A Dynamical Point of View on Quantum Optimization

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“Quantum Hamiltonian Descent”, arXiv:2303.01471
“A quantum-classical performance separation in nonconvex optimization”, manuscript in preparation

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JOINT CENTER FOR QUANTUM INFORMATION AND COMPUTER SCIENCE

Quantum computing 101

Classical (digital) Computer

- Unit of information: bit ($b \in \{0,1\}$)
- Classical information → bitstrings (e.g., 10001001)
- Computation = manipulation of finite-length bitstrings
- Readout/Return: bitstrings

Quantum Computer

- Unit of information: quantum bit, or **qubit**

$$|\psi> = a|0> + b|1>, a, b \in \mathbb{C}, |a|^2 + |b|^2 = 1$$

- Quantum information → quantum state (i.e., superposition of |*bitstring*>)

$$|GHZ> = \frac{1}{\sqrt{2}}\left(|000> + |111>\right)$$

- Computation = unitary (i.e., preserving 2-norm) operations on quantum states
- Readout: quantum measurement → a sample of bitstrings

Measure GHZ state:
000: 50%, 111: 50%, others: 0%

Digital Quantum Computers

Use quantum gates & quantum circuits, not ready in 5-10 years. Must do error correction.

Analog Quantum Computers

Solving problems by emulating a real quantum system. Ready & easy to scale. No error correction.

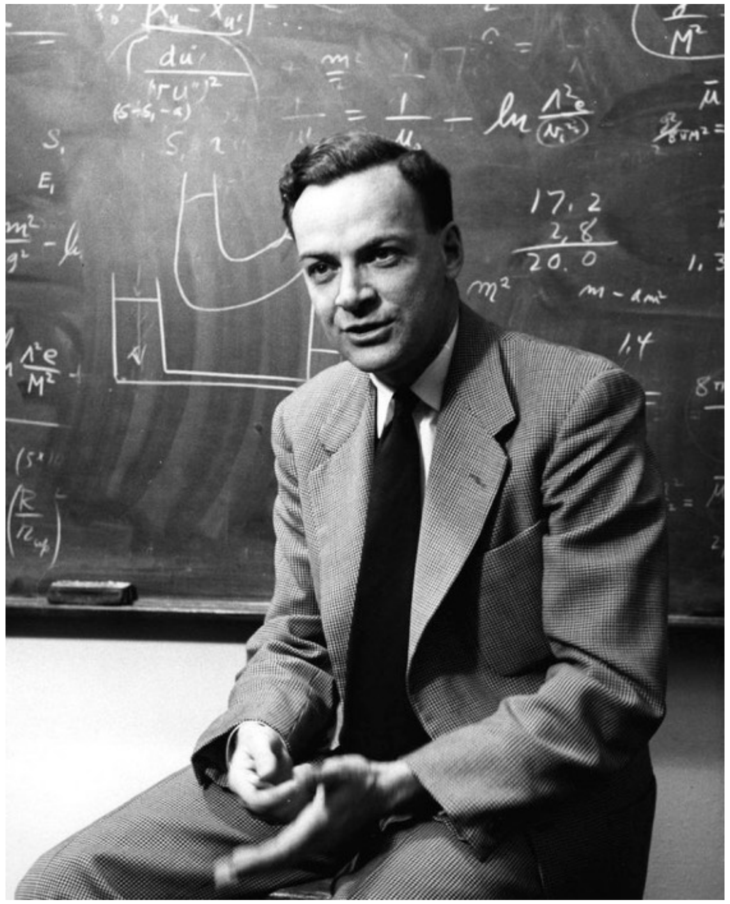
Hamiltonian simulation

- **Quantum simulation** (or **Hamiltonian simulation**): a prominent application of quantum computers. Exponential quantum speedup expected.

$$i\frac{\partial}{\partial t}\psi = \hat{H}(t)\psi$$

$\hat{H}(t)$: *quantum Hamiltonian (Hermitian/self-adjoint)*

- **Feynman** (*"Simulating Physics with Computers", 1982*): to simulate quantum systems, we would need to build quantum computers.



- **Applications**: quantum chemistry, quantum field theory, condensed matter physics, numerical optimization, etc.

Overview

- Part I: Quantum Hamiltonian Descent (QHD)
- Part II: A Quantum-Classical Performance Separation
- Part III: Implementation on Quantum Computers

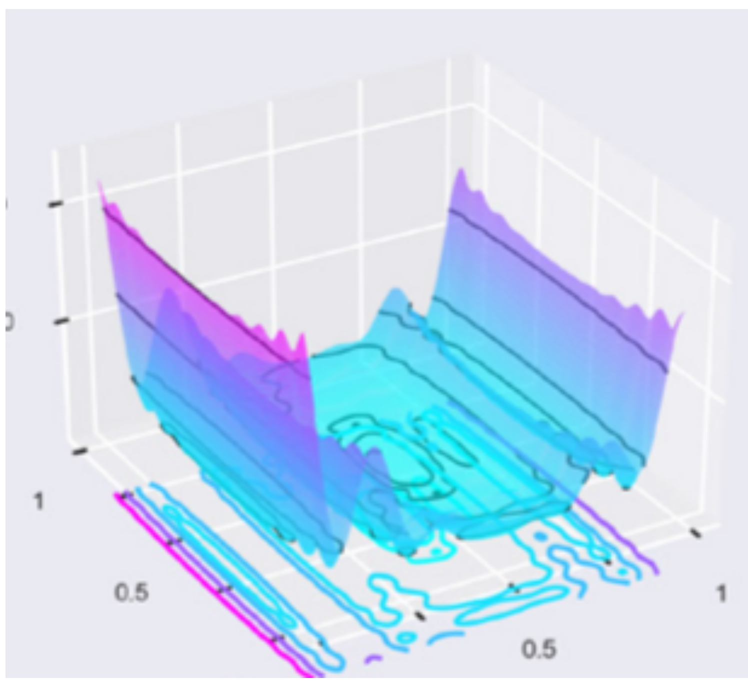
Part I:

Quantum Hamiltonian Descent

Problem formulation

Continuous optimization

$$\boxed{\min_{x \in \mathbb{R}^d} f(x)}$$



- Important in practice: machine learning, operations research, scientific computing, etc.
- A **challenging problem** for quantum: different nature in (quantum) algorithm design, requires new mathematical tools to prove convergence.
- **Opportunity**: new *primitives* of quantum speedups!

Classical algorithms: Gradient Descent (GD)

- Standard GD: $x_{k+1} = x_k - s\nabla f(x_k)$.
- Nesterov's accelerated GD: $x_{k+1} = y_k - s\nabla f(y_k)$, $y_{k+1} = x_{k+1} + \dfrac{k}{k+3}\left(x_{k+1} - x_k\right)$.

A Lagrangian formulation of accelerated methods

Su, Boyd, & Candes
NeurIPS 2014

$$x_k = y_{k-1} - s\nabla f(y_{k-1}),$$
$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1}).$$

Nesterov's accelerated GD

$$\longrightarrow$$

$$\ddot{X} + \frac{3}{t}\dot{X} + \nabla f(X) = 0,$$

ODE model

Wibisono, Wilson, & Jordan
PNAS Nov 2016, 113 (47)

$$x_k = y_{k-1} - s\nabla f(y_{k-1}),$$
$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1}).$$

Nesterov's accelerated GD

$$\longrightarrow$$

$$\mathcal{L}(t, \dot{X}, X) = t^3 \left(\frac{1}{2}|\dot{X}|^2 - f(X)\right)$$

Lagrangian formulation

$$H(t, X, P) = \frac{1}{2t^3}|P|^2 + t^3 f(X)$$

Hamiltonian formulation

- Accelerated GD can be modeled by accelerated gradient flows.
- GD algorithms can be generated by discretizing continuous-time dynamics.

Accelerated Hamiltonian flows: classical v.s. quantum

We can make the classical dynamics quantum!!

