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The Capabilities and Limitations of Quantum Learning Models

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Contents

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I. The power of QNN in the view of optimization and learning theory *[On the learnability of quantum neural networks, arXiv:2007.12369]*

II. QAS: An efficient scheme to enhance the trainability of QNN and supress its error *[Quantum circuit architecture search: error mitigation and trainability enhancement for variational quantum solvers, arXiv:2010.10217]*

III. The power of quantum kernels in the NISQ era *[Towards understanding the power of quantum kernels in the NISQ era, arXiv:2103.16774]*

Noisy intermediate-scale quantum (NISQ) era

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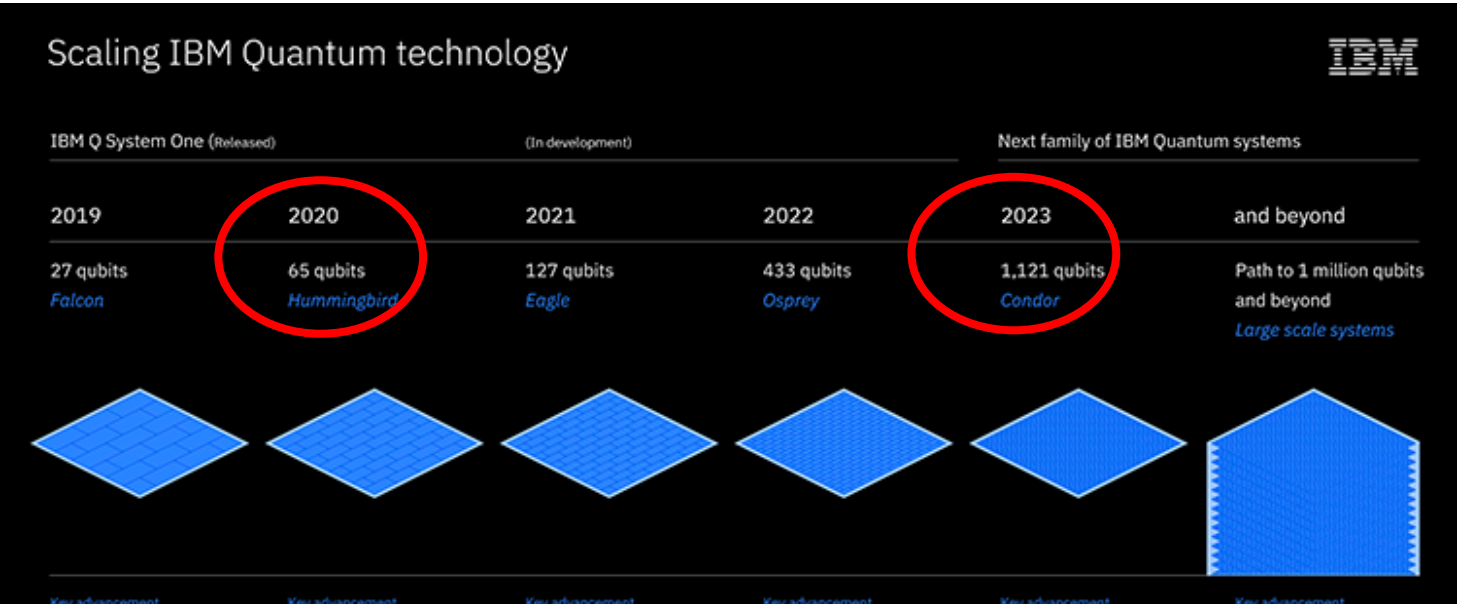
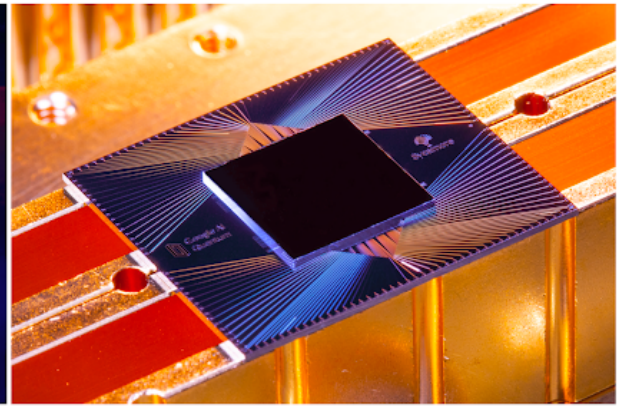
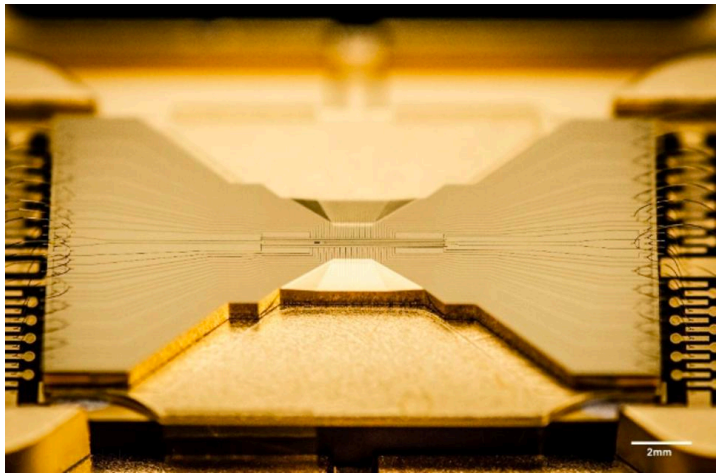
Super-conducting

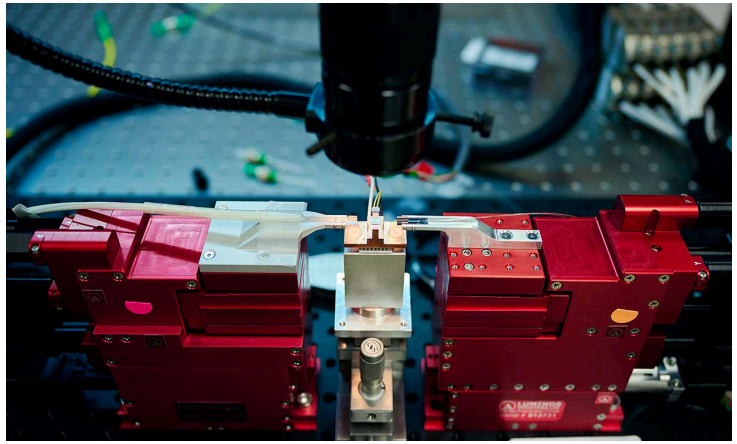




Trap-ion



Photonic chips



https://www.ibm.com/blogs/research/2020/09/ibm-quantum-roadmap/, https://www.forbes.com/sites/ibm/2020/01/16/the-quantum-computing-era-is-here-why-it-mattersand-how-it-may-change-our-world/, https://ai.googleblog.com/2019/10/quantum-supremacy-using-programmable.html, https://www.forbes.com/sites/moorinsights/2020/10/07/ionq-releases-a-new-32-qubit-trapped-ion-quantum-computer-with-massive-quantum-volume-claims, https://spectrum.ieee.org/tech-talk/computing/hardware/photonic-quantum

Noisy intermediate-scale quantum (NISQ) era

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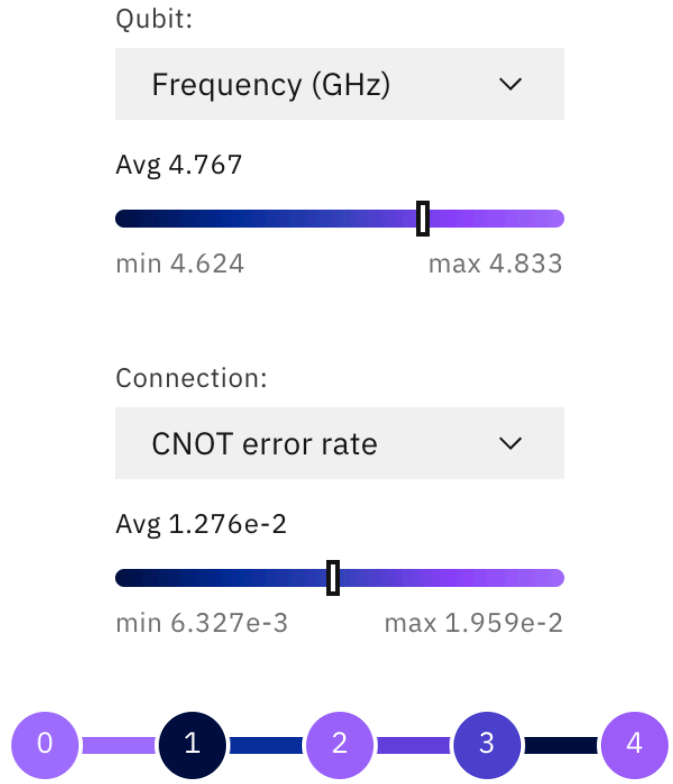
The caveats of NISQ processors are:

- a limited number of qubits;
- shallow circuit depth;
- connectivity restriction;
- unavoidable system noise.



