Variational Quantum Semi-Definite Programming

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Motivation and Goal

- Optimization is a key task for which quantum computers could possibly provide a speedup over classical algorithms
- Semi-definite programs (SDPs) have wide applicability in computer science, engineering, mathematics, and physics
- This talk:
  1) brief overview of SDP theory
  2) QSlack method for estimating their optimal values

Background on
Semi-Definite Programming

Background on Semi-Definite Programming

- An SDP involves optimizing a linear objective function over the cone of positive semi-definite matrices, with affine constraints
- Every SDP (called primal SDP) has a corresponding dual SDP
- Dual SDP involves opposite kind of optimization and provides a bound on primal SDP

Primal and Dual SDPs

- SDP inputs are Hermitian matrices A and B and a Hermiticity-preserving superoperator Φ
- Primal SDP: $\alpha := \sup_{X \geq 0} \{\mathrm{Tr}[AX] : \Phi(X) \leq B\}$
- Dual SDP: $\beta := \inf_{Y \geq 0} \left\{\mathrm{Tr}[BY] : \Phi^\dagger(Y) \geq A\right\}$

Adjoint of a Superoperator

- Recall Hilbert-Schmidt inner product: $\langle C, D\rangle := \mathrm{Tr}[C^\dagger D]$
- Superoperator $\Phi^\dagger$ is adjoint of Φ
- It is the unique superoperator satisfying $\langle Y, \Phi(X)\rangle = \left\langle \Phi^\dagger(Y), X\right\rangle$ for all X, Y

SDP Duality Theory

- Weak duality $\alpha \leq \beta$ always holds

$$\alpha := \sup_{X \geq 0} \{\mathrm{Tr}[AX] : \Phi(X) \leq B\}$$

$$\beta := \inf_{Y \geq 0} \left\{\mathrm{Tr}[BY] : \Phi^\dagger(Y) \geq A\right\}$$

- Indeed, for all feasible X and Y,

$$\mathrm{Tr}[AX] \leq \mathrm{Tr}[\Phi^\dagger(Y)X] = \mathrm{Tr}[Y\Phi(X)] \leq \mathrm{Tr}[YB]$$

- Slater's condition $\Rightarrow$ strong duality $\alpha = \beta$

- Strong duality holds in practice for many SDPs

Application of SDP Duality

- SDP duality theory allows for bounding the optimal value α from both above and below
- Key feature that we make use of in QSlack, for providing certified bounds on the optimal value

Quantum Mechanics and Semi-Definite Constraints

- Postulates of quantum mechanics: all its constituents are described by constrained positive semi-definite matrices
- Quantum state $\rho \in \mathscr{D}$ satisfies $\rho \geq 0$ and $\mathrm{Tr}[\rho] = 1$
- Quantum measurement $(\Lambda_x)_{x \in \mathscr{X}}$ satisfies $\Lambda_x \geq 0 \ \ \forall x \in \mathscr{X}$ and $\displaystyle\sum_{x \in \mathscr{X}} \Lambda_x = I$
- Choi matrix of a channel $\mathscr{N}$ satisfies $\Gamma^{\mathscr{N}}_{RB} \geq 0$ and $\mathrm{Tr}_B[\Gamma^{\mathscr{N}}_{RB}] = I_R$
- Thus natural for SDPs to play a role in q. information and vice versa

Ground-State Energy as an SDP

- Finding the ground-state energy of a Hamiltonian H is an SDP:

$$\lambda_{\min}(H) = \inf_{\rho \in \mathcal{D}} \mathrm{Tr}[H\rho]$$

- Dual SDP is

$$\lambda_{\min}(H) = \sup_{\eta \in \mathbb{R}} \left\{ \eta : \eta I \leq H \right\}$$

- Key example of interest in physics

Normalized Trace Distance as an SDP

- Key distinguishability measure of quantum states ρ and σ is normalized trace distance

- Can be written as primal and dual SDPs:

$$\frac{1}{2}\|\rho-\sigma\|_1 = \sup_{\Lambda\geq 0}\left\{\mathrm{Tr}[\Lambda(\rho-\sigma)] : \Lambda \leq I\right\} = \inf_{Z\geq 0}\left\{\mathrm{Tr}[Z] : Z \geq \rho-\sigma\right\}$$