Classical Hamiltonian Systems $\xrightarrow{\text{Path integral formulation of Quantum Mechanics}}$ **Quantum Hamiltonian Evolution**

Due to Feynman

$$\boxed{H(t,X,P) = \frac{1}{2t^3}|P|^2 + t^3 f(X)} \longrightarrow \boxed{\hat{H}(t) = \frac{1}{t^3}\left(-\frac{1}{2}\Delta\right) + t^3 f(x)}$$

Bregman Lagrangian

$$\mathcal{L}(X,\dot{X},t) = e^{-\varphi_t}\left(\frac{1}{2}|\dot{X}|^2\right) - e^{\chi_t} f(X)$$

→

Quantum propagator

$$K(b,t_b;a,t_a) \propto \sum_{\text{paths from a to b}} e^{\frac{i}{\hbar}S[X(t)]}$$

↓

Infinitesimal expansion

$$\Psi(x,t+\epsilon) \propto \int \exp\left\{\frac{i}{\hbar}\epsilon\mathcal{L}\left(\frac{x+y}{2},\frac{x-y}{\epsilon},t\right)\right\}\Psi(y,t)\,dy$$

←

Schrodinger equation (QHD)

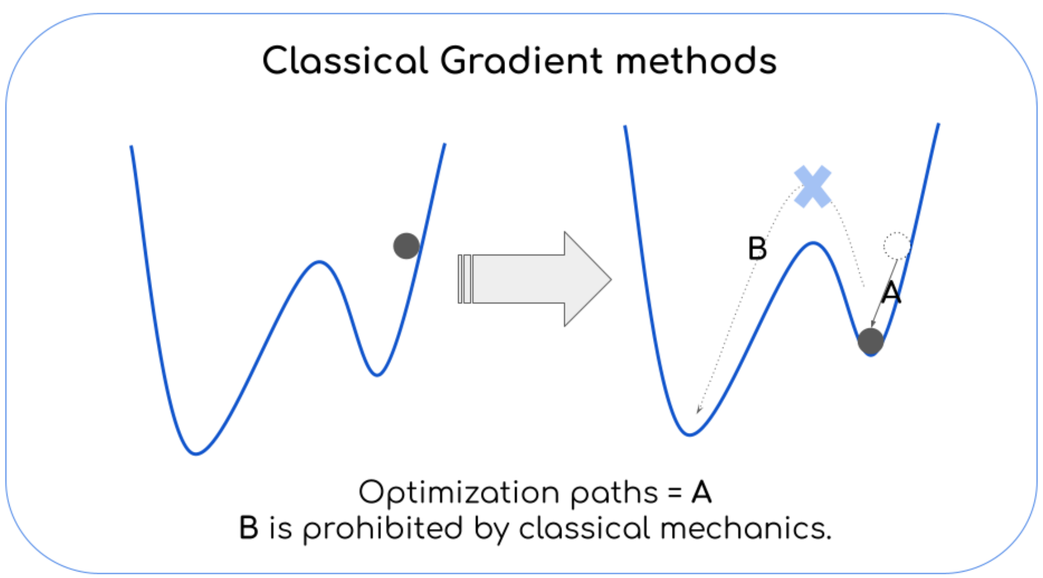
$$i\hbar\frac{\partial\Psi}{\partial t} = \left[e^{\varphi_t}\left(-\frac{\hbar^2}{2}\nabla^2\right) + e^{\chi_t} f(x)\right]\Psi$$

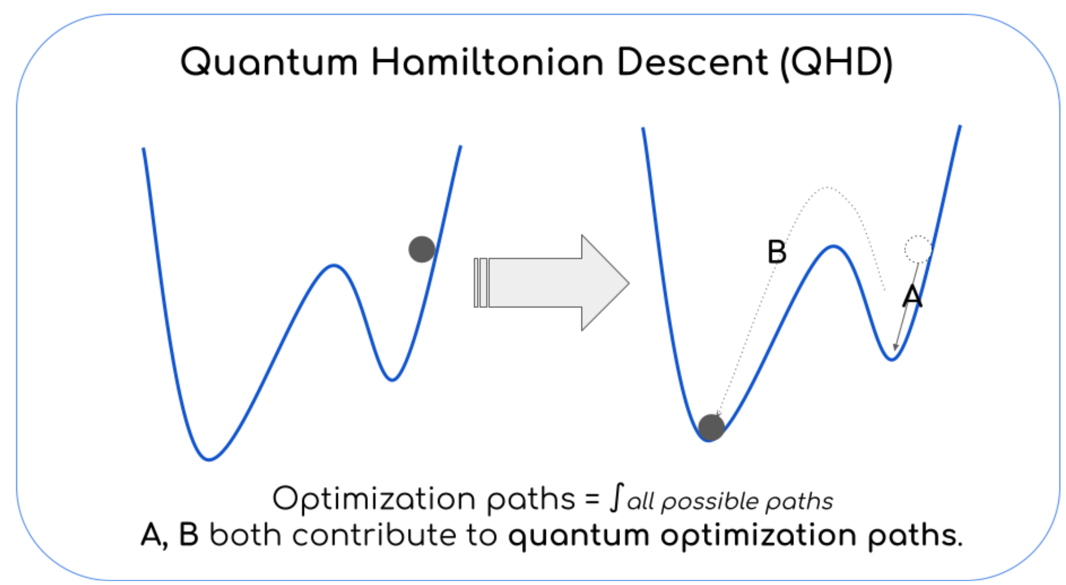
Quantum Hamiltonian Descent

$$H(t, X, P) = e^{\varphi_t}\left(\frac{1}{2}|P|^2\right) + e^{\chi_t} f(X) \longrightarrow \hat{H}(t) = e^{\varphi_t}\left(-\frac{1}{2}\nabla^2\right) + e^{\chi_t} f(x).$$

Accelerated gradient flows → Quantum Hamiltonian Descent (QHD)

- This is a quantum dynamical system with *damping* ($e^{\varphi_t - \chi_t} \to 0$).
- The energy damping allows the quantum system to *converge* to a low-energy configuration (i.e., minimizing the objective f).
- **Intuition**: "Path integral" of classical GD → does it help **nonconvex** optimization?



