Tunneling Effect of quantization-based optimization

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***Abstract*—In this paper, we present an analysis of the tunneling effect in the quantization-based optimization. We prove that, when the quantization step size is an exponential decay function with respect to an iteration, the quantized objective function admits a decomposition into longitudinal and transverse fields. From the perspective of quantum mechanics, since the transverse field gives the quantum tunneling effect, quantization-based optimization can outperform a conventional thermodynamics-based optimization scheme. Experimental results for a vanilla objective function and a typical combinatorial optimization problem, such as the traveling salesman problem, demonstrate that the presented analysis is valid.**

***Index Terms*—quantization, optimization, tunneling effect, quantum mechanics, Schrödinger**

I. Introduction

Although the quantization-based optimization algorithm outperforms conventional combinatorial optimization algorithms[8], the underlying dynamic mechanism responsible for its enhanced optimization performance remains unclear. However, from the perspective of the quantized energy level, we can anticipate that quantum mechanical analysis for a Hamiltonian is a key attribute in quantization-based optimization. The prominent property of the quantum mechanical search algorithm is the tunneling effect, which is the fundamental theory in quantum computing for optimization, such as the quantum approximate optimization algorithm. Accordingly, we expect that the quantization-based optimization embeds equal dynamics to those of the quantum mechanics-based optimization scheme. In this paper, we demonstrate through numerical analysis that the Hamiltonian derived from the quantization-based optimization algorithm is equivalent to the dynamics inspired by quantum mechanics, which are used to avoid local minima in the search algorithm. Based on the presented analysis, we can conclude that quantization-based optimization employs the quantum tunneling effect as a prominent search mechanism. Furthermore, we argue that quantization-based optimization is an alternative implementation of a quantum computation method for an optimization problem.

II. Preliminaries

Beginning with this conjecture, we derive the Hamiltonian, which is composed of longitudinal fields and transverse fields in an Ising glass system[4], for a quantized objective function extracted from the quantization-based optimization algorithm. According to the above-mentioned Ising model, we can write the Hamiltonian as follows:

$$H(t) = H_0 - H_k(t) = -\sum_{i,j} J_{i,j}\sigma_i^z\sigma_j^z - \Gamma(t)\sum_i \sigma_i^x \tag{1}$$

where the potential energy $H_0 \triangleq -\sum_{i,j} J_{i,j}\sigma_i^z\sigma_j^z = -\sum_{i,j} J_{i,j}\sigma_i^z \otimes \sigma_j^z$ is an Edward-Anderson disordered Ising model as a longitude field, and the time-dependent Hamiltonian $H_k(t) \triangleq -\Gamma(t)\sum_i \sigma_i^x = -\Gamma(t)\sum_i \sigma_i^x \otimes I$ is a kinetic energy as a transverse field. Additionally, $\sigma_i^x \in \mathcal{B}(\mathcal{H}_N)$ is the Pauli-X operator acting non-trivially on the i-th qubit (i.e., 1/2-spin particle), where $\mathcal{H}_N := (\mathbb{C}^2)^{\otimes N}$ denotes the Hilbert space for N spins and $\mathcal{B}(\mathcal{H}_N)$ represents the set of bounded linear operators on $\mathcal{H}_N$. $\Gamma(t) \in \mathbb{R}^+$ denotes the amplitude of the transverse field, which decreases from a large initial value satisfying $\Gamma(0) \gg H_{\text{cl}}$ to zero as t increases, and $J_{ij} \in \mathbb{R}$ denotes coupling parameter The transverse Ising model (1) naturally leads to the following time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H(t)|\psi(t)\rangle. \tag{2}$$

From the definition of the Hamiltonian in the Schrödinger equation, i.e., $H = -\frac{\hbar^2}{2m}\nabla^2 + V_0$, where V_0 is a potential energy, we can see that quantum tunneling appears in stationary solutions($\partial_t\psi = 0$), straightforwardly. Therefore, the solution of (2) describes quantum tunneling under a time-dependent potential barrier, which is modulated by $\Gamma(t)$ in the transverse field.