https://quantum-computing.ibm.com/

Noisy intermediate-scale quantum (NISQ) era

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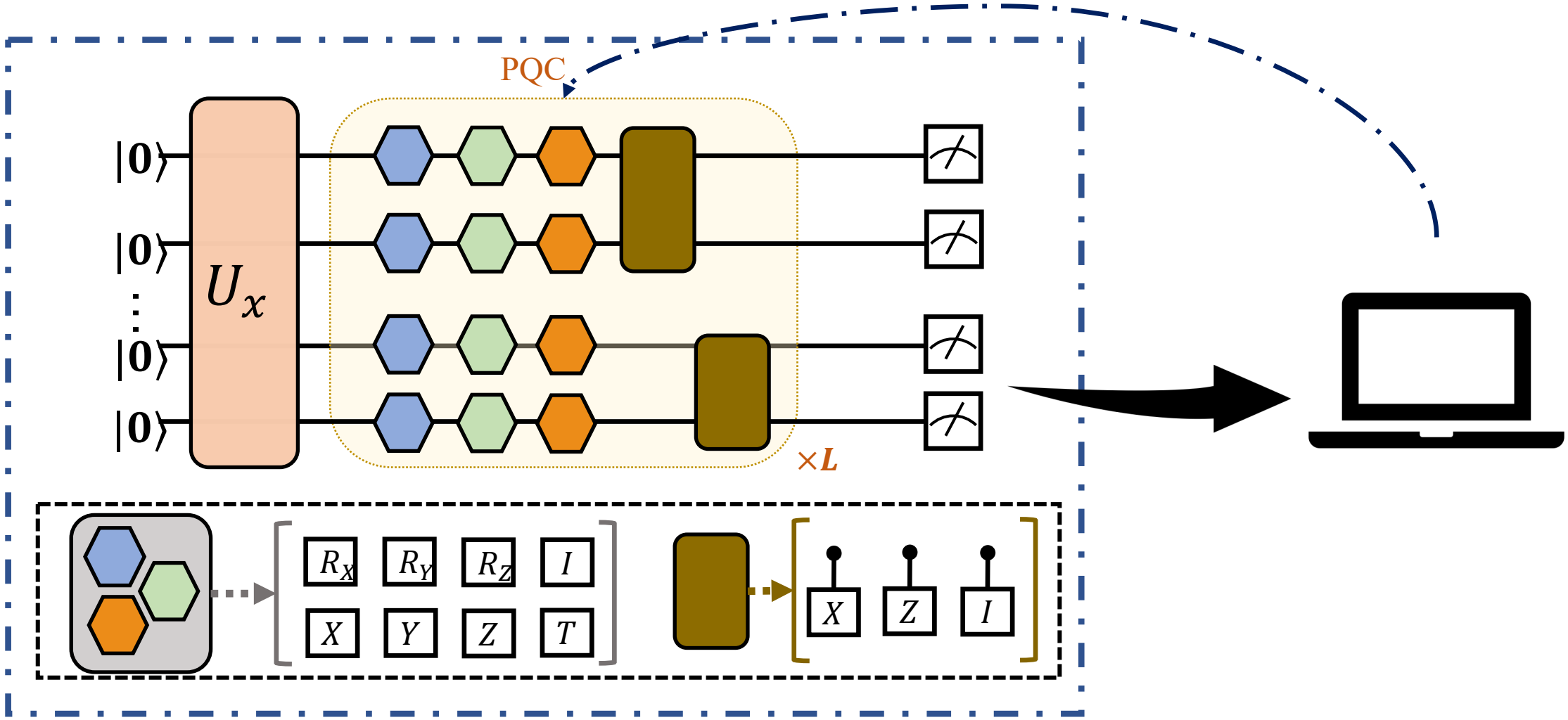
Variational quantum algorithm



Noisy intermediate-scale quantum (NISQ) applications

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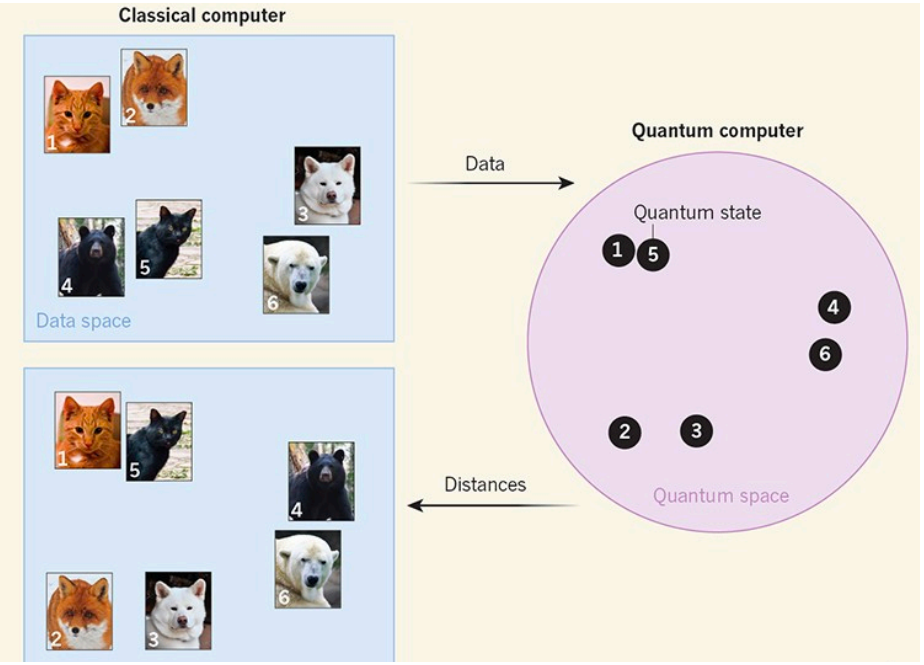
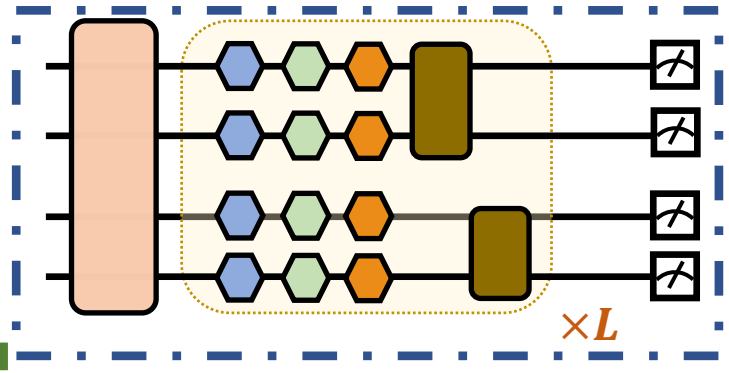
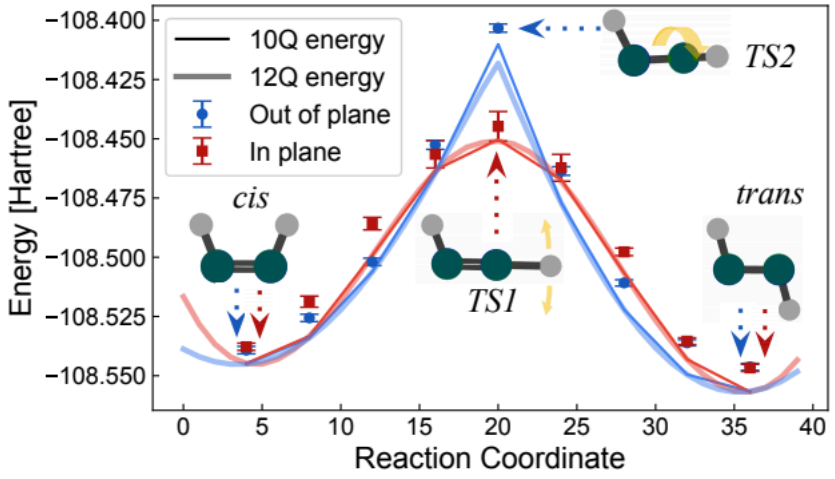


Machine learning

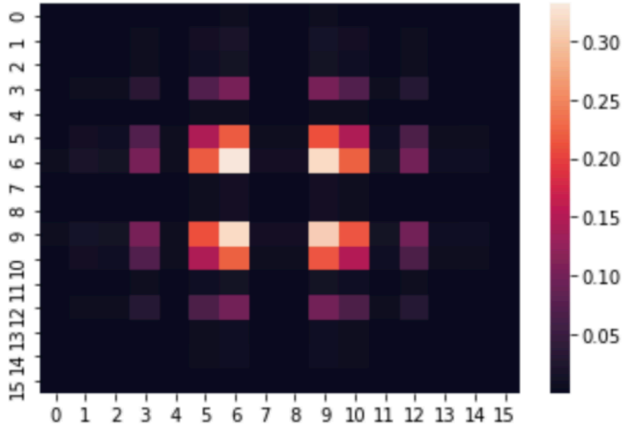
Variational quantum algorithm





Chemistry

Quantum information processing,
Quantum metrology, …



https://science.sciencemag.org/content/369, https://www.nature.com/articles/d41586-019-00771-0, https://arxiv.org/pdf/2003.02989.pdf

Problem setup

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ERM: The empirical risk minimization (ERM) principle is a learning paradigm that has been broadly employed to benchmark the performance of supervised learning algorithms.

When QNN is employed to tackle ERM, the optimization yields:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}\in\mathcal{C}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}) := \frac{1}{n}\sum_{j=1}^{n} l\left(y_j, \hat{y}_j\right) + r(\boldsymbol{\theta}).$$

$\boldsymbol{z} = \{\boldsymbol{z}_j\}_{j=1}^{N} \in \mathcal{Z}$: Input dataset with N samples;

$\boldsymbol{z}_j = (\boldsymbol{x}_j, y_j)$: The j-th sample, the feature vector as $\boldsymbol{x}_j \in \mathbb{R}^{D_c}$, the label as $\boldsymbol{y}_j \in \mathbb{R}^1$,

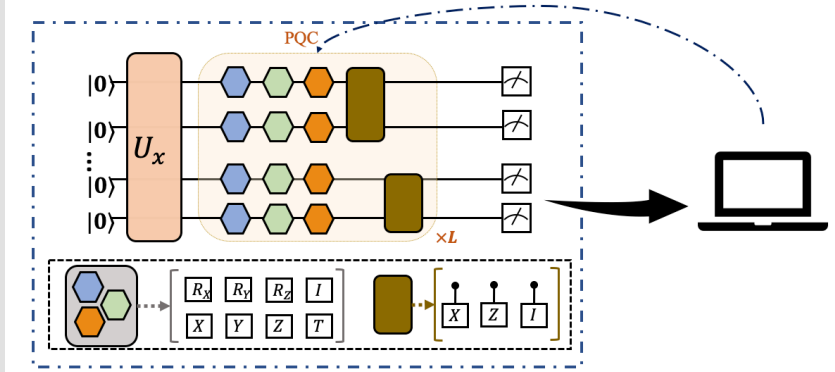
$\hat{y}_j = \mathrm{Tr}\left((\boldsymbol{\Pi}|\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})|\right)$: The predicted label of the j-th sample;

$|\psi(\boldsymbol{\theta})\rangle$: quantum states prepared by $U(\boldsymbol{\theta})$ and $\boldsymbol{z}_j$;

$U(\boldsymbol{\theta})$: The trainable quantum circuit as.