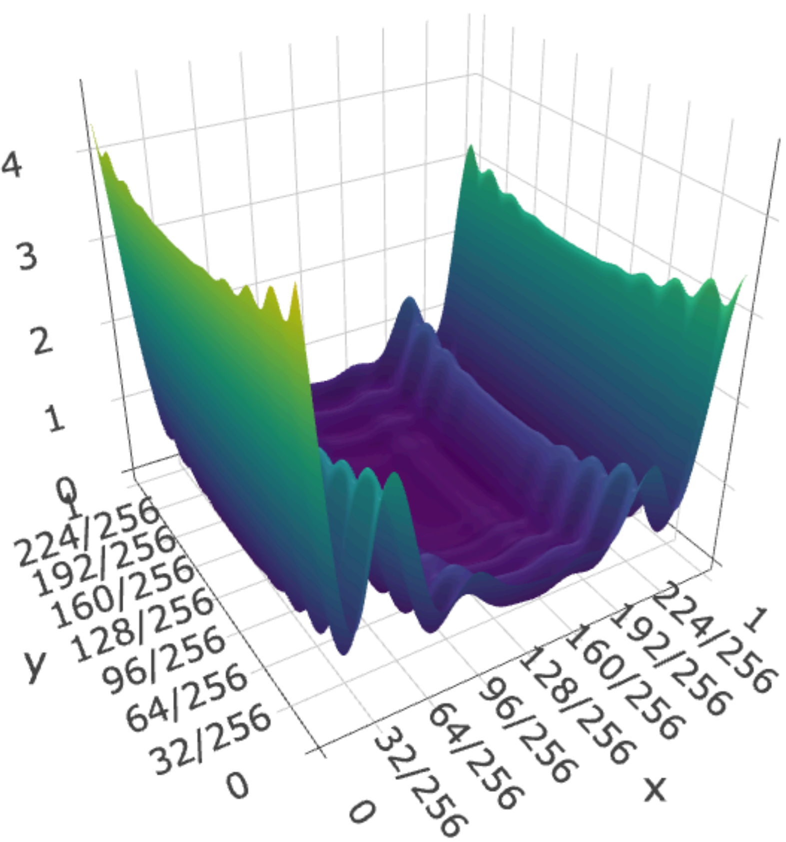


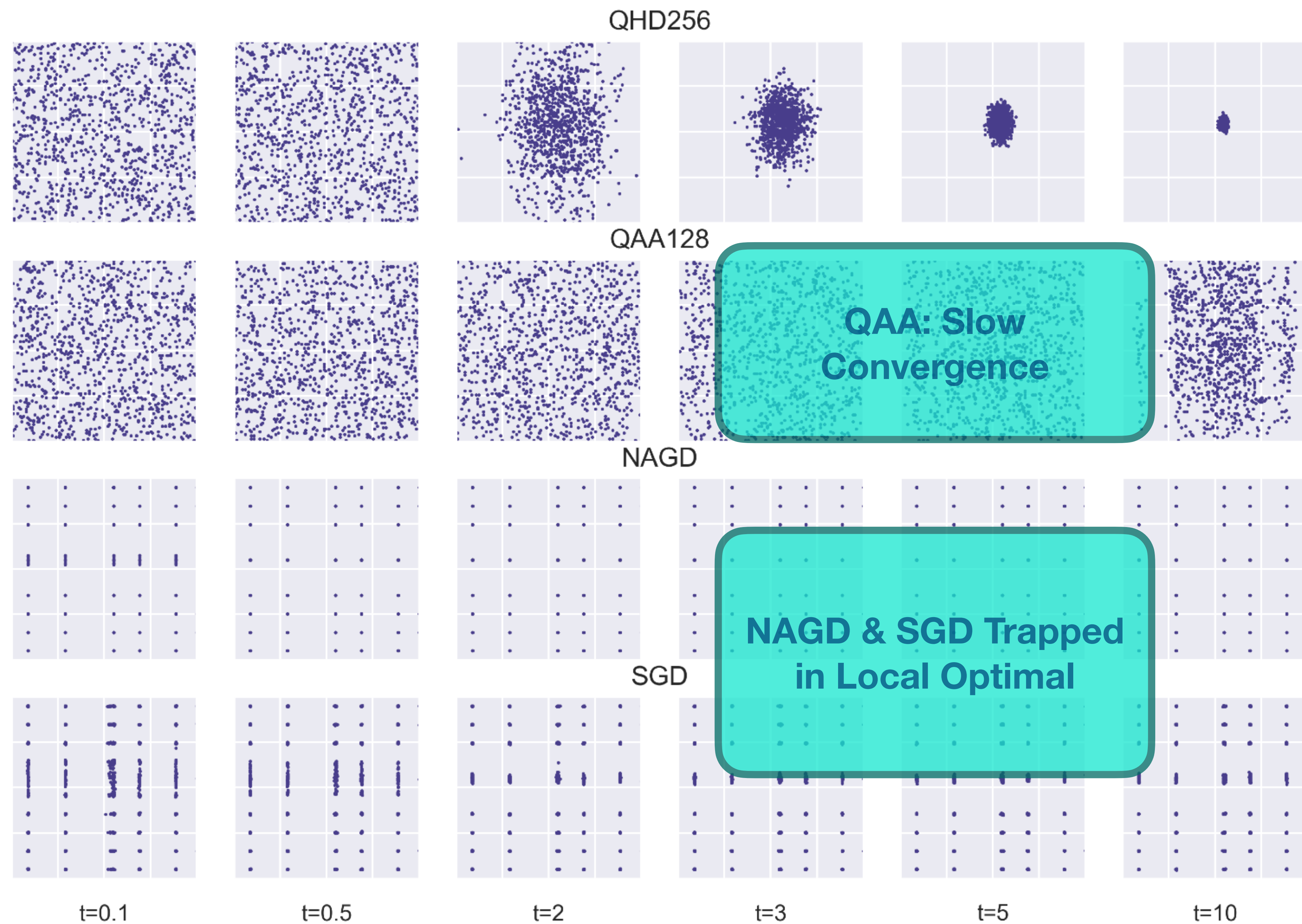
Quantum Hamiltonian Descent - numerical example

QAA: quantum adiabatic algorithm. **NAGD:** Nesterov's accelerated gradient descent.

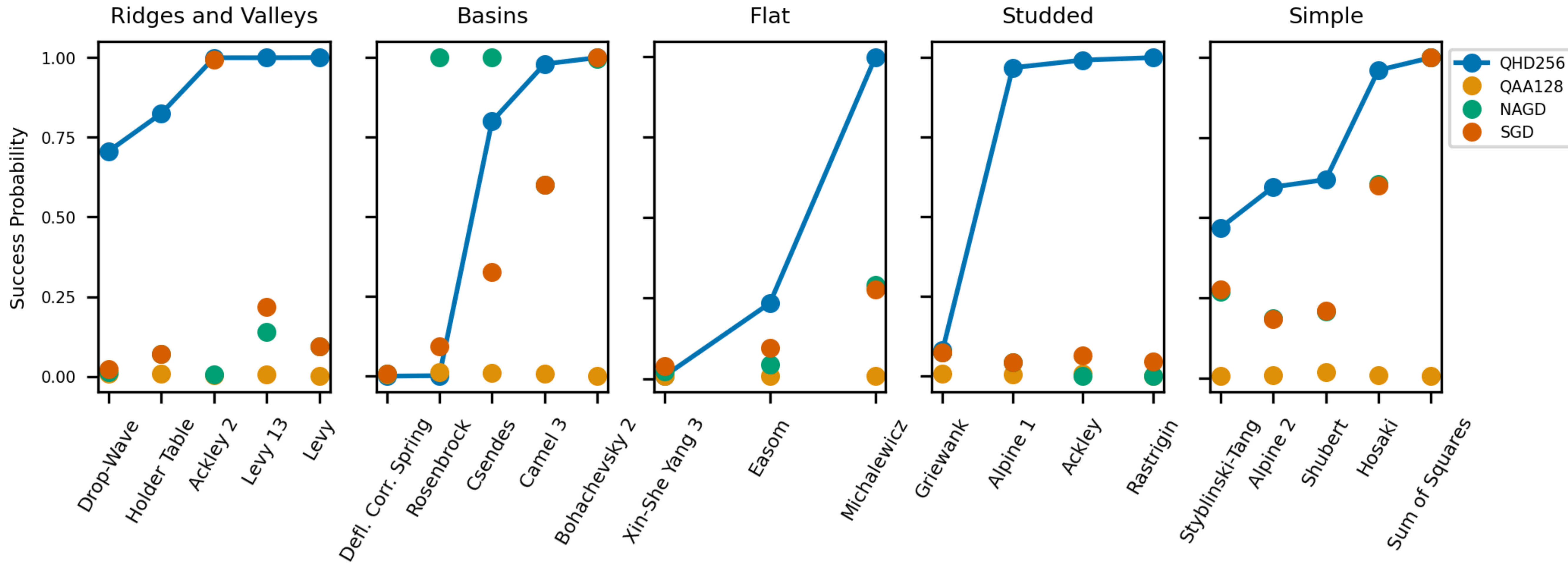
SGD: stochastic gradient descent.

QHD showcase: the Levy function.





Behavior of QHD on 2D benchmark



Measure in Success Probability for some given time:

the probability of generating a solution within radius r of the optimal solution from random initial points.

QAA: use standard *linear interpolation* in the adiabatic method (i.e., $H_T(t) = (1 - t/T)H_0 + (t/T)H_1$) and simulate $H_T(t)$ for T=10 over a **128-by-128** grid on $[0,1] \times [0,1]$.

QHD: simulate QHD Hamiltonian with Nesterov's AGD parameters (i.e., $H(t) = -\frac{1}{2t^3}\nabla^2 + t^3 f(x)$) from $t = 0$ to 10 over a **256-by-256** grid on $[0,1] \times [0,1]$.

Convergence guarantee: convex optimization

$$H(t, P, X) = e^{\alpha_t}\left(-\frac{e^{-\gamma_t}}{2}P^2 + e^{\gamma_t+\beta_t}f(X)\right) \longrightarrow \frac{d}{dt}\left(e^{-\alpha_t}\dot{X}_t + X_t\right) = e^{\alpha_t+\beta_t}\nabla f(X_t)$$

Theorem [Wibisono, Wilson, Jordan (2016)]

Assume $f(x)$ is continuously differentiable and convex, and $\dot{\beta}_t \leq e^{\alpha_t}$, $\dot{\gamma}_t = e^{\alpha_t}$ (aka, *ideal scaling condition*). Then, the solution $X(t)$ satisfies

$$f(X_t) - f(x^*) \leq O(e^{-\beta_t}).$$

$$\hat{H}(t) = e^{\alpha_t}\left(-\frac{e^{-\gamma_t}}{2}\Delta + e^{\gamma_t+\beta_t}f(x)\right) \longrightarrow \frac{\partial}{\partial t}\Psi(t, x) = \hat{H}(t)\Psi(t, x)$$

Theorem [Leng, Hickman, Li, Wu (2023)]

Assume $f(x)$ is continuously differentiable and convex, and $\dot{\beta}_t \leq e^{\alpha_t}$, $\dot{\gamma}_t = e^{\alpha_t}$ (aka, ideal scaling condition). Define $\mathbb{E}[f]_{\sim\Psi(t)} = \langle\Psi(t)|f|\Psi(t)\rangle = \int f|\Psi(t)|^2\,dx$, then we have

$$\mathbb{E}[f]_{\sim\Psi(t)} - f(x^*) \leq O(e^{-\beta_t}).$$

A Lyapunov function approach

Theorem [Leng, Hickman, Li, Wu (2023)]