Four Steps of QSlack

(focusing on primal SDP)

Step 1 of QSlack: Introduce Slack Variables

- Introduce slack variable $W \geq 0$ to replace inequality constraint $\Phi(X) \leq B$ with equality constraint $B - \Phi(X) = W$:

$$
\begin{aligned}
\alpha &= \sup_{X \geq 0} \{\mathrm{Tr}[AX] : \Phi(X) \leq B\} \\
&= \sup_{X, W \geq 0} \{\mathrm{Tr}[AX] : B - \Phi(X) = W\}
\end{aligned}
$$

- Follows because $\Phi(X) \leq B$ is equivalent to existence of $W \geq 0$ such that $B - \Phi(X) = W$

Step 2 of QSlack: Introduce Penalty Terms

- Use penalty term to move equality constraint into objective function:

$$\alpha(c) := \sup_{X,W\geq 0} \left\{ \mathrm{Tr}[AX] - c \left\| B - \Phi(X) - W \right\|_2^2 \right\}$$

where $c > 0$ is a penalty constant

- From optimization theory, we know that $\lim_{c\to\infty} \alpha(c) = \alpha$

- Use finite but large value of c to approximate $\lim_{c\to\infty} \alpha(c) = \alpha$

Step 3 of QSlack: Introduce Density Matrices

- Replace optimization over PSD matrices with scaled density matrices:

$$\alpha(c) = \sup_{X,W \geq 0} \left\{ \mathrm{Tr}[AX] - c \left\| B - \Phi(X) - W \right\|_2^2 \right\}$$

$$= \sup_{\substack{\lambda, \mu \geq 0, \\ \rho, \sigma \in \mathcal{D}}} \left\{ \lambda \, \mathrm{Tr}[A\rho] - c \left\| B - \lambda\Phi(\rho) - \mu\sigma \right\|_2^2 \right\}$$

- As before, $\lim_{c \to \infty} \alpha(c) = \alpha$

Step 4 of QSlack: Parameterize States

- Final step: Replace optimization over all states with optimization over parameterized states:

$$\tilde{\alpha}(c) := \sup_{\lambda,\mu\geq 0,\theta_1,\theta_2\in\Theta} \left\{ \lambda \operatorname{Tr}[A\rho(\theta_1)] - c \left\| B - \lambda\Phi(\rho(\theta_1)) - \mu\sigma(\theta_2) \right\|_2^2 \right\},$$

- Then $\alpha(c) \geq \tilde{\alpha}(c)$ holds because set of parameterized states is contained in set of all states

Steps of QSlack for Dual SDP

- Steps are similar and shown concisely here

$$\beta := \inf_{Y \geq 0} \left\{ \mathrm{Tr}[BY] : \Phi^\dagger(Y) \geq A \right\}$$

$$= \inf_{Y, Z \geq 0} \left\{ \mathrm{Tr}[BY] : \Phi^\dagger(Y) - A = Z \right\}$$

$$\beta(c) := \inf_{Y, Z \geq 0} \left\{ \mathrm{Tr}[BY] + c \left\| \Phi^\dagger(Y) - A - Z \right\|_2^2 \right\}$$

$$\lim_{c \to \infty} \beta(c) = \beta$$

$$= \inf_{\substack{\kappa, \nu \geq 0, \\ \tau, \omega \in \mathscr{D}}} \left\{ \kappa \, \mathrm{Tr}[B\tau] + c \left\| \kappa \Phi^\dagger(\tau) - A - \nu\omega \right\|_2^2 \right\}$$

$$\geq \tilde{\beta}(c) := \inf_{\kappa, \nu \geq 0, \theta_3, \theta_4 \in \Theta} \left\{ \kappa \, \mathrm{Tr}[B\tau(\theta_3)] + c \left\| \kappa \Phi^\dagger(\tau(\theta_3)) - A - \nu\omega(\theta_4) \right\|_2^2 \right\},$$