$l(\cdot,\cdot)$: the loss function measures the difference between y_j and $\hat{y}_j$;

$r(\boldsymbol{\theta})$: the regularizer.



Challenges of QNN

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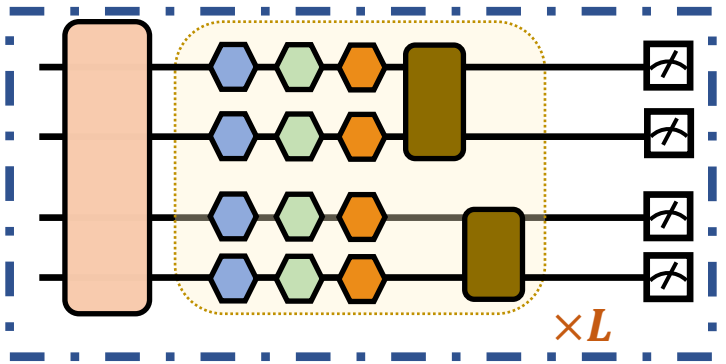
$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}\in\mathcal{C}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}) \coloneqq \frac{1}{n}\sum_{j=1}^{n} l\left(y_j, \hat{y}_j\right) + r(\boldsymbol{\theta}).$$

The difficulties to theoretically understand QNN are:

- the versatile structures;
- the non-convex optimization landscapes;
- the unavoidable gate noise and measurement errors.



Part I. Understanding the power of QNN

Challenges of QNN

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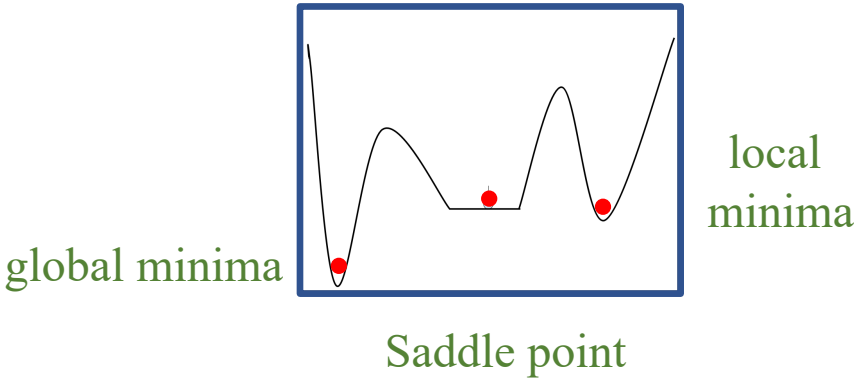
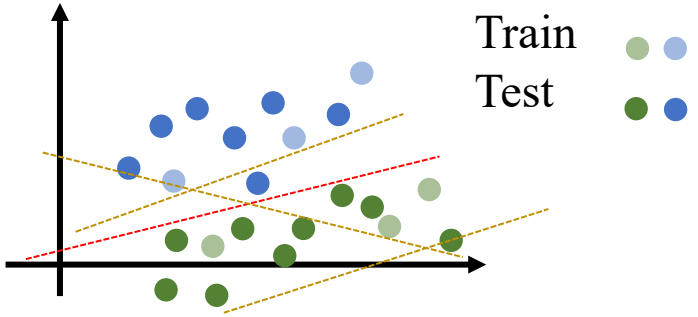
Key issue: what is the learnability of QNN, where

$$learnability = \text{`}trainability\text{'} + \text{`}generalization\text{'}.$$

- *Trainability* ←→ stationary point;



- *Generalization* ←→ find a good hypothesis in a poly sample complexity.



Allen-Zhu, Zeyuan, Yuanzhi Li, and Yingyu Liang. "Learning and generalization in overparameterized neural networks, going beyond two layers." Advances in neural information processing systems. 2019. https://machinelearningmastery.com/why-training-a-neural-network-is-hard/

Why we need to understand the learnability of QNN

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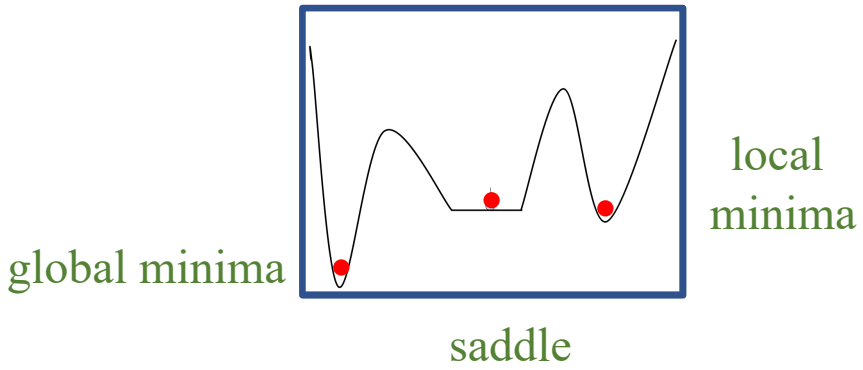
Trainability:

- ❖ Evaluation of the performance of various QNN-based learning algorithms;

- ❖ Guide to design better quantum learning protocols to avoid barren plateaus.



Why we need to understand the learnability of QNN

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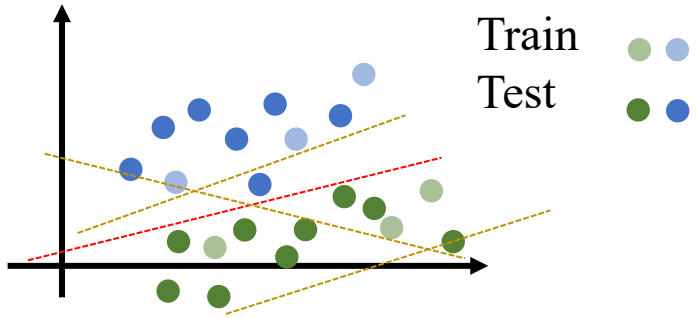
Generalization:

- Answer whether there exists any class of concepts that can be efficiently learned by (noisy) QNN but are computationally hard for the classical learning models.

- Use QNN implemented on NISQ devices to accomplish certain tasks with theoretical advantages.



Problem setup of the trainability of QNN towards ERM

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QNN towards ERM:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{C}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}) := \frac{1}{n}\sum_{j=1}^{n} l\left(y_j, \hat{y}_j\right) + r(\boldsymbol{\theta}).$$

Setting: the mean square error loss with $l\left(y_j, \hat{y}_j\right) = (y_j - \hat{y}_j)^2$;

the L2-norm regularizer $r(\boldsymbol{\theta}) = \frac{\lambda||\boldsymbol{\theta}||^2}{2}$,

depolarization noise.

Our analysis can be easily generalized to other loss functions, regularizer, noise model.

Problem setup of the trainability of QNN towards ERM

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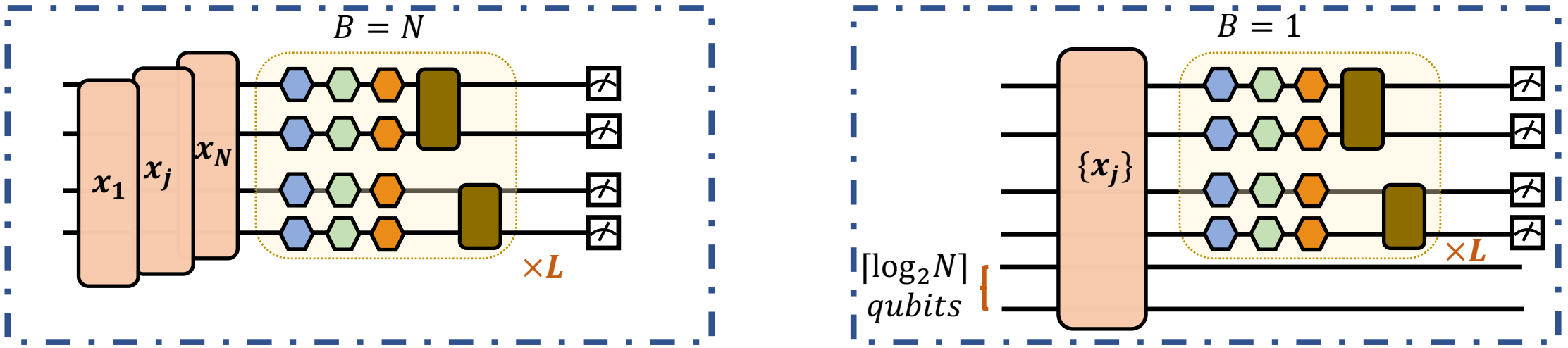
The optimization rule is the batch gradient descent method. At the t-th iteration, the parameters are updated to

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \frac{\eta}{B}\sum_{i=1}^{B} \nabla \mathcal{L}(\boldsymbol{\theta}, B_i)\,,$$

where η is the learning rate and $\nabla \mathcal{L}(\boldsymbol{\theta}, B_i)$ is obtained by *the parameter shift rule*.