Assume $f(x)$ is continuously differentiable and convex, and $\dot{\beta}_t \leq e^{\alpha_t}$, $\dot{\gamma}_t = e^{\alpha_t}$ (aka, ideal scaling condition). Define $\mathbb{E}[f]_{\sim\Psi(t)} = \langle \Psi(t) \,|\, f \,|\, \Psi(t) \rangle = \int f \,|\, \Psi(t) \,|^2 \; dx$, then we have

$$\mathbb{E}[f]_{\sim\Psi(t)} - f(x^*) \leq O(e^{-\beta_t}).$$

- We construct a Lyapunov function ($< O >_t = < \Psi_t \,|\, O \,|\, \Psi_t >$, $\hat{p} = -i\nabla$):

$$\mathcal{W}(t) = \langle \hat{J}^2/2 \rangle_t + e^{\beta_t} \langle f \rangle_t$$

$$\hat{J} := e^{-\gamma_t} \hat{p} + \hat{x}.$$

- We can prove this Lyapunov function is **non-increasing in t**.
- Therefore, we have $e^{\beta_t} \mathbb{E}[f]_{\sim\Psi_t} \leq \mathcal{W}(t) \leq \mathcal{W}(0), \quad \mathbb{E}[f]_{\sim\Psi_t} \leq \mathcal{W}(0) e^{-\beta_t} \leq O(e^{-\beta_t}).$

- A sanity check: we have the same converge rate as classical [WWJ16].
- Nesterov's GD: $e^{\alpha_t} = 2/t, \; e^{\beta_t} = e^{\gamma_t} = t^2$, implies the convergence rate $O(t^{-2})$.
- QHD is more stable & robust with larger time discretization steps.

- <u>Question: can we achieve $O(e^{-\sqrt{\beta}t})$ convergence rate for β-strongly convex f ?</u>

Convergence guarantee: nonconvex optimization

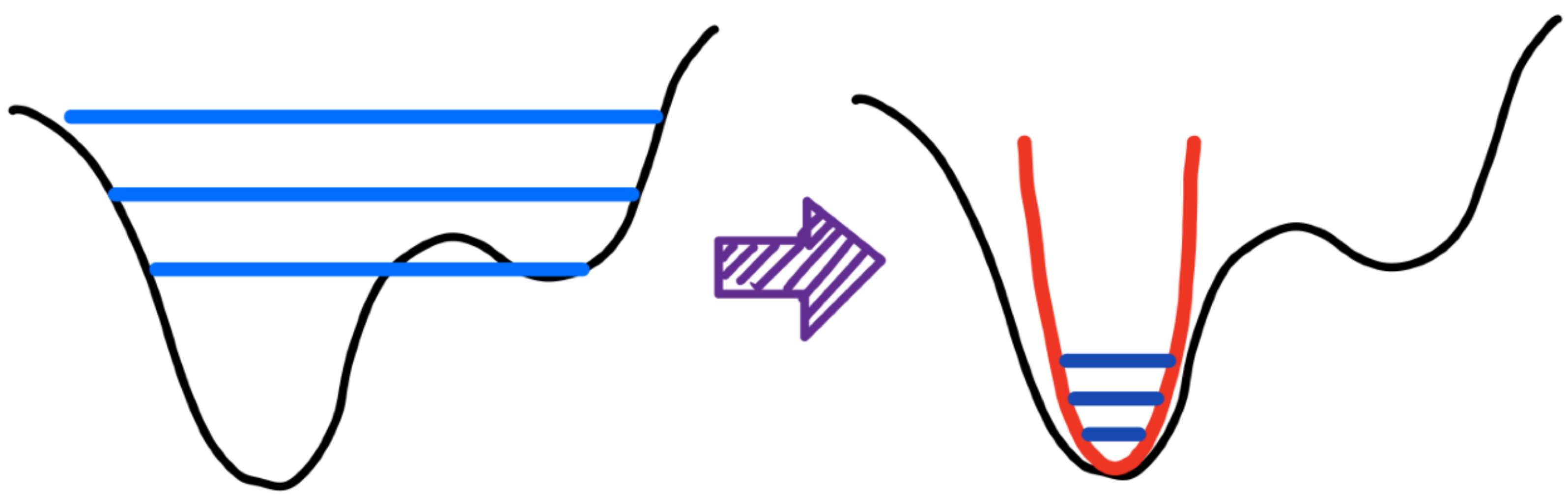
$$\hat{H}(t) = \left(-\frac{e^{\varphi_t}}{2}\Delta + e^{\chi_t} f(x)\right) \longrightarrow \frac{\partial}{\partial t}\Psi(t,x) = \hat{H}(t)\Psi(t,x)$$

Theorem (informal) [Leng, Hickman, Li , Wu (2023)]

Suppose $f(x)$ be smooth, unbounded at infinity, and has a unique non-degenerate global minimum x^*. Let the initial wave Ψ_0 be in the low-energy subspace of $H(0)$ and $e^{\varphi_t - \chi_t} \to 0$, $|\dot{\varphi}_t|, |\dot{\chi}_t| \ll 1$ (i.e., $H(t)$ is slow-varying), then

$$\lim_{t\to\infty} \mathbb{E}[f]_{\sim\Psi_t} = f(x^*)\,.$$

- Slow-varying $H(t)$ -> the wave function $\Psi(t)$ stays in the low-energy subspace for all t.
- The low-energy subspace of $H(t)$ will *migrate* to the global minimum of f as $t \to \infty$.



Quantum Hamiltonian Descent: complexity analysis

1. Prepare an initial state $|\psi_0>$.
2. Simulating the Schrodinger equation: $i\partial_t\psi = \hat{H}(t)\psi,\ \psi(0) = \psi_0$.
3. At time t = T, *measure* the final state $|\Psi_T>$ (i.e., to sample from the corresponding distribution $|\Psi(T)|^2$).
4. Ideally, the measurement results will cluster around the global minimizer of f.

$$\hat{H}(t) = e^{\varphi_t}\left(-\frac{1}{2}\nabla^2\right) + e^{\chi_t} f(x)$$

Runtime of QHD

QHD is comparable to GD in terms of simplicity and resource cost:

- Running QHD = time-dependent Hamiltonian simulation [Childs, Leng, Li, Liu & Zhang, 2022]
- The runtime of QHD is $\tilde{O}(dT)$ (d: dimension of f , T: total evolution time).
- Resource cost (on quantum computer) is comparable to that of classical GD.
- Resource cost (on classical computer) is exponential in d.

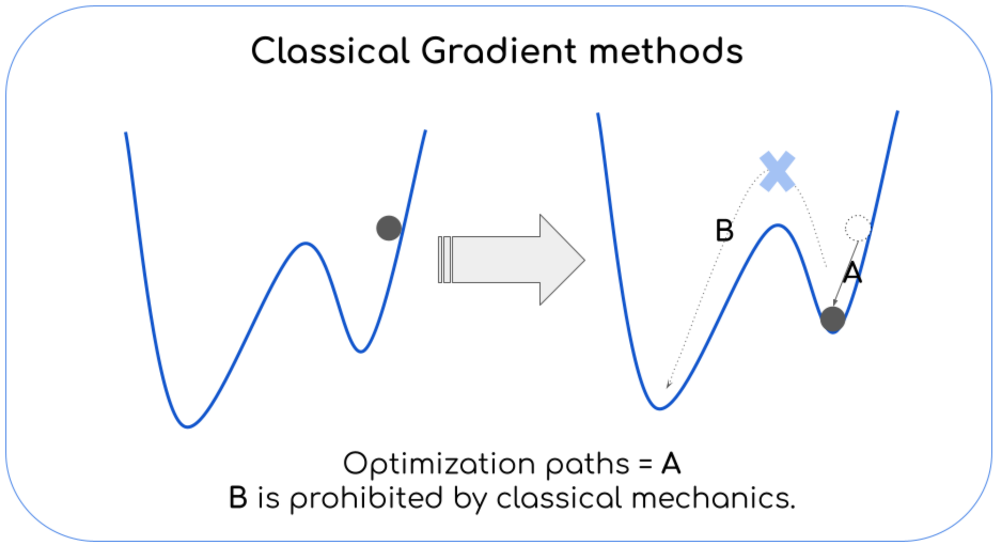
Therefore, *QHD is a quantum-upgraded version of GD*. We will demonstrate how powerful QHD could be by itself. One could also build on top of QHD like what we've done with GD.

