E-01
A	20	0.17/2.07E+00/**1.17E+04**/7.67E-01	0.92/1.51E-01/**1.10E+04**/7.34E-01	0.99/2.52E-02/**1.06E+04**/7.26E-01	**1.00/0.00E+00/1.10E+04**/6.45E-01	**1.00/0.00E+00/1.10E+04**/6.63E-01
E	25	0.08/2.52E+00/**1.35E+04**/9.07E-01	0.85/2.82E-01/**1.29E+04**/8.64E-01	0.98/5.04E-02/**1.29E+04**/8.56E-01	0.99/3.00E-02/**1.40E+04**/7.75E-01	**1.00/0.00E+00/1.25E+04**/7.92E-01
S	30	0.01/3.65E+00/**1.51E+04**/1.05E+00	0.79/3.95E-01/**1.40E+04**/9.94E-01	0.94/1.51E-01/**1.40E+04**/9.81E-01	0.99/3.00E-02/**1.35E+04**/8.97E-01	**1.00/0.00E+00/1.37E+04**/9.58E-01
	35	0.01/5.35E+00/**1.64E+04**/1.19E+00	0.70/6.96E-01/**1.57E+04**/1.13E+00	0.93/2.01E-01/**1.57E+04**/1.12E+00	**1.00/0.00E+00/1.56E+04**/1.03E+00	**1.00/0.00E+00/1.58E+04**/1.11E+00
	40	0.00/6.50E+00/**1.84E+04**/1.31E+00	0.61/1.05E+00/**1.71E+04**/1.26E+00	0.90/2.52E-01/**1.73E+04**/1.25E+00	0.99/3.00E-02/**2.11E+04**/1.15E+00	**1.00/0.00E+00/1.64E+04**/1.24E+00
	5	0.48/8.87E-02/5.00E+04/4.26E-01	0.55/1.88E-02/5.00E+04/4.23E-01	0.38/3.36E-06/5.00E+04/4.25E-01	0.39/3.08E-06/5.00E+04/4.37E-01	0.43/3.19E-06/5.00E+04/4.24E-01
B	10	0.14/1.23E+00/1.00E+05/9.92E-01	0.78/4.70E-01/1.00E+05/9.75E-01	0.95/1.26E-01/1.00E+05/9.93E-01	**1.00**/3.63E-08/1.00E+05/9.92E-01	**1.00**/3.31E-08/1.00E+05/9.82E-01
B	15	0.03/2.71E+00/1.50E+05/1.65E+00	0.49/1.43E+00/1.50E+05/1.64E+00	0.87/3.78E-01/1.50E+05/1.64E+00	0.98/6.00E-02/1.50E+05/1.64E+00	**1.00**/5.87E-10/1.50E+05/1.63E+00
F	20	0.00/4.23E+00/2.00E+05/2.40E+00	0.35/1.94E+00/2.00E+05/2.39E+00	0.69/9.82E-01/2.00E+05/2.40E+00	0.92/2.40E-01/2.00E+05/2.41E+00	**1.00**/3.11E-11/2.00E+05/2.43E+00
W	25	0.00/5.46E+00/2.50E+05/3.27E+00	0.13/3.71E+00/2.50E+05/3.24E+00	0.66/1.28E+00/2.50E+05/3.23E+00	0.88/3.30E-01/2.50E+05/3.26E+00	**1.00**/5.36E-12/2.50E+05/3.26E+00
A	30	0.00/6.68E+00/3.00E+05/4.23E+00	0.08/4.55E+00/3.00E+05/4.21E+00	0.43/2.54E+00/3.00E+05/4.23E+00	0.84/4.80E-01/3.00E+05/4.35E+00	**1.00**/2.35E-12/3.00E+05/4.23E+00
	35	0.00/8.24E+00/3.50E+05/5.31E+00	0.03/5.80E+00/3.50E+05/5.31E+00	0.32/2.87E+00/3.50E+05/5.30E+00	0.85/4.20E-01/3.50E+05/5.32E+00	**1.00**/5.60E-12/3.50E+05/5.27E+00
	40	0.00/1.00E+01/4.00E+05/6.55E+00	0.01/7.47E+00/4.00E+05/6.52E+00	0.22/4.28E+00/4.00E+05/6.46E+00	0.79/6.94E-01/4.00E+05/6.57E+00	**1.00/0.00E+00**/4.00E+05/6.46E+00