Problem setup of the trainability of QNN towards ERM

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The trainability (convergence performance) of QNN is measured by the following two standard utility metrics:

$$R_1\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}\left[\left\|\nabla \mathcal{L}(\boldsymbol{\theta}^{(T)})\right\|^2\right],$$

$$R_2\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}[\mathcal{L}(\boldsymbol{\theta}^{(T)})] - \mathcal{L}(\boldsymbol{\theta}^*),$$

where the expectation is taken over the randomness of QNN resulted from the measurement error and gate noise.

Problem setup of the trainability of QNN towards ERM

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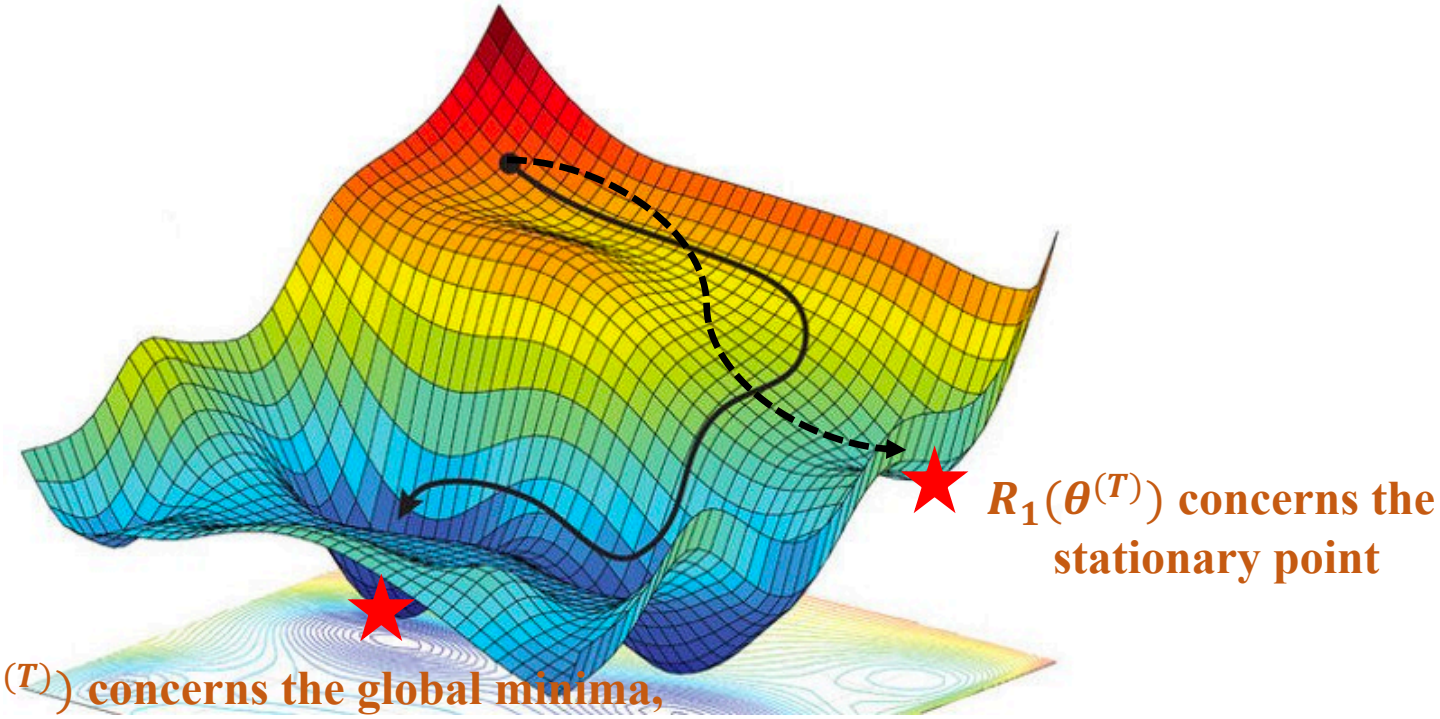
- $R_1(\boldsymbol{\theta}^{(T)})$ evaluates how far QNN is away from the stationary point, i.e., $\left|\left|\nabla\mathcal{L}\left(\boldsymbol{\theta}^{(T)}, \boldsymbol{z}\right)\right|\right| = 0$.
- $R_2(\boldsymbol{\theta}^{(T)})$ evaluates how far QNN is away from the optimal result $\mathcal{L}(\boldsymbol{\theta}^*, \boldsymbol{z})$.



https://medium.com/swlh/non-convex-optimization-in-deep-learning-26fa30a2b2b3

Main results of the trainability of QNN towards ERM

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Theorem 1. Let K be the number of measurements, L be the circuit depth, p be the depolarization noise of quantum gates, and B be the batch size. QNN outputs $\boldsymbol{\theta}^{(T)} \in \mathbb{R}^{\boldsymbol{d}}$ after training T iterations with the utility bound

$$R_1\left(\boldsymbol{\theta}^{(T)}\right) \leq \tilde{O}\left(poly\left(\frac{d}{TBK(1-p)^L}\right)\right).$$

When λ satisfies a technical assumption, QNN outputs $\boldsymbol{\theta}^{(T)} \in \mathbb{R}^{\boldsymbol{d}}$ after $T = \tilde{O}(d^3/(1-p)^L)$ training iterations with the utility bound

$$R_2\left(\boldsymbol{\theta}^{(T)}\right) \leq \tilde{O}\left(poly\left(\frac{d}{BK^2(1-p)^L}\right)\right).$$

Main results of the trainability of QNN towards ERM

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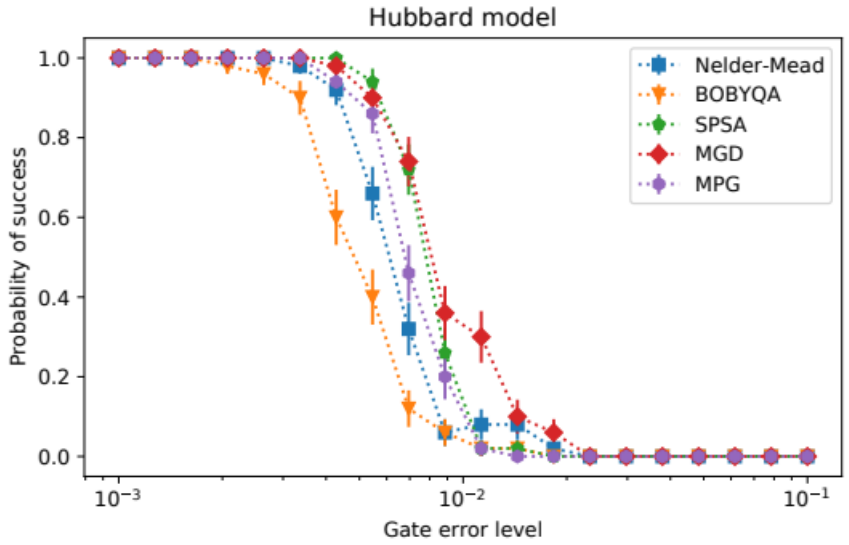
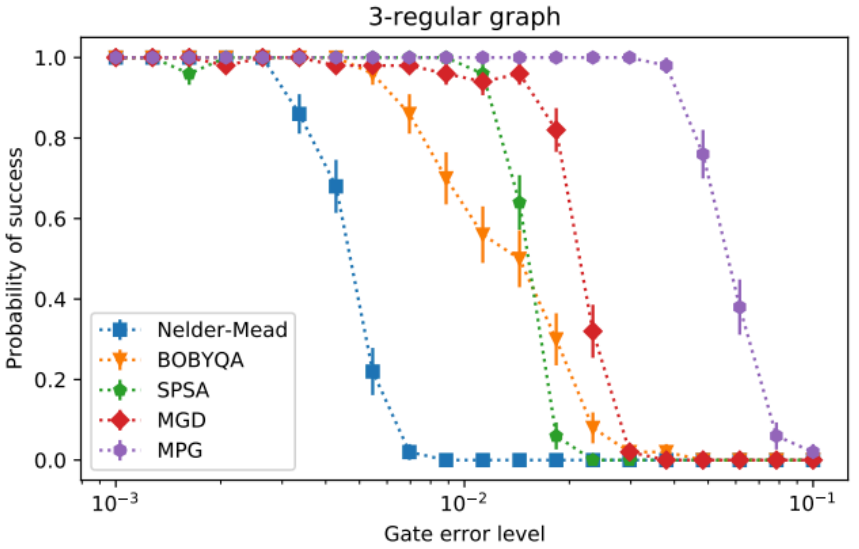
Implications of Theorem 1:

- $K\uparrow$, B $\uparrow$, $p\downarrow$, $d\downarrow$, and L $\downarrow$ yield better utility bounds $R_1\left(\boldsymbol{\theta}^{(T)}\right)$ and $R_2\left(\boldsymbol{\theta}^{(T)}\right)$;





Sung, Kevin J., et al. "Using models to improve optimizers for variational quantum algorithms." *Quantum Science and Technology* 5.4 (2020): 044008.