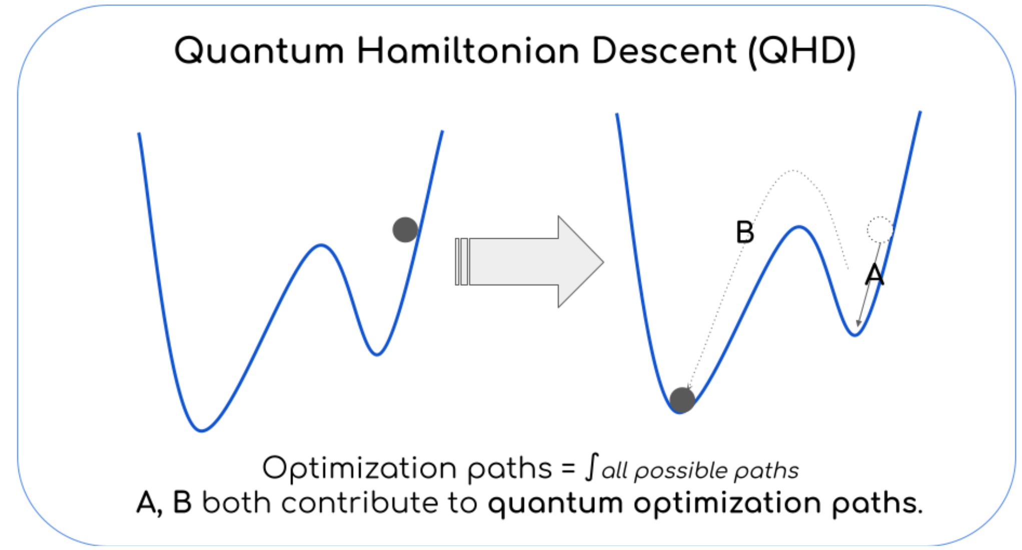
Part II:

A Quantum-Classical Performance Separation

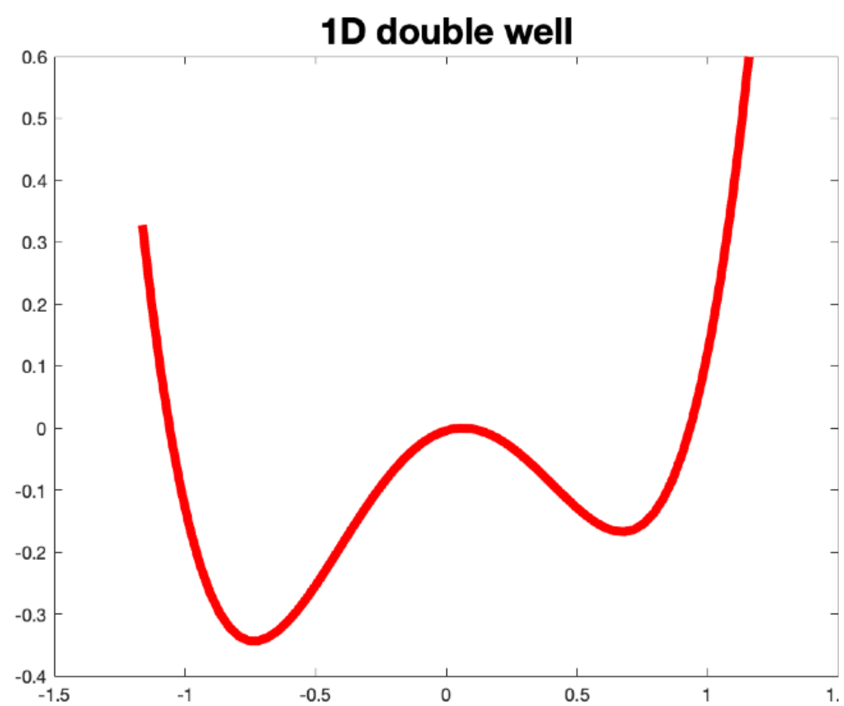
Quantum Hamiltonian Descent — practical setting?

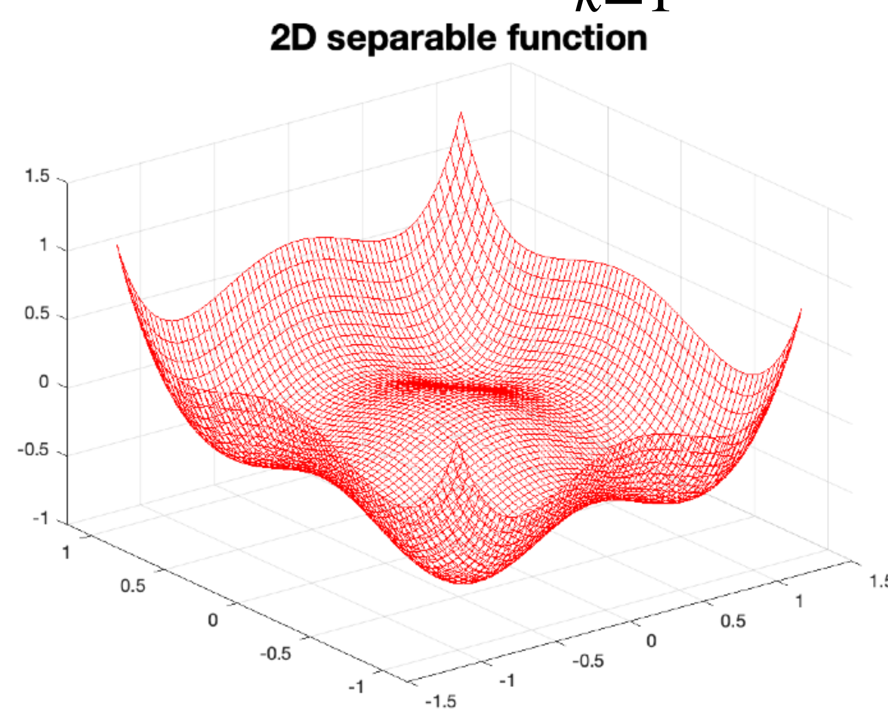
1-dim nonconvex model problem: double-well potential — $f(x)$





d-dim objective function: $F(x_1, \ldots, x_d) = \sum_{k=1}^{d} f(x_k)$,

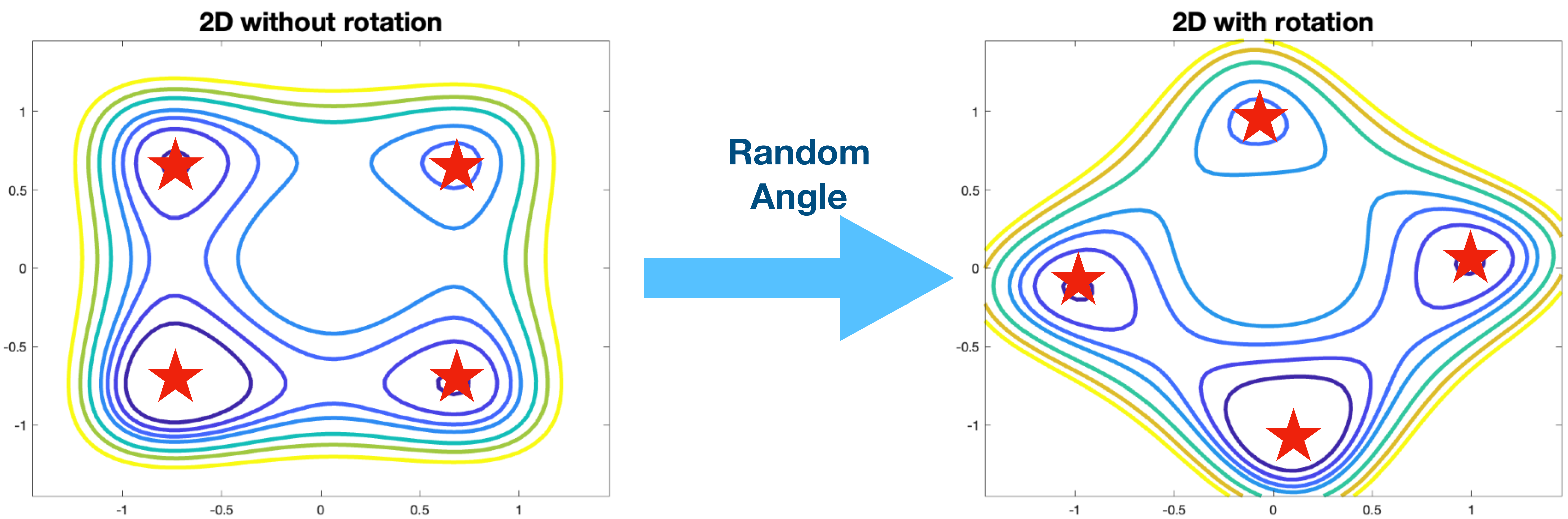




- $F(x)$ has 2^d local minima! (Only **one unique** global minimum).
- $F(x)$ is separable: not difficult for classical algorithms if the closed-form formula is given.

Construction of the optimization instances

Our instances = d-dim separable functions + random rotation



$$F(x_1, \ldots, x_d) = \sum_{k=1}^{d} f(x_k) \mapsto F_U(x) = F(Ux)$$

- $F_U(x)$ still has 2^d local minima, with a **unique** global minimum.
- $F(x)$ is non-separable: difficult to recover the rotation even with the closed-form formula!