QSlack

Primal		Dual
$\alpha = \sup_{X \geq 0} \{\mathrm{Tr}[AX] : \Phi(X) \leq B\}$	Constrained forms Weak duality: $\alpha \leq \beta$	$\beta = \inf_{Y \geq 0} \{\mathrm{Tr}[BY] : \Phi^\dagger(Y) \geq A\}$
$\alpha = \sup_{X,W \geq 0} \{\mathrm{Tr}[AX] : B - \Phi(X) = W\}$	Introduce slack variables	$\beta = \inf_{Y,Z \geq 0} \{\mathrm{Tr}[BY] : \Phi^\dagger(Y) - A = Z\}$
$\alpha(c) = \sup_{X,W \geq 0} \left\{\mathrm{Tr}[AX] - c\Vert B - \Phi(X) - W\Vert_2^2\right\}$ $\alpha = \lim_{c\to\infty} \alpha(c)$	Unconstrained forms (introduce penalty terms)	$\beta(c) = \inf_{Y,Z \geq 0} \left\{\mathrm{Tr}[BY] + c\left\Vert \Phi^\dagger(Y) - A - Z\right\Vert_2^2\right\}$ $\beta = \lim_{c\to\infty} \beta(c)$
$\alpha(c) = \sup_{\substack{\lambda,\mu \geq 0, \\ \rho,\sigma \in \mathcal{D}}} \left\{\lambda \,\mathrm{Tr}[A\rho] - c\Vert B - \lambda\Phi(\rho) - \mu\sigma\Vert_2^2\right\}$ $\alpha = \lim_{c\to\infty} \alpha(c)$	Write positive semi-definite matrices as scaled density matrices	$\beta(c) = \inf_{\substack{\kappa,\nu \geq 0, \\ \tau,\omega \in \mathcal{D}}} \left\{\kappa \,\mathrm{Tr}[B\tau] + c\left\Vert \kappa\Phi^\dagger(\tau) - A - \nu\omega\right\Vert_2^2\right\}$ $\beta = \lim_{c\to\infty} \beta(c)$
$\tilde{\alpha}(c) = \sup_{\substack{\lambda,\mu \geq 0, \\ \theta_1,\theta_2 \in \Theta}} \left\{\lambda \,\mathrm{Tr}[A\rho(\theta_1)] - c\Vert B - \lambda\Phi(\rho(\theta_1)) - \mu\sigma(\theta_2)\Vert_2^2\right\}$ $\lim_{c\to\infty} \tilde{\alpha}(c) \leq \alpha$	Parameterize density matrices	$\tilde{\beta}(c) = \inf_{\substack{\kappa,\nu \geq 0, \\ \theta_3,\theta_4 \in \Theta}} \left\{\kappa \,\mathrm{Tr}[B\tau(\theta_3)] + c\left\Vert \kappa\Phi^\dagger(\tau(\theta_3)) - A - \nu\omega(\theta_4)\right\Vert_2^2\right\}$ $\beta \leq \lim_{c\to\infty} \tilde{\beta}(c)$

Estimate the objective function using a quantum computer + Perform the optimization using a classical optimizer

Key Theoretical Insight of QSlack

- QSlack bounds on the optimal SDP values α and β:

$$\tilde{\alpha} \leq \alpha \leq \beta \leq \tilde{\beta}$$

where

$$\tilde{\alpha} := \sup_{\substack{\lambda, \mu \geq 0, \\ \theta_1, \theta_2 \in \Theta}} \left\{ \lambda \operatorname{Tr}[A\rho(\theta_1)] : B - \lambda \Phi(\rho(\theta_1)) = \mu \sigma(\theta_2) \right\},$$

$$\tilde{\beta} := \inf_{\substack{\kappa, \nu \geq 0, \\ \theta_3, \theta_4 \in \Theta}} \left\{ \kappa \operatorname{Tr}[B\tau(\theta_3)] : \kappa \Phi^\dagger(\tau(\theta_3)) - A = \nu \omega(\theta_4) \right\},$$

- In the ideal case in which the optimal $\tilde{\alpha}$ and $\tilde{\beta}$ can be found, then QSlack bounds the optimal SDP values α and β from above and below

How to Parameterize n-Qubit Mixed States?