However, the optimization perspective primarily focuses on the average energy or the eigenvalue of energy, as given by $E(t) = \frac{\langle\psi(t)|H|\psi(t)\rangle}{\langle\psi(t)|\psi(t)\rangle}$, rather than on the detailed quantum dynamics of the system. Accordingly, by replacing the spin variables with the eigenvalues of σ^z and σ^x (i.e., ± 1), the Hamiltonian becomes a scalar function over binary fields, providing a more tractable formulation for constructing optimization algorithms:

$$H(t) = (1 - \lambda(t))H_0 + \lambda(t)H_k, \tag{3}$$

where $\lambda(t) \in \mathbb{R}[0, 1]$ is a monotone decreasing function such that $\lambda(t) \downarrow 0$ as $t \uparrow \infty$. The Hamiltonian described by (3) is known as the adiabatic quantum evolution, and the optimization technique based on this formulation is called quantum annealing(QA) or adiabatic quantum computation[3, 6]. As is well known, adiabatic quantum computation solves combinatorial optimization problems that can be formulated as the ground state of the quadratic unconstrained binary optimization(QUBO). The state vector of QUBO is in $\mathbb{R}^n\{0,1\}$, which shows that an eigen model of an Ising model is equivalent to the QUBO. Hence, as equivalent to the transverse Ising model, quantum tunneling is the primary feature in the search process to avoid local minima during adiabatic quantum evolution. Consequently, if we formulate the quantization-based optimization algorithm presented in Algorithm 1 as the adiabatic quantum evolution described by Equation (3), we conclude that time-varying quantization to an objective function on a scalar field is equivalent to quantum computational optimization.

III. Fundamental Analysis

A. Definitions and Assumptions

Suppose that an objective function $f(\boldsymbol{x}) \in \mathbb{R}^+$, where $\boldsymbol{x} \in \mathbb{R}^n$ denotes a state vector. Consider the optimization problem such that $\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$. According to Algorithm 1, we establish the following definitions:

Definition 1: For $f \in \mathbf{R}$, we define the quantization of f as follows:

$$f^Q \triangleq \frac{1}{Q_p}\left\lfloor Q_p \cdot (f + \tfrac{1}{2Q_p})\right\rfloor = \frac{1}{Q_p}\left(Q_p \cdot f + \varepsilon^q\right) = f + \varepsilon^q Q_p^{-1}, \tag{4}$$

where $\lfloor f \rfloor \in \mathbf{Z}$ denotes the floor function, defined as the greatest integer less than or equal to for all $f \in \mathbb{R}$, $Q_p \in \mathbb{Q}^+$ is the resolution of quantization, and ε^q represents the fraction for quantization such that $\varepsilon^q : \Omega \mapsto \mathbb{R}[-\frac{1}{2}, \frac{1}{2})$. Thus, $f^Q \in \mathbb{Q}$. In Definition 1, the quantization step size Q_p is a constant parameter. To implement a search process, we redefine Q_p as a time-dependent function as follows:

Definition 2: The quantization parameter Q_p is a monotone-increasing function of $t \in \mathbb{R}^+$ such that $Q_p(t) = \gamma \cdot b^{\bar{h}(t)}$, where $\gamma \in \mathbb{Q}^{++}$ denotes the fixed constant parameter, $b \in \mathbb{Z}^+$ represents the base (typically 2), and $\bar{h} : \mathbb{R}^{++} \mapsto \mathbb{Z}^+$ denotes the power function satisfying $\bar{h}(t) \uparrow \infty$ as $t \to \infty$.

For the analysis of the feature of the adiabatic quantum evolution in quantization-based optimization, we assume that the quantization step size depends on the time index as follows:

Assumption 1: For a given time index $t \in \mathbb{Z}^+$, the quantization step size is defined as $Q_p(t) = b^t$.