Main results of the trainability of QNN towards ERM

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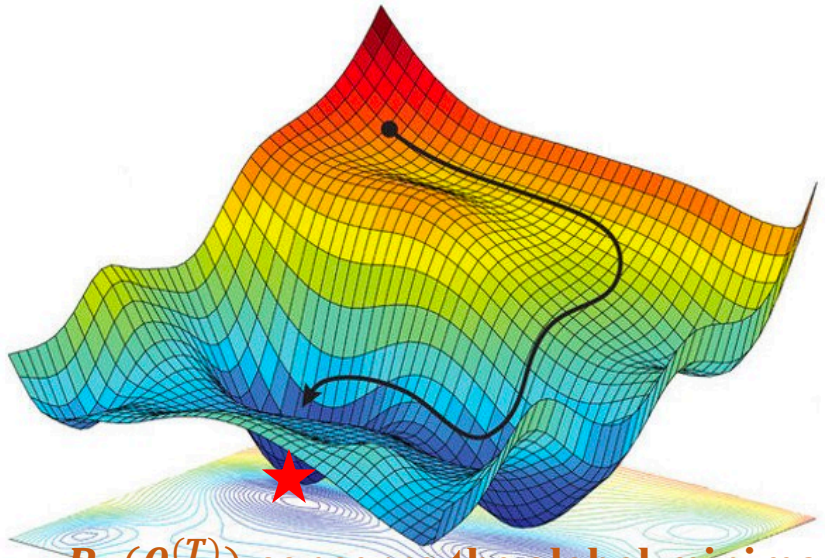
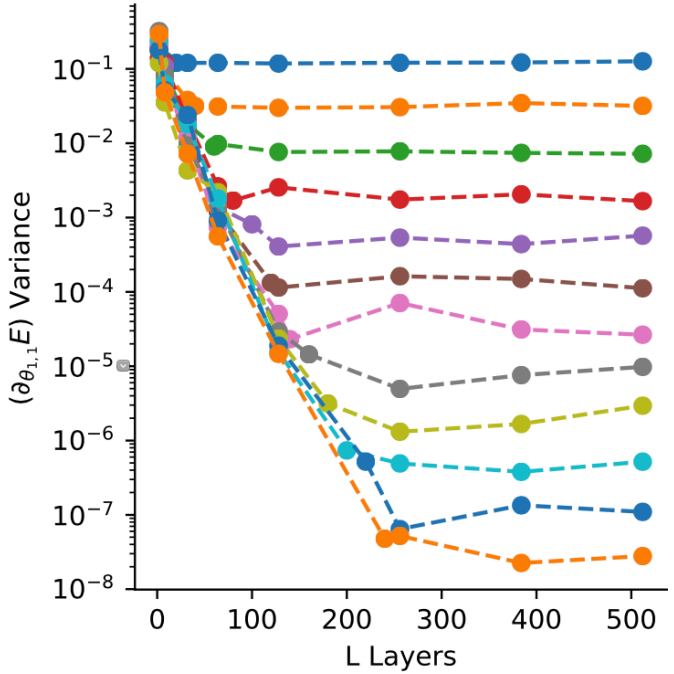
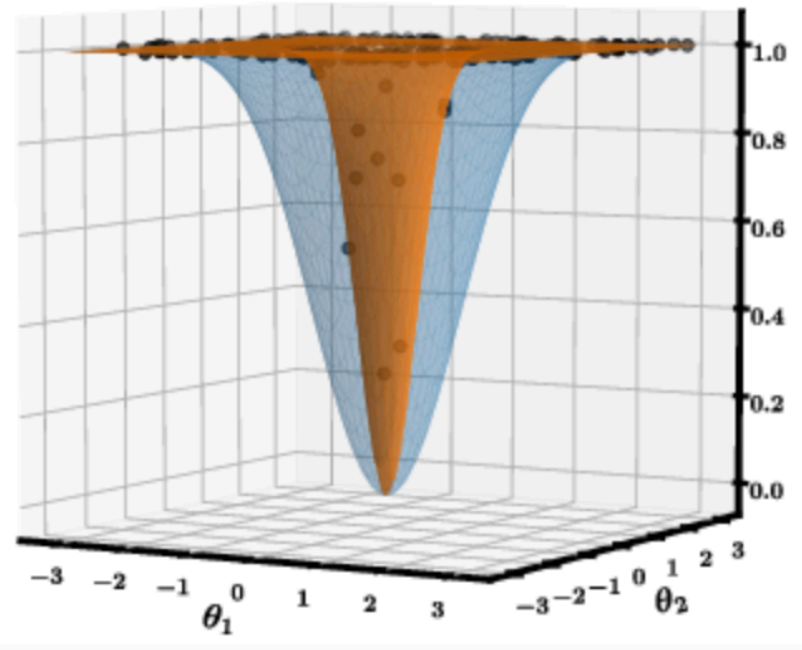
- $K\uparrow$, B $\uparrow$, $p\downarrow$, $d\downarrow$, and L $\downarrow$ yield better utility bounds $R_1\left(\boldsymbol{\theta}^{(T)}\right)$ and $R_2\left(\boldsymbol{\theta}^{(T)}\right)$;
- The convergence towards the global optima as shown in $R_2\left(\boldsymbol{\theta}^{(T)}\right)$ provides an insight about how to employ regularization techniques to avoid barren plateaus.



$R_2(\theta^{(T)})$ concerns the global minima, the target result of QNN





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Main results of the trainability of QNN towards ERM

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Implications of Theorem 1:

- $K\uparrow$, B $\uparrow$, $p\downarrow$, $d\downarrow$, and L $\downarrow$ yield better utility bounds $R_1\left(\boldsymbol{\theta}^{(T)}\right)$ and $R_2\left(\boldsymbol{\theta}^{(T)}\right)$;
- The convergence towards the global optima as shown in $R_2\left(\boldsymbol{\theta}^{(T)}\right)$ provides an insight about how to employ regularization techniques to avoid barren plateaus.
- The utility bound $R_1\left(\boldsymbol{\theta}^{(T)}\right)$ indicates that the optimization of QNN can diverge for large d and p, no matter how large T or K would become;

$$R_1 \leq \frac{2S(1+90\lambda d)}{T(1-\tilde{p})^2} + \frac{(2\tilde{p}-\tilde{p}^2)(2G+d)(1+10\lambda)^2}{(1-\tilde{p})^2} + \frac{6dK+8d}{(1-\tilde{p})^2 BK^2}\,.$$

Sketch of proof

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$$R_1 \leq \tilde{O}\left(poly\left(\frac{d}{T(1-p)^{L_Q}}, \frac{d}{BK(1-p)^{L_Q}}, \frac{d}{(1-p)^{L_Q}}\right)\right) \qquad R_1\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}\left[\left\|\nabla \mathcal{L}(\boldsymbol{\theta}^{(T)})\right\|^2\right]$$

The objective function $\mathcal{L}(\boldsymbol{\theta})$ is S-smooth, i.e.,

$$\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)}) \leq \langle \nabla \mathcal{L}(\boldsymbol{\theta}^{(t)}), \boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)} \rangle + \frac{S}{2}\|\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\|^2 .$$

The optimization rule of **noisy** QNN at the t-th iteration follows

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta \nabla \bar{\mathcal{L}}(\boldsymbol{\theta}^{(t)}) .$$

$$\begin{aligned} &\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)}) \\ \leq &-\frac{1}{S}\langle \nabla \mathcal{L}(\boldsymbol{\theta}^{(t+1)}), \nabla \bar{\mathcal{L}}(\boldsymbol{\theta}^{(t)}) \rangle \\ &+ \frac{1}{2S}\|\nabla \bar{\mathcal{L}}(\boldsymbol{\theta}^{(t)})\|^2 \end{aligned}$$

Sketch of proof

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$$R_1 \leq \tilde{O}\left(poly\left(\frac{d}{T(1-p)^{L_Q}}, \frac{d}{BK(1-p)^{L_Q}}, \frac{d}{(1-p)^{L_Q}}\right)\right) \qquad R_1\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}\left[\left\|\nabla \mathcal{L}(\boldsymbol{\theta}^{(T)})\right\|^2\right]$$

$$\begin{aligned}
&\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)}) \\
\leq &-\frac{1}{S}\langle \nabla \mathcal{L}(\boldsymbol{\theta}^{(t+1)}), \nabla \bar{\mathcal{L}}(\boldsymbol{\theta}^{(t)})\rangle \\
&+\frac{1}{2S}\|\nabla \bar{\mathcal{L}}(\boldsymbol{\theta}^{(t)})\|^2
\end{aligned}$$

Theorem 3. *It follows that*

$$\nabla_j \bar{\mathcal{L}}_i(\boldsymbol{\theta}^{(t)}) = (1-\tilde{p})^2 \nabla_j \mathcal{L}_i(\boldsymbol{\theta}^{(t)}) + C_{j,1}^{(i,t)} + \varsigma_i^{(t,j)},$$

where $\tilde{p} = 1-(1-p)^{L_Q}$, L_Q *is the circuit depth, the constant* $C_{j,1}^{(i,t)}$ *only depends on* Y_i, $\boldsymbol{\theta}^{(t)}$, *and* $\tilde{p}$, *and* $\varsigma_i^{(t,j)}$ *follows the distribution* $\mathcal{P}_Q$ *that is formed by* Y_i, $\boldsymbol{\theta}^{(t)}$, *the number of measurements* K, *and* $\tilde{p}$ *with zero mean.*

$$\mathbb{E}_{\xi_i^{(t)}, \xi_i^{(t,j)}}[\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)})] \leq -\frac{1}{2S}(1-\tilde{p})^2 \|\nabla \mathcal{L}(\boldsymbol{\theta}^{(t)})\|^2 + \frac{2G+d}{2S}(2-\tilde{p})\tilde{p}(1+10\lambda)^2 + \frac{6dK+8d}{2SBK^2}.$$

Sketch of proof

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$$R_1 \leq \tilde{O}\left(poly\left(\frac{d}{T(1-p)^{L_Q}}, \frac{d}{BK(1-p)^{L_Q}}, \frac{d}{(1-p)^{L_Q}}\right)\right) \qquad R_1\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}\left[\left\|\nabla \mathcal{L}(\boldsymbol{\theta}^{(T)})\right\|^2\right]$$

$$\mathbb{E}_{\xi_i^{(t)}, \xi_i^{(t,j)}}[\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)})] \leq -\frac{1}{2S}(1-\tilde{p})^2 \|\nabla \mathcal{L}(\boldsymbol{\theta}^{(t)})\|^2 + \frac{2G+d}{2S}(2-\tilde{p})\tilde{p}(1+10\lambda)^2 + \frac{6dK+8d}{2SBK^2}.$$

By induction, with summing over t = 0, ..., T − 1 and taking expectation, we obtain

$$\mathbb{E}_t\left[\|\nabla \mathcal{L}(\boldsymbol{\theta}^{(t)})\|^2\right] \leq \frac{2S(1+90\lambda d)}{T(1-\tilde{p})^2} + \frac{(2\tilde{p}-\tilde{p}^2)(2G+d)(1+10\lambda)^2}{(1-\tilde{p})^2} + \frac{6dK+8d}{(1-\tilde{p})^2 BK^2}.$$

Sketch of proof

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$$R_2 \leq (1+90\lambda d)\exp\left(-\frac{\mu(1-\tilde{p})^2 T}{S}\right) + T\frac{(2\tilde{p}-\tilde{p}^2)(G+2d)(1+10\lambda)^2 BK^2 + 6dK + 8d}{2SBK^2}$$

$$R_2\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}[\mathcal{L}(\boldsymbol{\theta}^{(T)})] - \mathcal{L}(\boldsymbol{\theta}^*),$$

PL condition: a function f satisfies PL condition if there exists $\mu > 0$ and for every possible $\boldsymbol{\theta} \in \boldsymbol{\mathcal{C}}$, $\left|\left|\nabla f(\boldsymbol{\theta})\right|\right|^2 \geq 2\mu(f(\boldsymbol{\theta}) - f^*)$, where $f^* = \min_{\boldsymbol{\theta}\in\boldsymbol{\mathcal{C}}} f(\boldsymbol{\theta})$.