QHD: a polynomial-time quantum algorithm

Given an optimization problem $f(x): \mathbb{R}^d \to \mathbb{R}$ with a unique global minimizer x^*.
x is a **δ-approximate** solution if $\|x - x^*\| < \delta$.

Theorem (Informal) [Leng, Zheng, Wu (2023)]

Let $f(x): \mathbb{R} \to \mathbb{R}$ be a double-well potential function. Define $F_U(x) = F(Ux)$ where $F(x) = \sum_{k=1}^{d} f(x_k)$ and U is an arbitrary orthogonal matrix. For any small $\delta > 0$, QHD can produce a δ-approximate solution with probability at least $2/3$ using

- $\tilde{\mathcal{O}}(d^3/\delta^2)$ quantum queries to F_U, and
- $\tilde{\mathcal{O}}(d^4/\delta^2)$ additional 1- and 2-qubit gates.

Manuscript in preparation.

- The QHD Hamiltonian (more precisely, the Laplacian operator) is rotationally invariant.
- The ground state of the QHD Hamiltonian is the *vehicle* of quantum optimization.
- We use an adiabatic theorem for unbounded Hamiltonian.

A quantum-classical performance separation

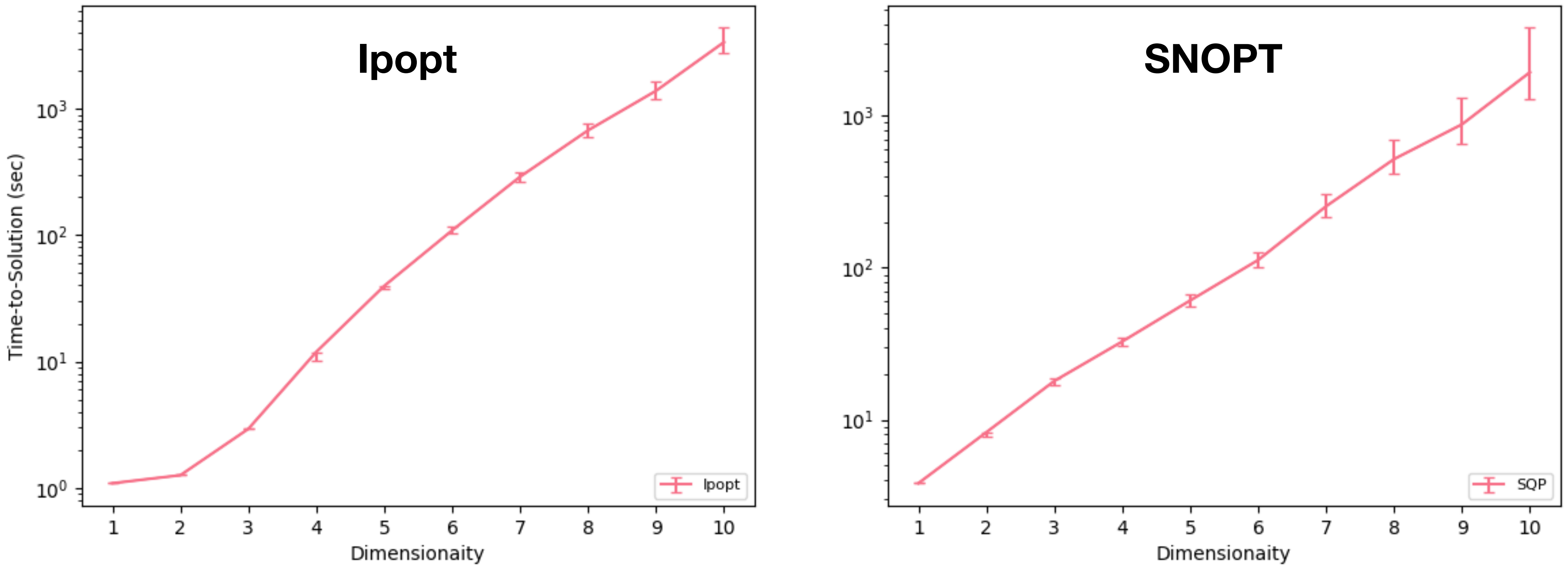
Time-To-Solution (TTS)

$$\mathrm{TTS} = t_{\mathrm{f}} \left\lceil \frac{\ln(1-0.99)}{\ln(1-P_g)} \right\rceil$$

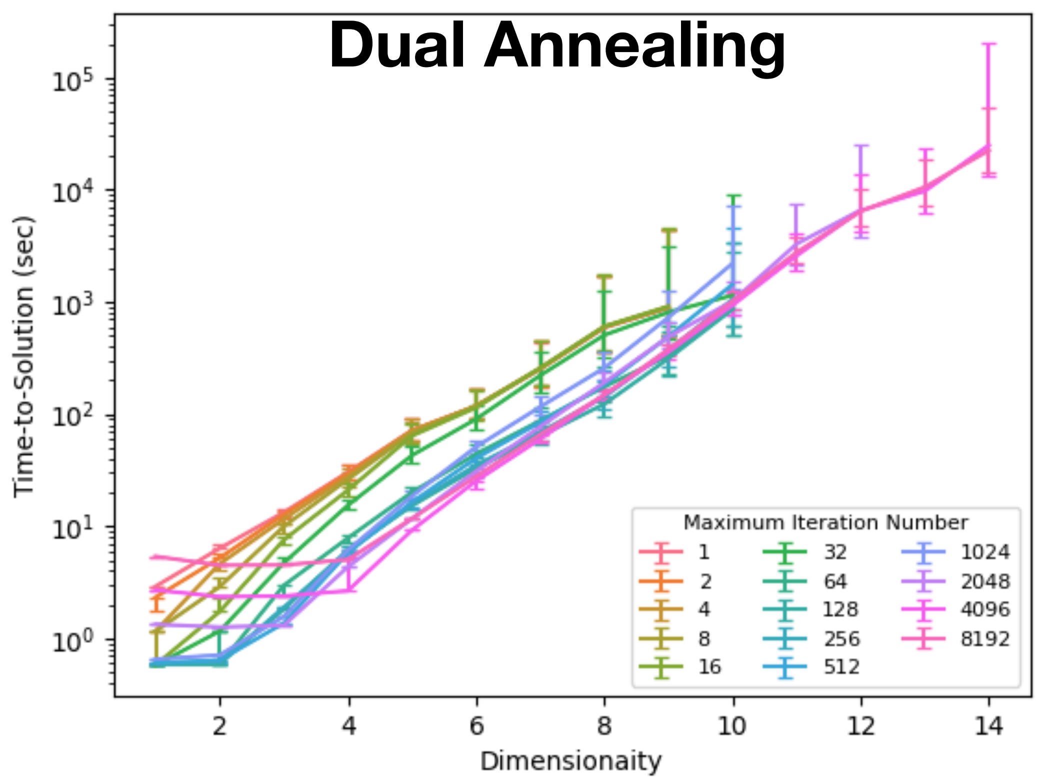
- t_f - algorithm/solver running time (wall clock time)
- p_g - success probability per run

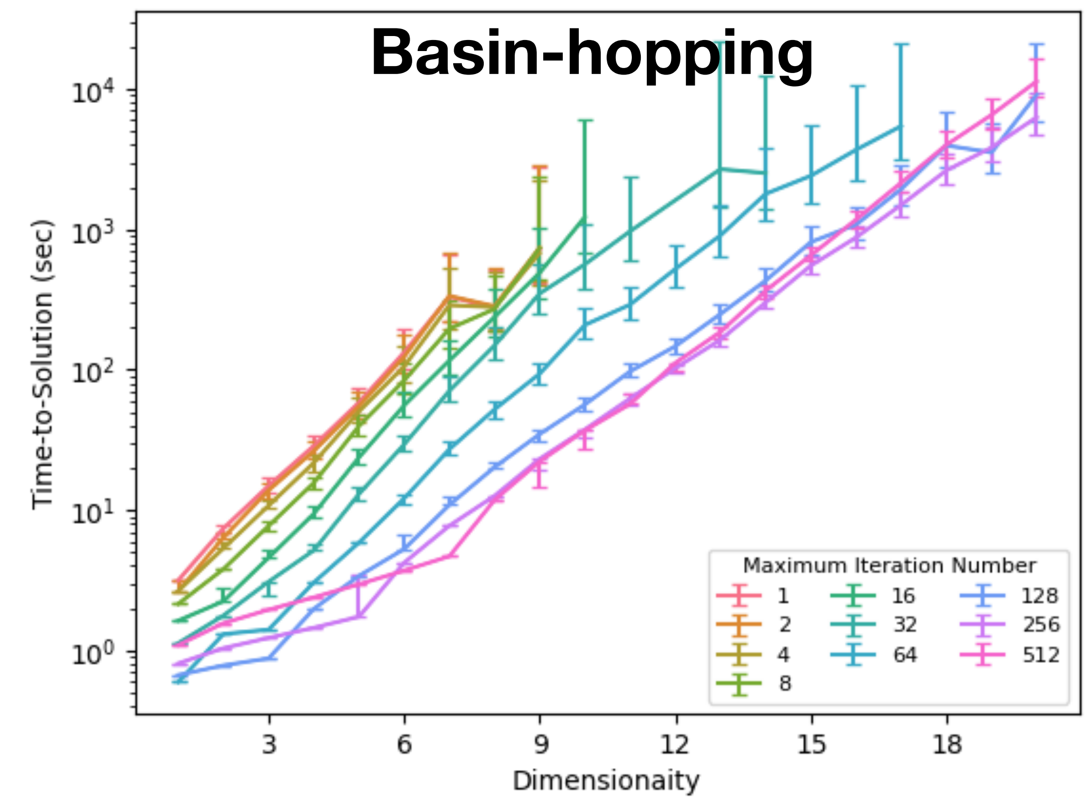
QHD TTS - $\mathcal{O}(d^4)$ (given fixed δ)