B. Equivalence of the Quantization-based Optimization and the Adiabatic Quantum Evolution

Theorem 3.1: The quantized objective function $f^Q(\boldsymbol{x}_t)$ derived by the quantization-based optimization described in Algorithm 1 is equivalent to the eigen value of the following Hamiltonian $\bar{H}$ represented by the formulation of the adiabatic quantum evolution:

$$\bar{H}(\boldsymbol{x}_t, t) = (1-\beta(t))H_0(\boldsymbol{x}_t, t) + \beta(t)H_k(\boldsymbol{x}_t, t), \tag{5}$$

where $\beta(t) \in \mathbb{R}[0,1]$ is a monotone decreasing function such that $\beta(0) = 1$ and $\beta(t) \downarrow 0$ as $t \uparrow \infty$.

a) Proof of Theorem: We rewrite the quantization of the objective function f using the base b for the quantization step size Q_p as defined in Definition 2, as follows:

$$f = f_b + \sum_{k=1}^{\infty} f_k b^{-k}, \quad f_k \in \mathbb{Z}^+[0,b) \tag{6}$$

Based on (6), we decompose the objective function as:

$$f = f_b + \sum_{k=1}^{t-1} f_k b^{-k} + \sum_{k=t}^{\infty} f_k b^{-k} = f^Q - \varepsilon^q Q_p^{-1}(t). \tag{7}$$

From the simple form of $Q_p(k)$, we define f_{t-1}^Q as the quantized objective function at the k-th resolution, i.e., $f_{t-1}^Q = f_b + \sum_{k=1}^{t-1} f_k b^{-k}$. Substituting f_{t-1}^Q into (7), we express the quantization error as the following power series:

$$f - f_{t-1}^Q = \sum_{k=t}^{\infty} f_k b^{-k} = \text{sign}(f - f_{t-1}^Q)\cdot b^{-(t-1)} \sum_{k=1}^{\infty} \epsilon_k b^{-k}, \tag{8}$$

where $\epsilon_k \in \mathbb{Z}[0,b)$ is a remaining coefficient for numerical representation. Furthermore, although the sequence $\{\epsilon_k\}_{k=1}^{\infty}$ and $\{f_k\}_{k=t}^{\infty}$, the quantized value f_b are not identical, he quantized value f_b coincides for both sequences. Therefore, by the above auxiliary equations, we rewrite f_{t-1}^Q such that

$$\begin{aligned} f_{t-1}^Q &= f + (f_{t-1}^Q - f) \\ &= f - \text{sign}(f - f_{t-1}^Q)\cdot b^{-(t-1)} \sum_{k=1}^{\infty} \epsilon_k b^{-k} \\ &= f - b^{-(t-1)}\,\text{sign}(f - f_0^Q) \sum_{k=1}^{\infty} \epsilon_k b^{-k} \\ &= f - b^{-(t-1)}(f - f_b) \\ &= f + b^{-(t-1)}(f_b - f) = b^{-(t-1)} f_b + (1 - b^{-(t-1)}) f. \end{aligned}$$

Therefore, we obtain

$$f_t^Q = b^{-t} f_b + (1 - b^{-t}) f \tag{9}$$

Since $b^{-1} < 1$, we designate $(1 - b^{-t})f$ as the eigenvalue of $(1 - \lambda(t))H_0$ and $b^{-t} f_b$ as $\lambda(t)H_k$ such that $f_b = \langle\psi|H_0|\psi\rangle / \langle\psi|\psi\rangle$. Finally, we set f_t^Q as the eigenvalue of the Hamiltonian $\hat{H}(t)$ for the Schrödinger equation. **(Q.E.D.)**