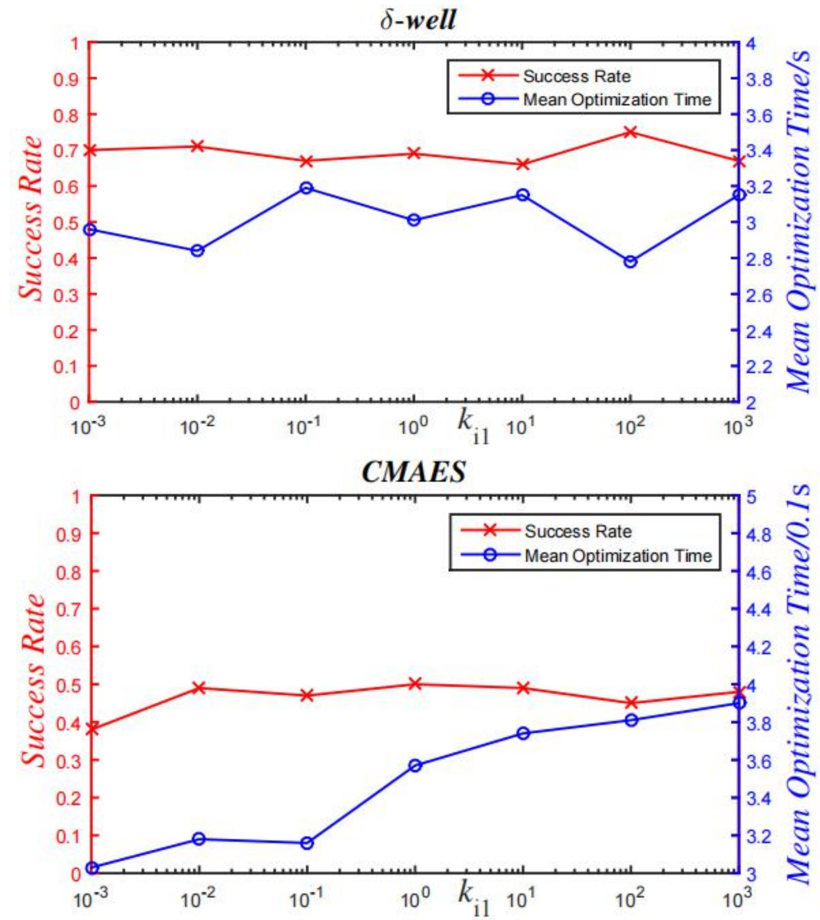
conclusion

- When Δ_i is positive, optimization is easy, and optimization difficulty is not very sensitive to the change in dimension.
- When Δ_i is negative, as Δ_i decreases the optimization task becomes more difficult for a fixed n.
- When Δ_i is negative, optimization difficulty increases as the dimension increases.

B. Optimization under different values of k_1

- In the second experiments, a series of k_{i1} values ranging from 10^{-3} to 10^3 was tested in multimodal optimization.
- To obtain reasonable SRs for these algorithms, different parameters of $H_n(x)$ were employed because their optimization performances are quite different.
- Specifically, l_i was set to 2.00, 2.50, 2.00, 3.00, and 2.50; k_{i2} was set to 0.150, 0.025, 0.050, 0.250, and 0.280; and n was set to 20, 20, 20, 12, and 10 for MQHOA, δ–well, QPSO, CMAES, and BBFWA, respectively.