Lemma Assume $\lambda \in \left(0, \frac{1}{3\pi}\right) \cup \left(\frac{1}{\pi}, \infty\right)$ the loss $\mathcal{L}$ used in QNN satisfies PL condition with $\mu = \frac{(-1+\lambda\pi)^2}{1+\lambda d(3\pi)^2}$.

Sketch of proof

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$$R_2 \leq (1+90\lambda d)\exp\left(-\frac{\mu(1-\tilde{p})^2 T}{S}\right) + T\frac{(2\tilde{p}-\tilde{p}^2)(G+2d)(1+10\lambda)^2 BK^2 + 6dK + 8d}{2SBK^2}$$

$$R_2\left(\boldsymbol{\theta}^{(T)}\right) := \mathbb{E}[\mathcal{L}(\boldsymbol{\theta}^{(T)})] - \mathcal{L}(\boldsymbol{\theta}^*),$$

Lemma Assume $\lambda \in \left(0, \frac{1}{3\pi}\right) \cup \left(\frac{1}{\pi}, \infty\right)$ the loss $\mathcal{L}$ used in QNN satisfies PL condition with $\mu = \frac{(-1+\lambda\pi)^2}{1+\lambda d(3\pi)^2}$.

$$+ \quad \left|\left|\nabla f(\boldsymbol{\theta})\right|\right|^2 \geq 2\mu(f(\boldsymbol{\theta}) - f^*)$$

$$\mathbb{E}_{\xi_i^{(t)},\xi_i^{(t,j)}}[\mathcal{L}(\boldsymbol{\theta}^{(t+1)}) - \mathcal{L}(\boldsymbol{\theta}^{(t)})] \leq -\frac{1}{2S}(1-\tilde{p})^2\left\|\nabla\mathcal{L}(\boldsymbol{\theta}^{(t)})\right\|^2 + \frac{2G+d}{2S}(2-\tilde{p})\tilde{p}(1+10\lambda)^2 + \frac{6dK+8d}{2SBK^2}.$$

By induction, with summing over t, and taking expectation

$$\mathbb{E}_{\boldsymbol{\varsigma}^{(t)}}[\mathcal{L}(\boldsymbol{\theta}^{(T)})] - \mathcal{L}^*$$

emma Assume $\lambda \in \left(0, \frac{1}{3\pi}\right) \cup \left(\frac{1}{\pi}, \infty\right)$ the loss $\mathcal{L}$ used in QNN satisfies PL condition with $= \frac{(-1+\lambda\pi)^2}{1+\lambda d(3\pi)^2}$.

Simulation results

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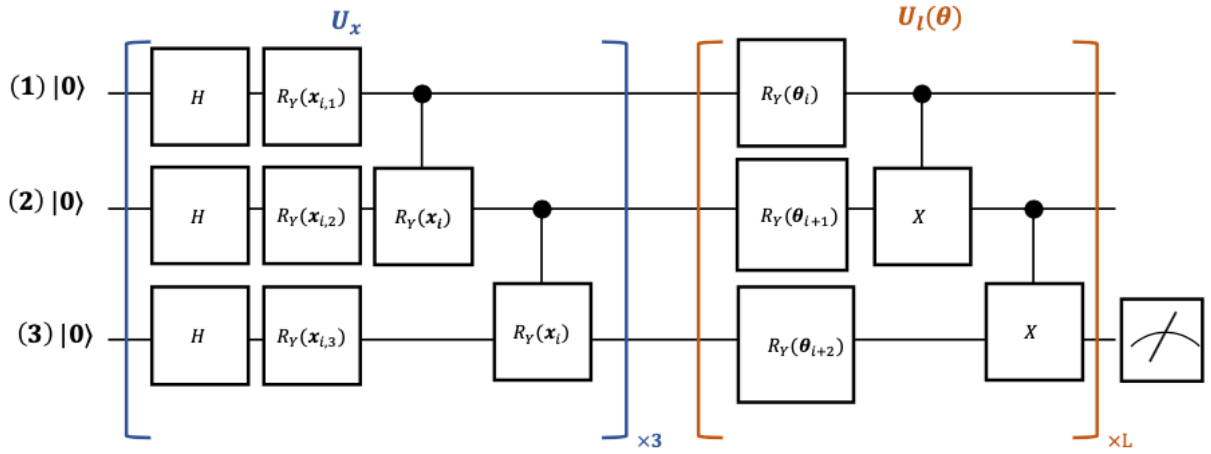