C. Time Independent Analysis of Schrödinger Equation for Tunneling Effect

To focus on the essential aspects, let Γ be an eigen-space of the Hamiltonian $\bar{H}(\boldsymbol{x}_t, t)$, which is homeomorphic to $\mathbb{R}$, at a fixed time t. Thus, the domain of the wave function $\psi(\boldsymbol{x}_t, t)$ is restricted to $\Gamma \cong \mathbb{R}$. First, considering the tunneling effect on Γ, we use the following time-independent Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\right)\psi(\boldsymbol{x}_t, t) = f_t^Q \psi(\boldsymbol{x}_t, t), \tag{10}$$

where $f_t^Q : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ denotes the eigenvalue function of $\bar{H}$ given in Theorem 3.1, and $V_0 \in \mathbb{R}$ is a potential representing an energy barrier of width d such that $\Gamma[0,d) \cong \mathbb{R}[0,d)$. In

Algorithm 1: Blind Random Search (BRS) with the proposed quantization scheme[8]

Input: Objective function $f(x) \in \mathbf{R}^+$
Output: $x_{opt},\ f(x_{opt})$
Data: $x \in \mathbf{R}^n$
Initialization
$\tau \leftarrow 0$ and $\bar{h}(0) \leftarrow 0$
Set initial candidate x_0 and $x_{opt} \leftarrow x_0$
Compute the initial objective function $f(x_0)$
Set $b = 2$ and $\gamma = b^{-\lfloor \log_b(f(x_0)+1) \rfloor}$, $Q_p \leftarrow \gamma$
$f^Q_{opt} \leftarrow \frac{1}{Q_p}\left\lfloor Q_p \cdot (f + \frac{1}{2Q_p})\right\rfloor$
while *Stopping condition is not satisfied* **do**
  Set $\tau \leftarrow \tau + 1$
  Select x_τ randomly and compute $f(x_\tau)$
  Calculate $f^Q \leftarrow \frac{1}{Q_p}\left\lfloor Q_p \cdot (f + \frac{1}{2Q_p})\right\rfloor$ **if** $f^Q \leq f^Q_{opt}$ **then**
    $x_{opt} \leftarrow x_\tau$
    $\bar{h}(\tau) \leftarrow \bar{h}(\tau) + 1$ $Q_p \leftarrow \gamma \cdot b^{\bar{h}(\tau)}$
    $f^Q_{opt} \leftarrow \frac{1}{Q_p}\left\lfloor Q_p \cdot (f + \frac{1}{2Q_p})\right\rfloor$
  end
end

this setup, the potential satisfies $V_0 > f^Q_t$. Additionally, $x \in \mathbb{R}[0,d)$ denotes that x is in the barrier, whereas $x \in (\mathbb{R}[0,d))^c$ describes that x is outside of the barrier. The restriction to the eigen-space Γ yields the following simplified form:

$$\frac{d^2\psi}{dx^2}(x,t) = \frac{2m}{\hbar^2}\big(V_0 - f^Q_t\big)\psi(x,t), \tag{11}$$

where $x \in \Gamma$ denotes the state vector $\boldsymbol{x}_t$ on Γ.

From the perspective of classical mechanics, the mass of the particle is so heavy compared to the quantum particle. This provides the right-hand side of (11) is 0 and the primary solution of ψ is equal to 0. It means that the particle is impossible to penetrate the energy barrier to reach the other side. Meanwhile, from the perspective of quantum mechanics, the mass of the particle is sufficiently small, so we can discover the particle on the other side of the energy barrier with a transmission probability $T \in \mathbb{R}[0,1]$ defined as $T = |\psi_{\{x|x\in\mathbb{R}[0,d)\}}|^2/|\psi_{\{x|x\in(\mathbb{R}[0,d))^2\}}|^2$, which is exponentially decaying to the width d of the barrier, such that

$$T \propto \cdot \exp\left(-\frac{2}{\hbar}\int_x^{x+d}\sqrt{2m(V(x)-E)}\,dx\right). \tag{12}$$

Equation (12) shows a typical tunneling effect in the scalar domain [2]. We can regard the eigen-space provided by the gradient vector generated from a search algorithm. We expand this fundamental concept to the general analysis of the tunneling effect based on the adiabatic evolution.