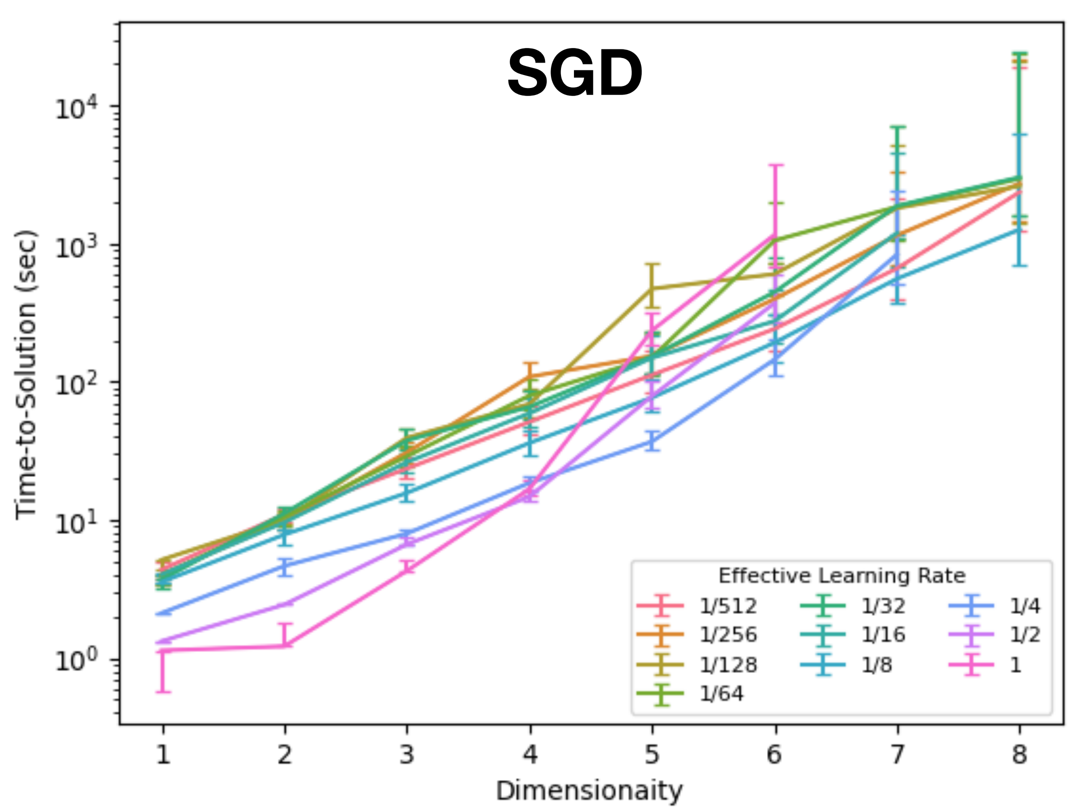
Classical TTS - numerical results suggest super-polynomial scaling in d

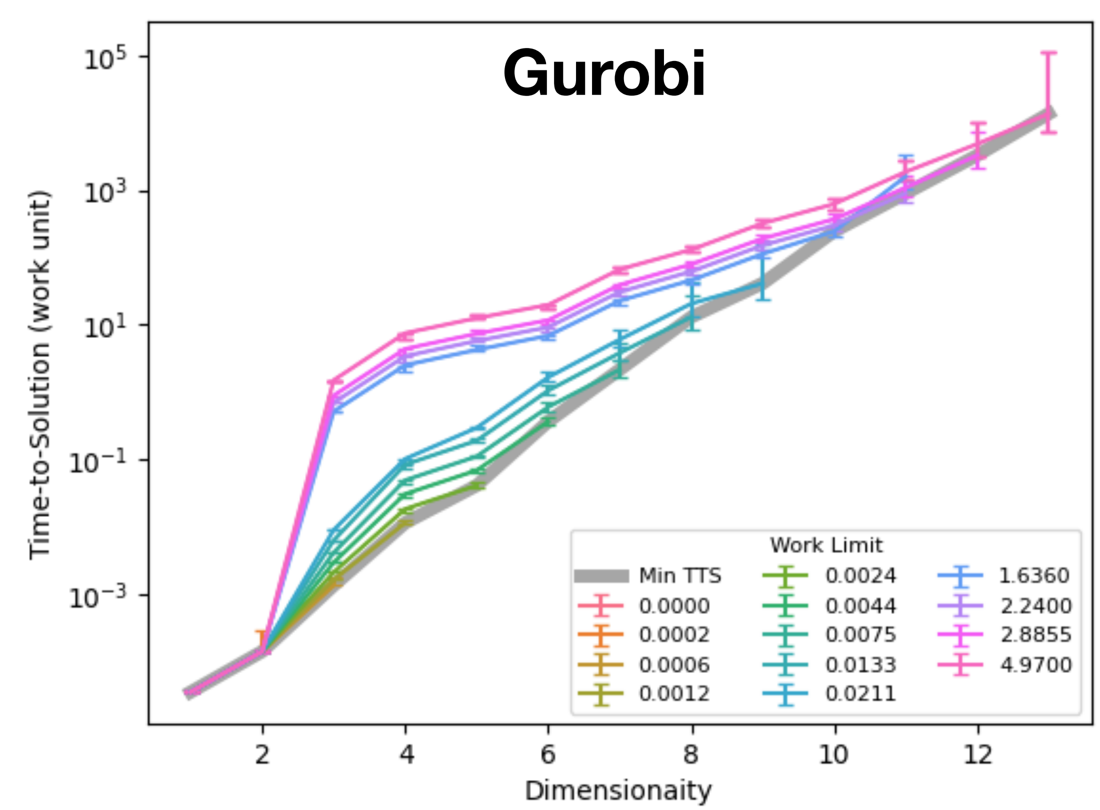


A quantum-classical performance separation









Part III:

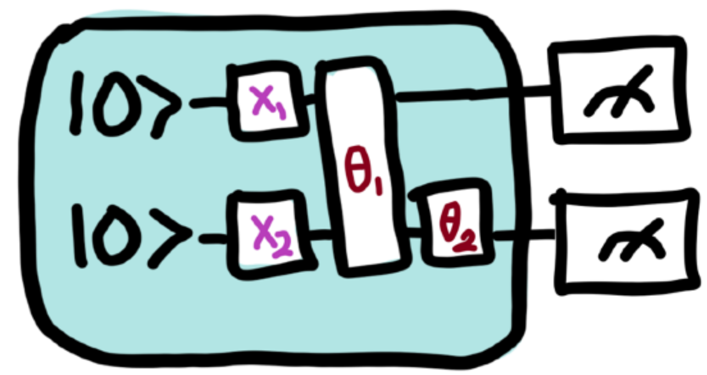
Implementation on Quantum Computers

QHD with digital quantum computers

$$H(t) = e^{\varphi(t)}(-\frac{1}{2}\nabla^2) + e^{\chi(t)}f(x), t \geq 0$$

Digital Quantum Implementation

- The algorithm is effectively a **time-dependent Hamiltonian simulation** in the real space (we know poly-time algorithms).
- Requires hundreds of millions of gates!
- **Conclusion**: the digital implementation is **far from being feasible** in near term!