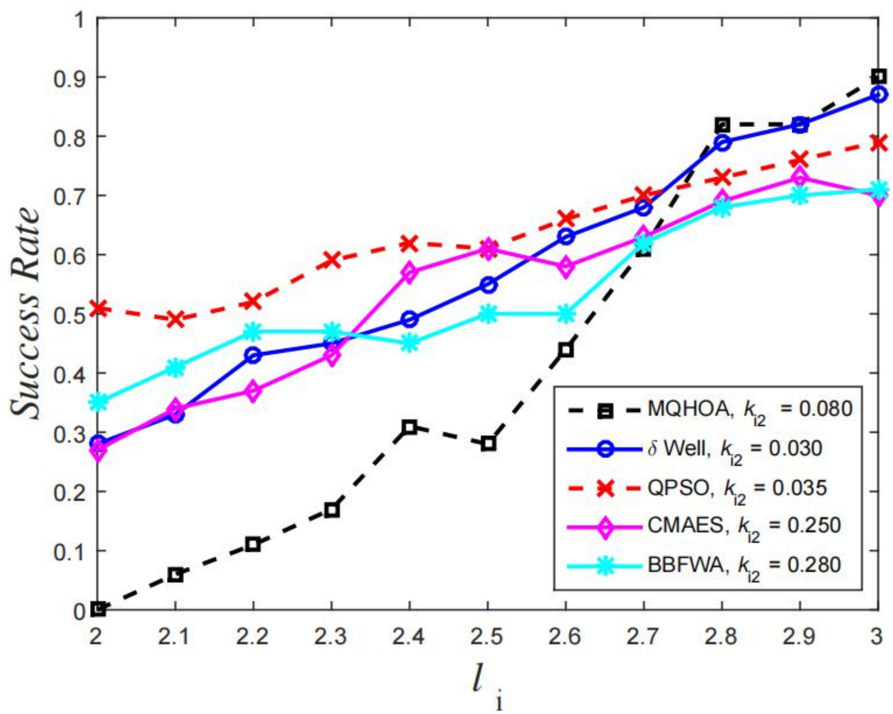


k_{i1} has a limited influence on the optimization result, especially if the change in k_{i1} is not significant.

Fig. 3. The optimization result of $k_1H_n(x)$, where k_{i1} range from 10^{-3} to 10^3.

C. Optimization under different values of l

- In the third experiment, a change in l_i was employed to study its influence on multimodal optimization.
- Setting: ki2 was set to 0.080, 0.030, 0.035, 0.250, and 0.280 for MQHOA, δ–well, QPSO, CMAES, and BBFWA, respectively, and n was set to 10 for all, and SR was chosen as the indicator of the optimization result.

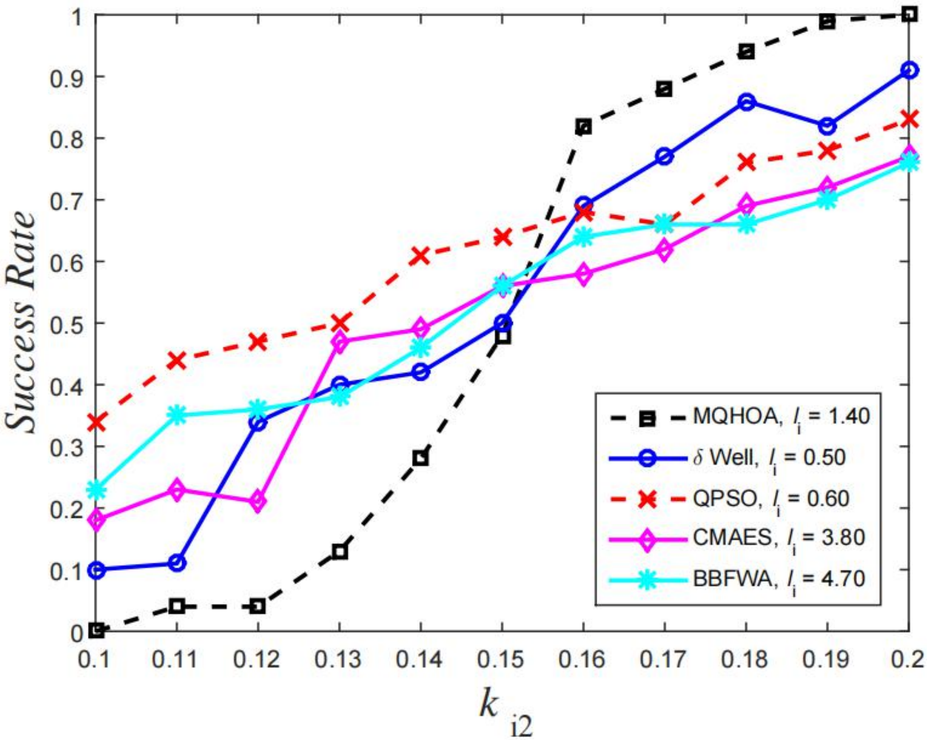


The optimization difficulty is reduced as l_i increases.

Fig. 4. The influence of l_i on the optimization of $H_n(x)$, where n = 10, and l_i range from 2 to 3

D. Optimization under different values of k_2

- In the fourth experiment, different values of k_{i2} increasing from 0.1 to 0.2 were tested to verify this conclusion.



As k_{i2} increases, the optimization difficulty of the DWF will decrease.

Fig. 5. The influence of k_{i2} on the optimization of $H_n(x)$, where n = 10, and k_{i2} range from 0.1 to 0.2

E. Unimodal optimization when all $\Delta_i > 0$

- We also conducted an experiment on unimodal optimization. As the first experiment has revealed, the optimization is too simple when n < 40 and Δ_i are large, and therefore, we set n = 100 and Δ_i =2.1E-05 here.