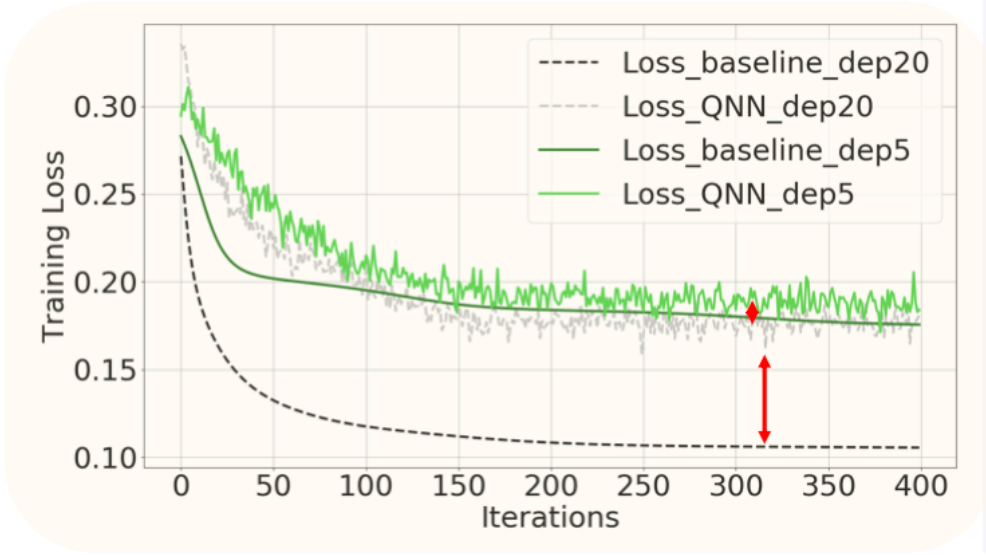

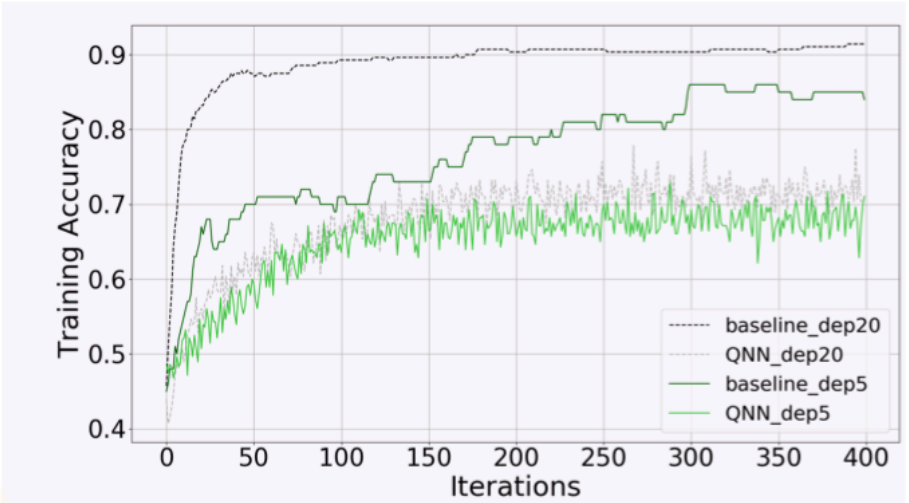

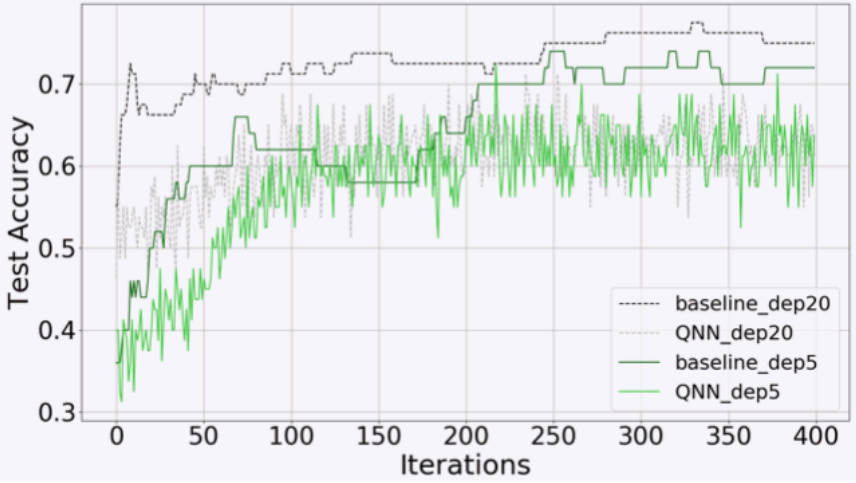

Problem setup of the generalization of QNN

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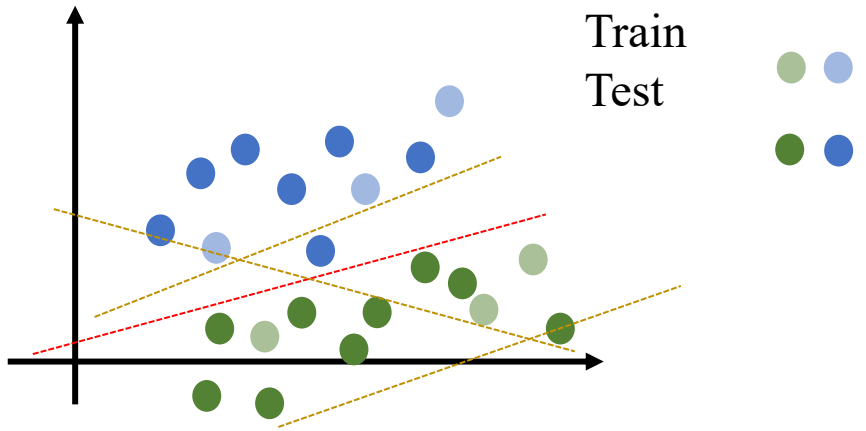
- **Generalization**: for a given learning problem, QNN requires a poly sample complexity to find a good hypothesis, while classical algorithms require an exp number of samples.

(Quantum) Leaning theory



Central tools to explore the generalization of QNN

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Quantum statistical query (QSQ) oracle: A QSQ oracle which takes a tolerance parameter τ and an observable $\mathbb{M} \in \mathbb{C}^{2^{N+1}\times 2^{N+1}}$ and returns a number α satisfies

$$|\alpha - \langle\psi_{c^*}|\mathbb{M}|\psi_{c^*}\rangle| \leq \tau.$$

$C \subseteq \{c: \{0,1\}^N \to \{0,1\}\}$: a concept class;

$D: \{0,1\}^N \to [0,1]$: an unknown distribution;

$|\psi_{c^*}\rangle = \sum_{\boldsymbol{x}\in\{\boldsymbol{0},\boldsymbol{1}\}^N} \sqrt{D(\boldsymbol{x})}|\boldsymbol{x}, \boldsymbol{c}^*(\boldsymbol{x})\rangle$: a quantum example.

Arunachalam, Srinivasan, Alex B. Grilo, and Henry Yuen. "Quantum statistical query learning." arXiv preprint arXiv:2002.08240 (2020).

Central tools to explore the generalization of QNN

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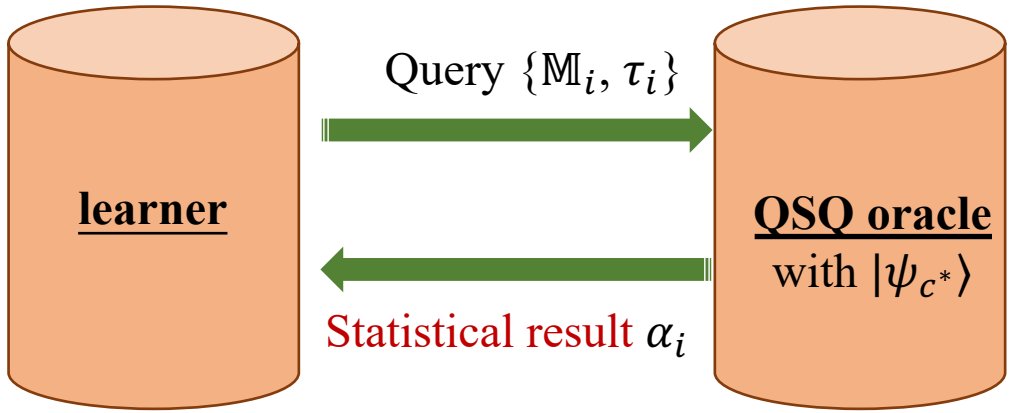
Quantum statistical query (QSQ) learning algorithm: The QSQ learning algorithm adaptively feeds a sequence of $\{\mathbb{M}_i, \tau_i\}$ into a QSQ oracle, and exploits the responses of $\{\alpha_i\}$ to output a hypothesis $h: \{0,1\}^N \rightarrow \{0,1\}$.

The goal of the learner is to achieve $\Pr_{\boldsymbol{x}\sim\boldsymbol{D}}\left(h(\boldsymbol{x}) = c^*(\boldsymbol{x})\right) \leq \epsilon$ for all possible D and c^*.



Central tools to explore the generalization of QNN

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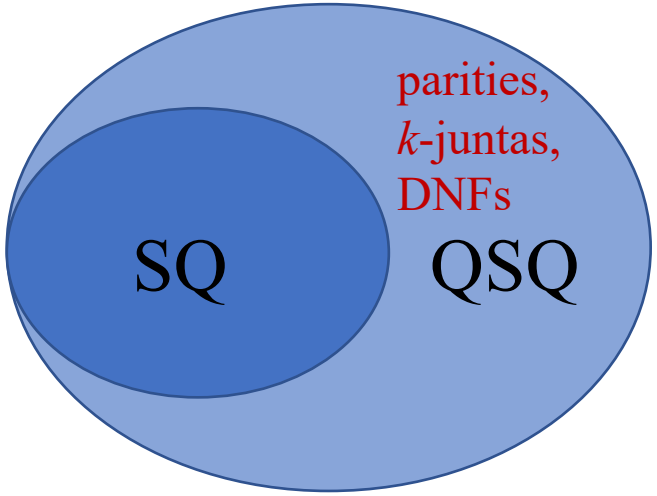
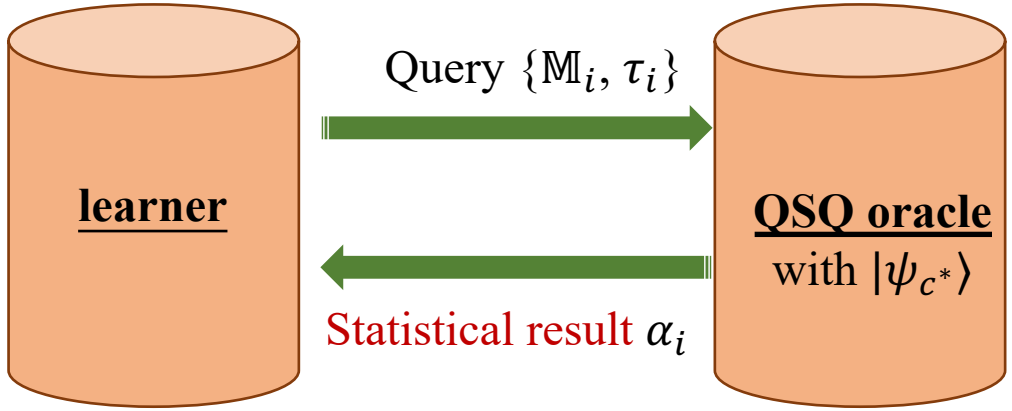
Lemma 1. Let C be the concept class of parities, k-juntas, or poly(N)-sized DNFs (Disjunctive Normal Forms), then there exists a poly(N)-query QSQ algorithm with tolerance $\tau = \tilde{O}(\epsilon)$ that efficiently learns C under the uniform distribution.





Arunachalam, Srinivasan, Alex B. Grilo, and Henry Yuen. "Quantum statistical query learning." arXiv preprint arXiv:2002.08240 (2020).

The generalization of QNN

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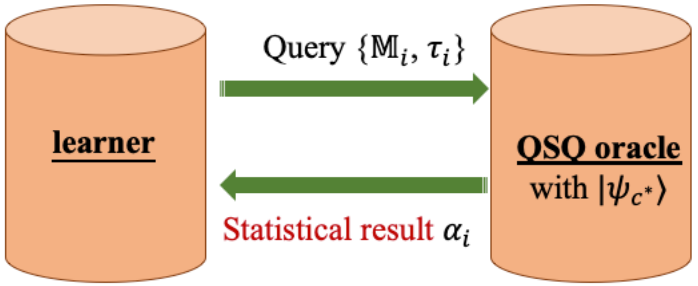
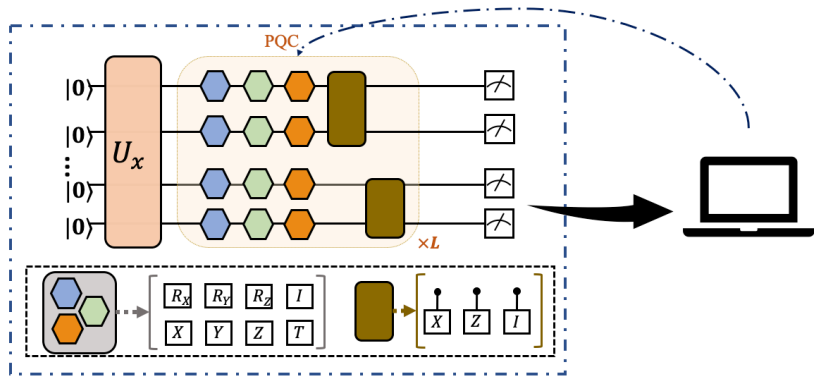
Motivation: the QSQ oracle yields a similar behavior of the variational quantum circuit used in QNN:

1) measurement statistics
2) noisy setting.