- Purification ansatz: generate parameterized pure state on $2n$ qubits and trace over half of them:

$$\rho(\theta) = \mathrm{Tr}_R[U(\theta)|0\rangle\langle 0|_{RS} U^\dagger(\theta)]$$

- Convex combination ansatz (CCA): sample x randomly from a parameterized neural net & then input $|x\rangle$ to a parameterized unitary:

$$\rho(\varphi, \gamma) = \sum_x p_\varphi(x) U(\gamma) |x\rangle\langle x| U^\dagger(\gamma)$$

- Advantage of CCA is that only n qubits are needed

Executing QSlack on a Quantum Computer

- Suppose A, B, and Φ correspond to efficiently measurable observables
- Then a q. computer can measure all objective-function terms efficiently (using expectations of observables or destructive SWAP tests)
- In general, it is not clear how to do so on a classical computer
- Hope is that QSlack might give a q. advantage over classical methods

Performing Optimization

- Estimate objective function and its gradient ∇_θ using q. computer and parameter-shift rule (can also use SPSA)
- Then employ gradient descent or its variants

Example: Ground-State Energy

- Recall the ground-state energy problem:

$$\lambda_{\min}(H) = \inf_{\rho \in \mathscr{D}} \operatorname{Tr}[H\rho] = \sup_{\eta \in \mathbb{R}} \left\{ \eta : \eta I \leq H \right\}$$

- For the minimization, apply the variational quantum eigensolver (VQE)
- VQE upper bounds $\lambda_{\min}(H)$, but quality of bound is unclear
- For the maximization, apply QSlack to lower bound $\lambda_{\min}(H)$ (called Dual-VQE for this application)

Example: Ground-State Energy (Ctd.)

- In more detail, Dual-VQE method:

$$\begin{aligned}
\sup_{\eta\in\mathbb{R}} \left\{\eta : \eta I \le H\right\} &= \sup_{\eta\in\mathbb{R}, W\ge 0} \left\{\eta : H - \eta I = W\right\} \\
&= \sup_{\eta \in \mathbb{R}, \nu \ge 0, \omega \in \mathscr{D}} \left\{\eta : H - \eta I = \nu\omega\right\} \\
&= \lim_{c\to\infty} \sup_{\eta \in \mathbb{R}, \nu \ge 0, \omega \in \mathscr{D}} \left\{\eta - c \left\| H - \eta I - \nu\omega \right\|_2^2\right\} \\
&\ge \lim_{c\to\infty} \sup_{\eta \in \mathbb{R}, \nu \ge 0, \theta \in \Theta} \left\{\eta - c \left\| H - \eta I - \nu\omega(\theta) \right\|_2^2\right\}
\end{aligned}$$

Example: Ground-State Energy (Ctd.)