Corresponding **T-gate** Count with Digital Quantum Computing (before fault-tolerance)

Dimensions	**3-qubit format**	**16-qubit format**	**32-qubit format**
50	5.49e+8	7.8386e+9	2.672e+10
60	6.588e+8	9.4063e+9	3.2064e+10
75	8.235e+8	1.1758e+10	4.008e+10

QHD with analog quantum computers

Analog Quantum Implementation

- **Analog simulation**: problem solving by *emulating real quantum systems*.
- Abstraction: **Quantum Ising Machine** (**QIM**, e,g., D-Wave, QuEra, etc.)

$$H(t) = -\frac{A(t)}{2}\left(\sum_j \sigma_x^{(j)}\right) + \frac{B(t)}{2}\left(\sum_j h_j \sigma_z^{(j)} + \sum_{j>k} J_{j,k}\sigma_z^{(j)}\sigma_z^{(k)}\right)$$

- **Programmability:** coefficients $h_j, J_{j,k}$ and functions $A(t), B(t)$.

- QHD is formulated as a quantum Hamiltonian evolution → suitable for analog implementation!
- Patter mismatch: QHD $H(t) = e^{\varphi_t}(-\Delta/2) + e^{\chi_t}f$
- We develop a new technique named **Hamiltonian embedding**: mapping our target Hamiltonian (QHD) to a “diagonal block” of the machine Hamiltonian (QIM).
- If $H = H_0 \oplus H_1$, we have $e^{-iHt} = e^{-iH_0t} \oplus e^{-iH_1t}$.
- We implement QHD on today’s analog quantum computers (D-Wave’s **advantage_system6.1**).
- **Advantage**: resource-efficiency → first large-scale empirical study for nonlinear optimization using quantum computers.

Hamiltonian embedding of QHD

$$i\frac{\partial}{\partial t}\Psi(t,x) = \left[\underbrace{-\frac{e^{\varphi_t}}{2}\nabla^2}_{\text{Kinetic part}} + \underbrace{e^{\chi_t} f(x)}_{\text{Potential part}}\right]\Psi(t,x), \quad \xrightarrow{\text{Finite difference}} \quad i\frac{\mathrm{d}}{\mathrm{d}t}|\phi_t\rangle = \left[\underbrace{-\frac{e^{\varphi_t}}{2}\hat{A}}_{\text{Kinetic part}} + \underbrace{e^{\chi_t}\hat{F}}_{\text{Potential part}}\right]|\phi_t\rangle$$

- **Kinetic operator:**

$$\hat{L} = \frac{1}{(1/r)^2}\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ \cdots & \cdots & \cdots & \cdots \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{bmatrix} \quad \Rightarrow \quad \hat{A} = \frac{1}{(1/r)^2}\begin{bmatrix} 0 & 1 & & \\ 1 & 0 & 1 & \\ \cdots & \cdots & \cdots & \cdots \\ & 1 & 0 & 1 \\ & & 1 & 0 \end{bmatrix}$$

Tri-diagonal

Diagonal

- **Potential operator:**

$$\hat{F} = \begin{bmatrix} f(a_0) & & & \\ & f(a_1) & & \\ \cdots & \cdots & \cdots & \cdots \\ & & f(a_{r-1}) & \\ & & & f(a_r) \end{bmatrix}$$

Hamming states — an orthonormal basis

$$|H_j> = \frac{1}{\sqrt{C_j}}\sum_{|b|=j}|b> \quad \text{where } C_j = \binom{N}{j} \text{ and } 0 \le j \le N$$

$$|H_0> = |0000> , |H_1> = \frac{1}{2}(|1000> + |0100> + |0010> + |0001>), etc.$$

Lemma (informal version). [Leng, Hickman, Li, Wu (2023)]

Given n qubits, the subspace $\mathcal{S}$ spanned by all $(n+1)$ Hamming states is an invariant subspace of the QIM Hamiltonian. The projection of the QIM Hamiltonian into the subspace $\mathcal{S}$ approximates the discretized QHD Hamiltonian.

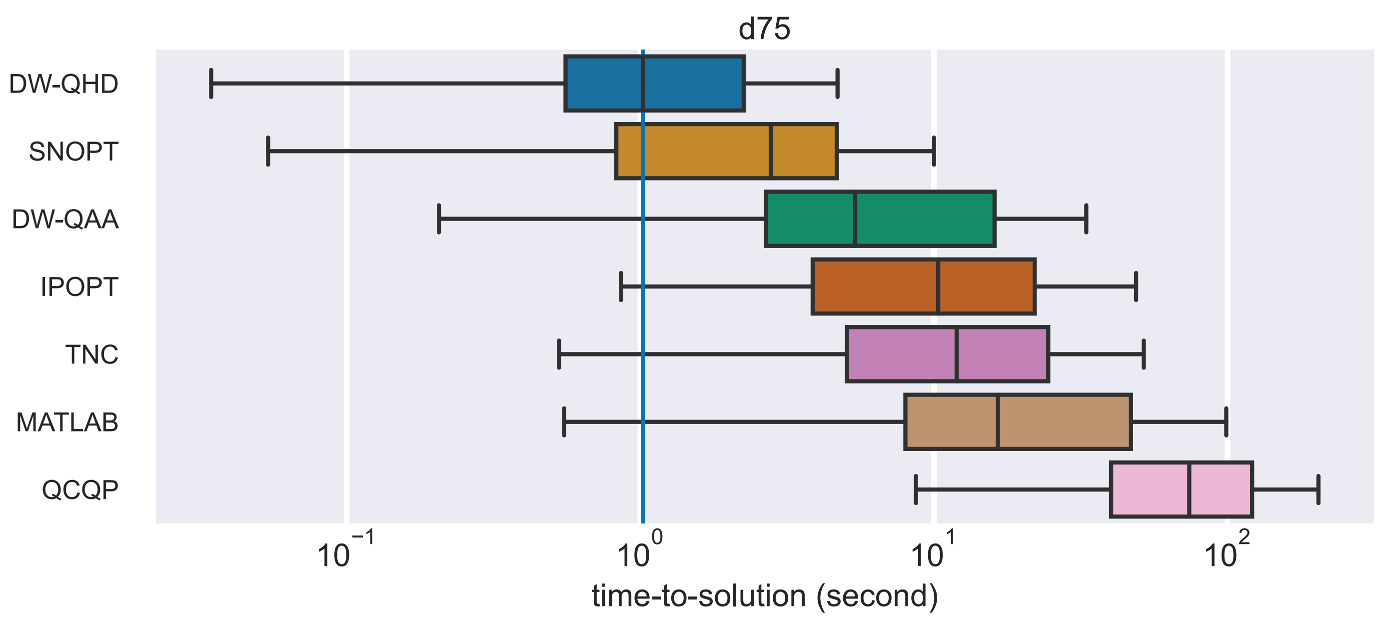
Large-scale empirical study on real quantum computers

We identify a class of *non-trivial* and *self-interesting* optimization problems that can be mapped to QIMs — **Quadratic Programming (QP) with box constraints**.

$$\begin{aligned} &\text{minimize} && f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{Q}\mathbf{x} + \mathbf{b}^\top \mathbf{x} \\ &\text{subject to} && \mathbf{0} \preccurlyeq \mathbf{x} \preccurlyeq \mathbf{1}, \end{aligned}$$

QP — NP-hard with indefinite Q

(For implementation details, see our paper arXiv:2303.01471 **Appendix F**)



Time-To-Solution (TTS)

The lower, the better!!

$$\mathrm{TTS} = t_f \left\lceil \frac{\ln(1-0.99)}{\ln(1-P_g)} \right\rceil$$

t_f - quantum anneal time + post-processing or classical runtime (**wall-clock time**)

p_g - success probability per run

- **DW-QHD** is better than the rest, including **DW-QAA**, and **classical GD, interior points**, and **some local search heuristic.**
- Assuming DW-QHD is no worse than the ideal QHD, this provides **a very strong empirical evidence supporting QHD**.
- QHD does not beat SOTA classical solvers (e.g., Gurobi, CPLEX) in D75. However, such branch-and-bound solvers are **not scalable!**

Summary & Future Work

- **QHD** is an upgraded version of classical GD and variants.
- QHD leverages the continuous structure of the problem and converges faster than QAA.
- QHD has different solution path compared to classical GD.

- **QHD** can be used as *subroutines* for more complicated algorithms like branch-and-bound.

All data & codes are available online!

- Source code (Github): https://github.com/jiaqileng/quantum-hamiltonian-descent
- Raw data (Box): https://umd.app.box.com/s/vq747fvjnt8qrkbxprexhoh44n0q9m0i
- Website: https://jiaqileng.github.io/quantum-hamiltonian-descent/

arXiv:2303.01471

Thank You!

QHD Website