TABLE II
OPTIMIZATION RESULT OF $H_{100}(\boldsymbol{x})$ WHERE Δ_i =2.1E-05

algorithm	SR	MeanErr	MeanFEs	MeanOT($/s$)	StdErr
MQHOA	0.98	7.35E-06	6.54E+05	1.22E+01	7.04E-05
$\delta-$well	**1.00**	2.08E-10	8.74E+04	**3.75E+00**	2.59E-11
QPSO	0.00	3.75E+01	1.00E+06	4.27E+01	7.71E+00
CMAES	**1.00**	**3.09E-13**	**2.52E+04**	4.39E+00	**1.28E-13**
BBFWA	**1.00**	4.21E-13	1.00E+06	3.07E+01	6.06E-13

The bold mark indicates the best results among all algorithms.

- $H_n(x)$ failed to detect their differences in optimization ability despite the change in n in a considerable range, this experiment and the first experiment indicate that $H_n(x)$ is not a perfect benchmark function for unimodal optimization when all $\Delta_i > 0$.

IV. CONCLUSION

- The DWF has been assumed to be a candidate for testing the optimization algorithm because it has many local minima in high-dimensional cases.

- To prove this, we mathematically analyzed a typical form of the DWF and found that its properties were controlled by a few adjustable parameters, which can be used to design ideal benchmark functions for testing.

- Furthermore, our analysis was also illustrated by numerical experiments, and the influences of the decisive factors that guide the design of an ideal DWF were also studied through a series of comparative experiments.

Reference

- [1] D. J. Griffiths, Introduction to Quantum Mechanics, 2nd ed, Pearson Education International: New York, 1995, pp.37–50.
- [2] H. Grabert and U. Weiss, “Quantum tunneling rates for asymmetric double-well systems with Ohmic Dissipation,” Phys. Rev. Lett. New York, vol. 54, no. 15, pp. 1605–1608, 1985.
- [3] J. Sj ¨ ostrand, “Potential wells in high dimensions II, more about the one well case,” Ann. Inst. H. Poincare´ Phys. the´ or. vol. 43, no. 1, pp. 43–45, 1993.
- [4] J. D. Swalen and J. A. Ibers, “Potential function for the inversion of Ammonia,” J. Chem. Phys. New York, vol. 36, no. 1, pp. 1914–1920, 1962.
- [5] H. Takeuchi, “ Clever and efficient method for searching optimal geometries of lennard-jones clusters,” J. Chem. Inf. Model. Washingtom, vol. 46, no. 5, pp. 2066–2070, 2006.
- [6] N. H. Awad, M. Z. Ali, J. J. Liang, B. Y. Qu, and P. N. Suganthan, “Problem definitions and evaluation criteria for the CEC 2017 special session and competition on single objective bound constrained real-parameter numerical optimization,” Technical Report, 2016. unpublished.
- [7] L. Stella, G. E. Santoro, and E. Tosatti, “Optimization by Quantum Annealing: lessons from simple cases,” Phys. Rev. B. Maryland, vol. 72, no. 1, 2005.
- [8] A. B. Finnila, M. A. Gomez, C. Sebenik, C. Stenson, and J.D. Doll, “ Quantum Annealing: a new method for minimizing multidimensional functions,” Chem Phys Lett. Amsterdam, vol. 219, no. 5–6, pp. 343-348, 2012.
- [9] M. W. Johnson, M. H. S. Amin, S. Gildert, T. Lanting, F. Hamze, N. Dickson et al, “Quantum Annealing with manufactured spins,” Nature. London, vol. 473, pp. 194–198, 2011.
- [10] S. J. Fan, “A new extracting formula and a new distinguishing means on the one variable three order equation,” Nat. Sci. J. Hainan. Teach. Coll. Haikou, vol. 2, no. 2, pp. 91–98, 1989.
- [11] P. Wang, Y. Huang, C. Ren, and Y. M. Guo, “Multi-Scale Quantum Harmonic Oscillator for high-dimensional function global optimization algorithm,” Acta. Electron. Sinica. Beijing, vol. 41, no. 12, pp. 2468–2473, 2013.
- [12] J. Sun, B. Feng, W. B. Xu, “Particle Swarm Optimization with particles having quantum behavior,” Congress on Evolutionary Computation. Portland, pp.325–331, 2004.
- [13] T. Suttorp, N. Hansen, and C. Igel, “Efficient Covariance Matrix Update for variable metric evolution strategies,” Mach. Learn. Dordrecht, vol. 75, no. 2, pp. 167–197, 2009.
- [14] J. Z. Li and Y. Tan, “ The bare bones fireworks algorithm: A minimalist global optimizer,” Appl. Soft. Comput, vol. 62, pp. 454–462, 2018.

Thank you for your time and attention!