D. Time-dependent Analysis of Schrödinger Equation for Tunneling Effect

In this section, we address that the primary process in Algorithm 1, i.e., $f^Q \leq f^Q_{OPT}$, is a tunneling effect in the adiabatic evolution.

For the analysis based on adiabatic evolution, we consider a state vector $|\psi(t)\rangle \in L^2(\mathbb{R}^n)$ corresponding to a wave function $\psi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$. Under this notation, the energy can be computed as the expectation value $E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$. If the state vector is normalized, i.e., $\langle\psi|\psi\rangle = 1$, this simplifies to $E = \langle\psi|H|\psi\rangle$. We assume throughout this section that each distinct state vector in $\psi_i,\ I \in \mathbb{Z}^+$, is orthonormal. Given the time-dependent Schrödinger equation (2), suppose the Hamiltonian corresponds to a two-level quantum model for different local minima:

$$H_{\text{2-level}}(s) = \begin{pmatrix} E_1(s) & \Delta(s)/2 \\ \Delta(s)/2 & E_2(s) \end{pmatrix}, \tag{13}$$

where s denotes the time index for this analysis instead of t or τ, E_k denotes the energy, i.e., the eigenvalue of the Hamiltonian $\bar{H}$ to the state $|\psi_k\rangle$ at x_k, and Δ is the tunneling matrix element defined as the square root of the transmission probability according to Wentzel–Kramers–Brillouin (WKB) theory [2]:

$$\Delta(s) = \sqrt{T} \propto \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x_2}\sqrt{2m(V(x)-\tilde{E}(s))}\,dx\right), \tag{14}$$

where $\tilde{E}(s)$ denotes that the eigenvalue of $H_{\text{2-level}}(s)$. Herein, by computing the eigenvalues of the two-level Hamiltonian $H_{\text{2-level}}(s)$, we obtain

$$\tilde{E}(s) = \frac{1}{2}\left[(E_1+E_2) \pm \sqrt{(E_1-E_2)^2 + \Delta^2(s)}\right]. \tag{15}$$

Based on Algorithm 1, we assume $E_1 = f^Q_t(x_1)$ and $E_2 = f^Q_t(x_2)$ for distinct $x_1, x_2 \in \mathbb{R}^d$ with distance $d = \|x_2 - x_1\|$. Furthermore, to illustrate the case when the quantized optimum f^Q_{opt} equals a quantized candidate f^Q_τ, we set $E_1 = E_2 = f^Q_s$. Under these assumptions, the eigenvalues reduce to

$$\tilde{E}(s) = f^Q_s \pm \frac{\Delta(s)}{2}. \tag{16}$$

The quantization property further yields

$$\int_{x_1}^{x_2}\sqrt{2m\left(V(x)-\tilde{E}(s)\right)}\,dx = \sqrt{2m\left(V(x)-\tilde{E}(s)\right)}\,d, \tag{17}$$

which implies

$$\Delta(s) \approx \exp\left[-\frac{1}{\hbar}\sqrt{2m\left(V(x)-\tilde{E}(s)\right)}\,d\right]. \tag{18}$$

Since all parameters in (18) are finite, the transmission probability is strictly positive, whereas in classical mechanics it vanishes. This phenomenon corresponds to the quantum tunneling effect in quantum adiabatic evolution. Even in the case where f^Q_{opt} equals f^Q_τ, quantum tunneling provides a feasible transition for Algorithm 1. As a consequence, the tunneling effect produces a non-strictly decreasing sequence of f_{opt}^Q without requiring smoothness or convexity, thereby ensuring the global convergence of Algorithm 1.

Moreover, the energy given by the eigenvalue of the Hamiltonian in (16) corresponds to the quantization of the objective function. This observation indicates that the dynamics of quantization-based optimization can be interpreted within the formalism of quantum mechanics.