- Expanding the objective function gives

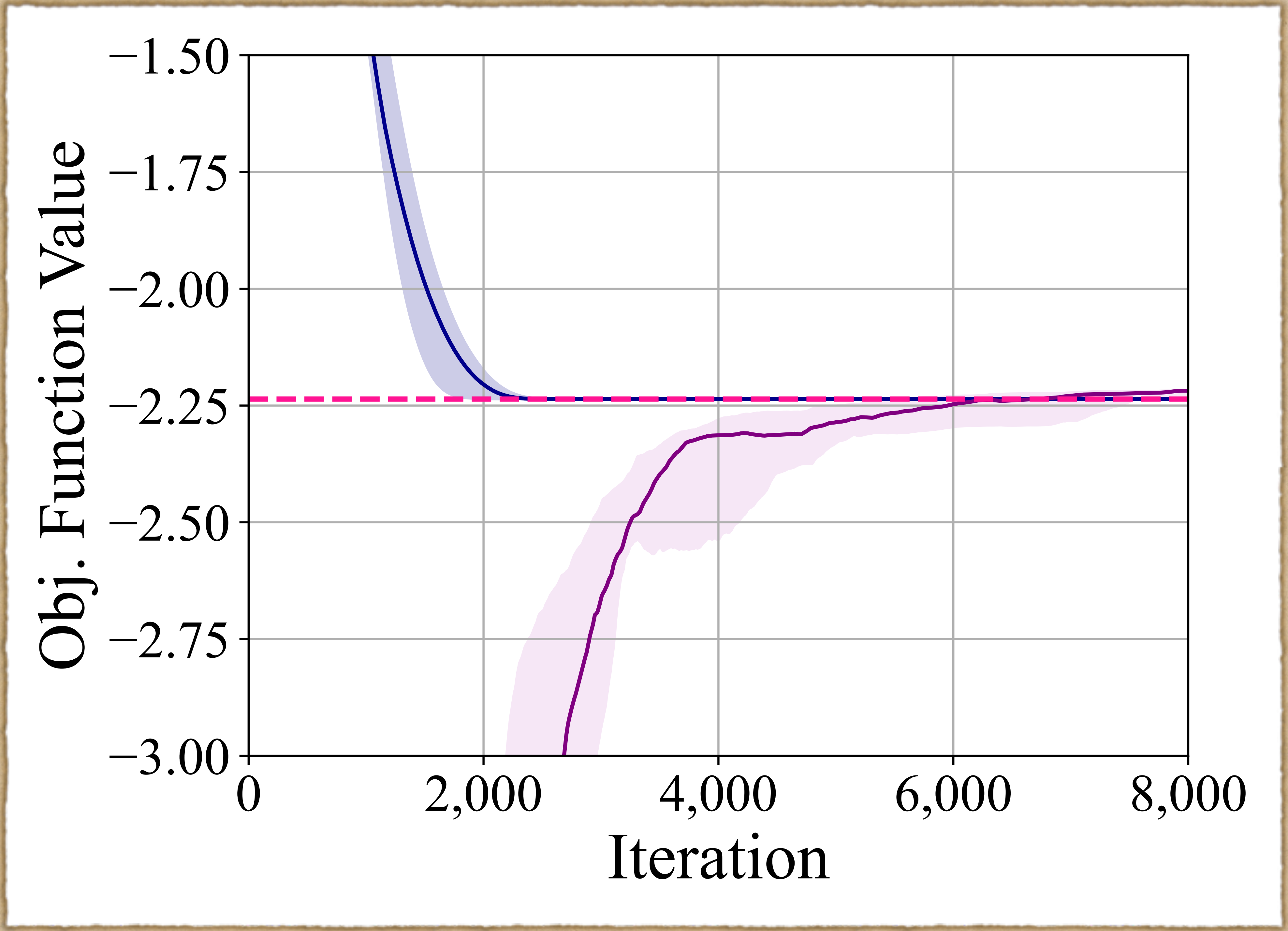
$$\sup_{\eta\in\mathbb{R},\nu\geq 0,\theta\in\Theta} \eta - c\Big(\mathrm{Tr}[H^2] + \eta^2 2^n + \nu^2\,\mathrm{Tr}[\omega(\theta)^2] - 2\eta\,\mathrm{Tr}[H] - 2\nu\,\mathrm{Tr}[H\omega(\theta)] + 2\eta\nu\Big)$$

- Various terms can be precomputed or easily calculated, the term $\mathrm{Tr}[\omega(\theta)^2]$ can be estimated by classical sampling, and the term $\mathrm{Tr}[H\omega(\theta)]$ can be estimated by a quantum computer