IV. Experimental Results

To validate the analysis presented in this paper, we evaluate the optimization performance on well-known benchmark functions, including Xin-She Yang N4[9], Salomon[5], Drop-Wave[1], and Shaffer N2[7]. All the benchmark functions used in our experiments are representative examples defined by the CEC 2017 and CEC 2022 optimization test standards. Each function has a unique global minimum and numerous local minima, which are located between relatively high energy barriers that hinder the search for better solutions. Additionally, some benchmark functions, such as Xin-She Yang N4, exhibit a wide energy barrier, which makes it difficult for algorithms based on quantum tunneling dynamics to find feasible states. We can verify this limitation of the quantum tunneling-based search process from the results of optimization performance comparison between tested algorithms in Table II. Herein, the quantum annealing fails to find the global minimum of the Xin-She Yang N4 benchmark function, whereas the simulated annealing and the quantized-based algorithm find it. Furthermore, although all algorithms succeed in finding the global minimum for complicated benchmark functions such as the Drop-Wave and the Shaffer N2, the quantization-based algorithm exhibits the best optimization performance compared to other algorithms. However, for the Salomon function, which is composed of the plain addition of a sinusoidal and a squared-quadratic function, so that it is relatively simple to find the global minimum, the simulated annealing demonstrates the best optimization performance. Consequently, even though the presented analysis demonstrates that the quantization-based algorithm optimizes the objective function through the quantum tunneling effect, we should recognize that other features of the quantization-based algorithm also contribute to the improvement of optimization performance.

V. Conclusion

We present an analysis of quantization-based optimization based on the adiabatic quantum evolution, which provides a quantum tunneling effect. The analysis shows that the quantum mechanical dynamics in quantization-based optimization are equivalent to those in quantum annealing. Such an equivalence suggests that quantization-based computation would be an alternative approach to quantum computation-based optimization.

However, the experimental results for optimization benchmark functions reveal that the quantization-based optimization outperforms the quantum mechanics-based algorithm that employs the quantum tunneling effect. These results indicate that additional search dynamics exist in the quantization-based algorithm that can enhance optimization performance.

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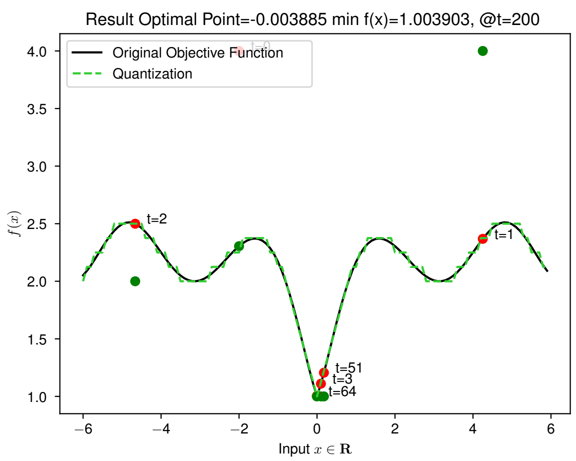
TABLE I
SPECIFICATION OF BENCHMARK TEST FUNCTIONS FOR PERFORMANCE TEST

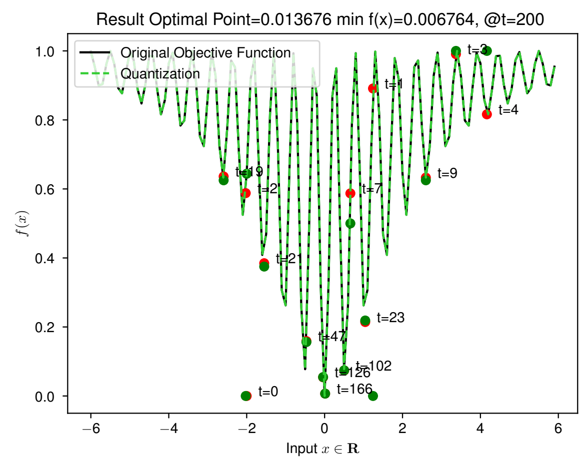
Function	Equation	optimal point
Xin-She Yang N4	$f(x) = 2.0 + (\sum_{i=1}^{d} \sin^2(x_i) - \exp(-\sum_{i=1}^{d} x_i^2) \exp(-\sum_{i=1}^{d} \sin^2 \sqrt{\lvert x_i \rvert})$	$\min f(x) = -1, \text{ at } x = 0$
Salomon	$f(x) = 1 - \cos\left(2\pi \sqrt{\sum_{i=1}^{d} x_i^2}\right) + 0.1 \sqrt{\sum_{i=1}^{d} x_i^2}$	$\min f(x) = 0, \text{ at } x = 0$
Drop-Wave	$f(x) = -\frac{1+\cos\left(12\sqrt{x^2+y^2}\right)}{0.5(x^2+y^2)+2}$	$\min f(x) = 0, \text{ at } x = 0$
Shaffel N2	$0.5 + \frac{\sin^2(x^2-y^2)-0.5}{(1+0.001(x^2+y^2)^2}$	$\min f(x) = 0, \text{ at } x = 0$

TABLE II
SIMULATION RESULTS OF STANDARD BENCHMARK TEST FUNCTION FOR NONLINEAR OPTIMIZATION

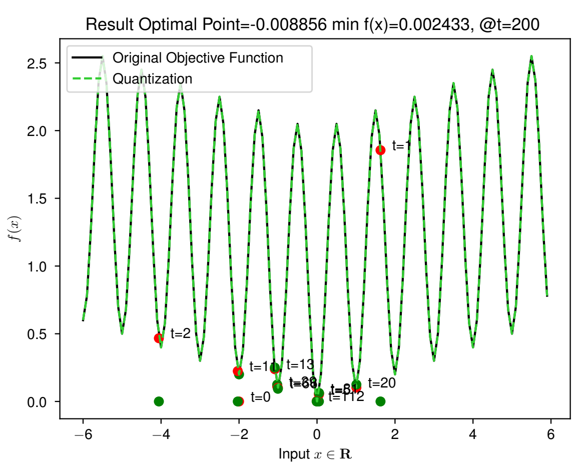
Function	Criterion	Simulated Annealing	Quantum Annealing	Quantization-Based Optimization
Xin-She Yang N4	Iteration	6420	17*	3144
	Improvement ratio	54.57%	35.22%	54.57%
Salomon	Iteration	1312	7092	1727
	Improvement ratio	99.99%	99.99%	100.0%
Drop-Wave	Iteration	907	3311	254
	Improvement ratio	100.0%	100.0%	100.0%
Shaffer N2	Iteration	7609	9657	2073
	Improvement ratio	100.0%	100.0%	100.0%



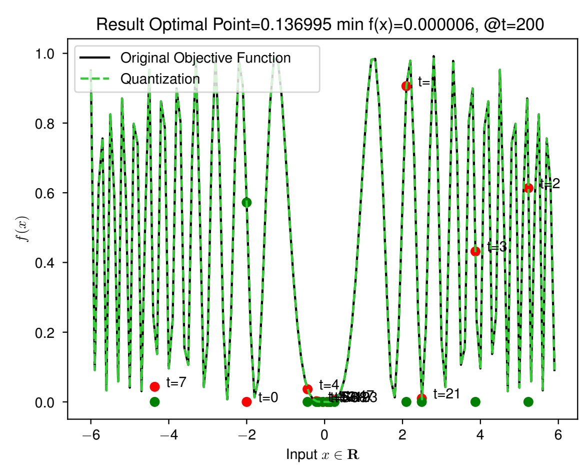
(a) Search process with respect to Xin She Yang N4 function



(b) Search process with respect to Drop wave function



(c) Search process with respect to Salomon function



(d) Search process with respect to Shaffel N2 function

Fig. 1. Visualization of the quantization-based search process on 1D benchmark functions