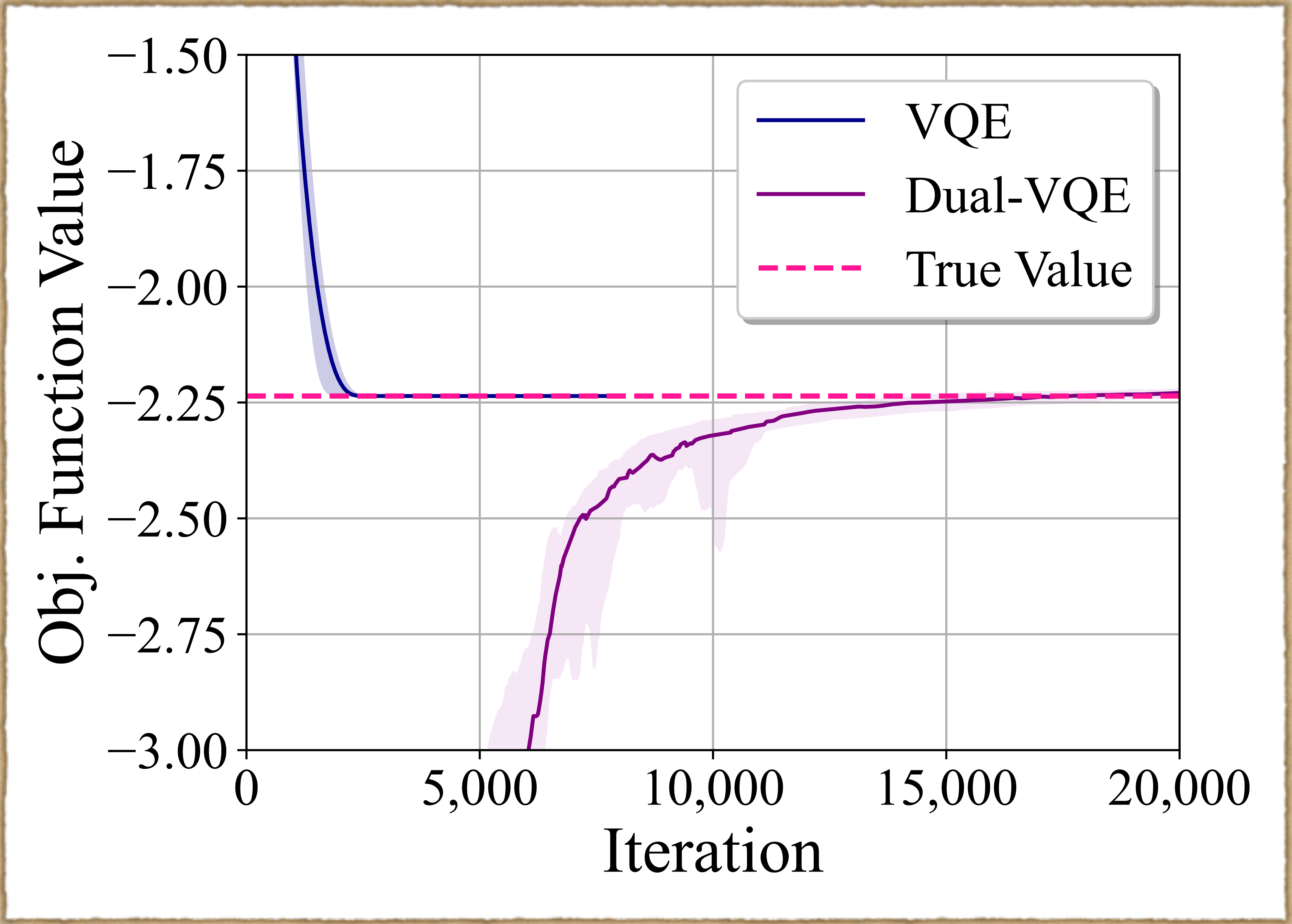
- Overhead of using quantum computer is the same as VQE

Simulation Results

Two-qubit, transverse-field Ising model



Purification ansatz



Convex combination ansatz

Comparing VQE and Dual-VQE

- In simulations, VQE converges faster than Dual-VQE does
- Possible reasons: Dual-VQE objective function is more complex, non-linear in $\omega(\theta)$, involves global term $\mathrm{Tr}[\omega(\theta)^2]$, and optimization over mixed states
- Differences in optimization landscapes can lead to different resource requirements for VQE and Dual-VQE

Obstacle: Barren Plateau Problem

- The barren plateau problem plagues variational quantum algorithms, and it can affect QSlack also
- In short, gradients of cost functions vanish exponentially with problem size
- Most promising approach (arXiv:2208.13673) seems to be finding a good initial state via tensor networks (classical simulation) and then continuing after this starting point with the usual hybrid quantum-classical algorithm
- This should work for Dual-VQE and constrained Hamiltonian optimization, but more work is needed to figure out how to apply it to other QSlack problems that have q. states as input

Conclusion

- QSlack is a general method for bounding the optimal value of an SDP from above and below
- All objective-function terms can be efficiently estimated on a q. computer if SDP inputs are efficiently measurable observables
- Showcased the method on the ground-state energy problem

Future Directions

- Determine behavior of QSlack for finite values of the penalty constant c
- Scale up simulations to larger numbers of qubits and incorporate error mitigation
- Modify QSlack to be an interior-point method