Main results of the generalization of QNN

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Theorem 2. A QSQ learning algorithm, where the distribution over the quantum example $|\psi_{c^*}\rangle$ is fixed to be uniform and the observable $\mathbb{M}$ can be implemented by at most poly(n) single and two-qubit gates, can be efficiently simulated by noisy QNN using **polynomial** samples.

Main results of the generalization of QNN

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Theorem 2. A QSQ learning algorithm, where the distribution over the quantum example $|\psi_{c^*}\rangle$ is fixed to be uniform and the observable $\mathbb{M}$ can be implemented by at most poly(n) single and two-qubit gates, can be efficiently simulated by noisy QNN using **polynomial** samples.

Implications:

- The noisy quantum circuit used in QNN has potential to tackle practical learning tasks, e.g., **support vector machines and linear and convex optimization**, with quantum advantages.

Sketch of Proof

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QSQ oracle: A QSQ oracle which takes a tolerance parameter τ and an observable $\mathbb{M} \in \mathbb{C}^{2^{N+1}\times 2^{N+1}}$ and returns a number α satisfies

$$|\alpha - \langle\psi_{c^*}|\mathbb{M}|\psi_{c^*}\rangle| \leq \tau.$$

ν

Let the encoding circuit U_x prepare the state $|\psi_{c^*}\rangle$ and the quantum measurement constructed from $\mathbb{M}$. Under the depolarization noise, the expectation value of quantum measurements of the noisy QNN yields

$$\tilde{\nu} = (1-\tilde{p})\nu + \frac{\tilde{p}\,\mathrm{Tr}(\mathbb{M})}{2^{N+1}}$$

Sketch of Proof

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$$\tilde{\nu} = (1-\tilde{p})\nu + \frac{\tilde{p}\,\mathrm{Tr}(\mathbb{M})}{2^{N+1}}$$

+

By the Chernoff-Hoeffding bound for real-valued variables, the relation between the sample mean $\frac{1}{K}\sum_{i=1} V_k$ and the result $\tilde{\nu}$ follows

$$\Pr\left(\left|\frac{1}{K}\sum_{i=1}^{K} V_k - \tilde{\nu}\right| \geq \frac{\delta}{2}\right) \leq 2\exp(-\delta^2 K/2)\ .$$

↓

$$\left|\frac{1}{K}\sum_{k=1}^{K} V_k - \nu\right| \leq \tilde{p}(\nu + \frac{1}{2^{N+1}}) + \frac{\delta}{2} \leq \frac{5}{4}\tilde{p} + \frac{\delta}{2} \leq \tau$$

→

With the successful probability $1-2b$, noisy QNN can efficiently simulate QSQ oracle using $K = 2\ln\left(\frac{2}{b}\right)/\delta^2$ examples.

Outlook

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- ✓ More measurements, lower noise, and shallower circuit depth contribute to a better performance of QNN.
- ✓ Theoretical guidance to devise more advanced QNN based learning models that are robust to inevitable gate noise and insensitive to the barren plateau phenomenon.
- ✓ QNN can efficiently learn parity, juntas, and DNF with quantum advantages even with gate noise.

❑ Exploit more advanced quantum models developed in quantum learning theory to explore the potential advantages that can be achieved by QNN.

Part II. QAS: An efficient scheme to enhance the trainability of QNN and suppress its error

Noisy intermediate-scale quantum (NISQ) era

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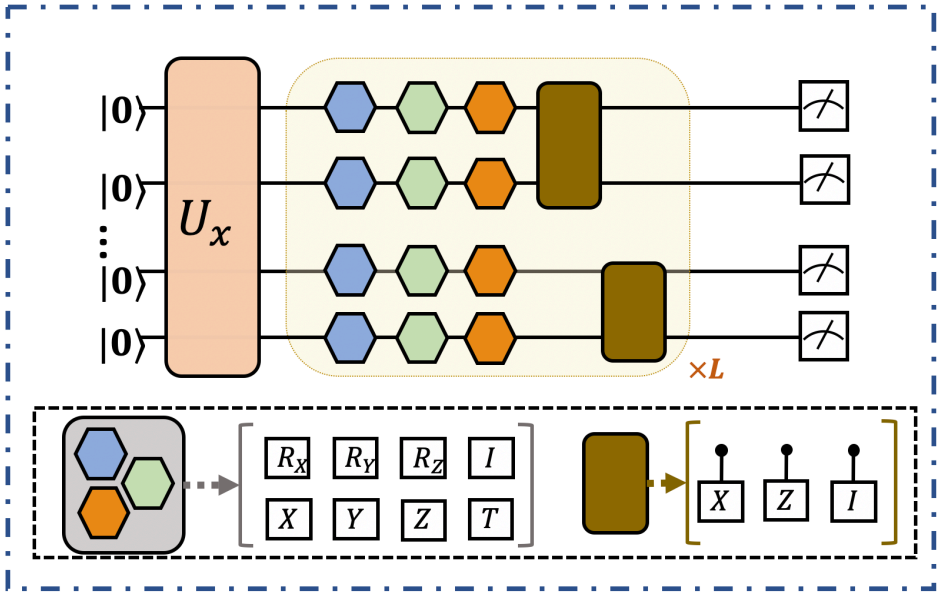
The caveats of NISQ processors are:

- limited number of qubits;
- shallow circuit depth;
- connectivity restriction;
- unavoidable system noise.



Problem setup

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Quantum neural networks (QNN) aims to find the optimal $\boldsymbol{\theta}^* \in \mathbb{R}^d$ that minimizes an objective function $\mathcal{L}$, i.e.,

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{C}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}) \coloneqq \frac{1}{n}\sum_{j=1}^{n} l\left(y_j, \hat{y}_j\right) + r(\boldsymbol{\theta}).$$

$\boldsymbol{z} = \{\boldsymbol{z}_j\}_{j=1}^{N} \in \mathcal{Z}$: Input dataset with N samples;

$\boldsymbol{z}_j = (\boldsymbol{x}_j, y_j)$: The j-th sample, the feature vector as $\boldsymbol{x}_j \in \mathbb{R}^{D_c}$, the label as $\boldsymbol{y}_j \in \mathbb{R}^1$,

$U(\boldsymbol{\theta})$: The trainable quantum circuit as.

$\hat{y}_j = \mathrm{Tr}\left((\boldsymbol{\Pi}|\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})|\right)$: The predicted label of the j-th sample;

$|\psi(\boldsymbol{\theta})\rangle$: quantum states prepared by $U(\boldsymbol{\theta})$ and $\boldsymbol{z}_j$;

$l(\cdot,\cdot)$: the loss function measures the difference between y_j and $\hat{y}_j$;

$r(\boldsymbol{\theta})$: the regularizer.

Challenges of VQLS

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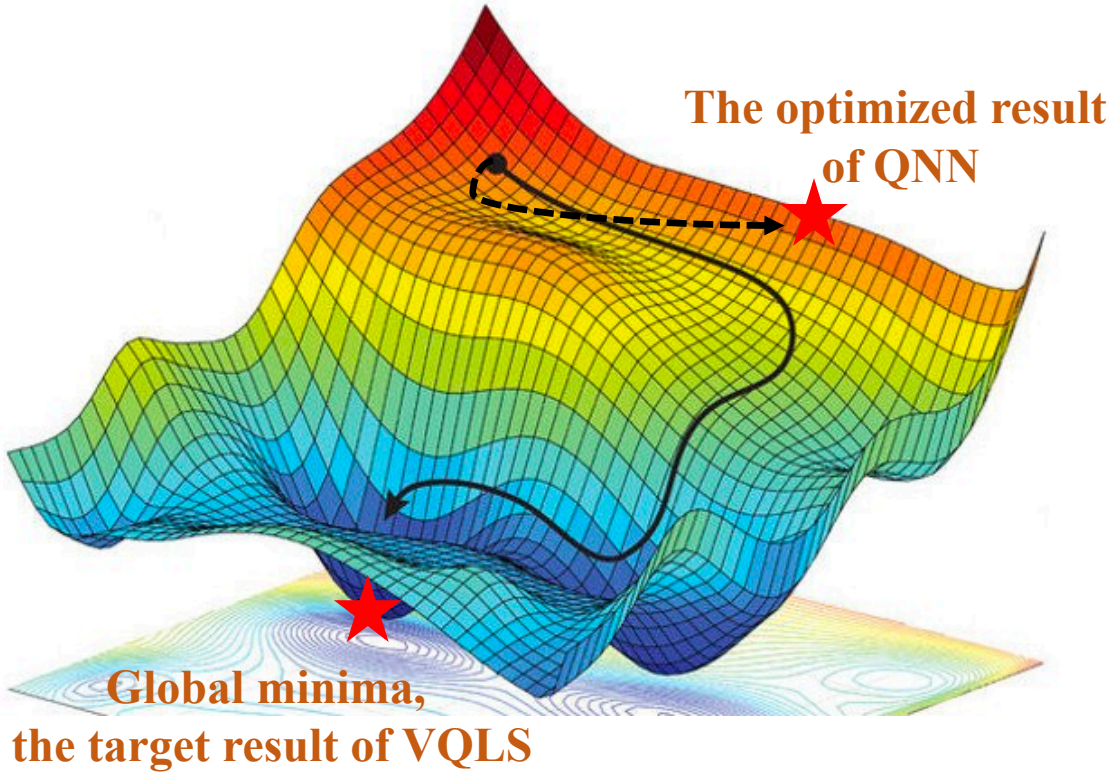
Two key issues that destroy the optimization of QNN are:

- barren plateaus,
- accumulated system noise.



https://medium.com/swlh/non-convex-optimization-in-deep-learning-26fa30a2b2b3

Some solutions

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- To avoid barren plateaus:
  - ❖ modify cost functions (*Cerezo, M. et al. "Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks."*),
  - ❖ adopt some strategies to initialize parameters (*Grant, Edward, et al. "An initialization strategy for addressing barren plateaus in parametrized quantum circuits."*).

- To suppress quantum system noise:
  - ❖ quantum error mitigation techniques (*Endo, Suguru, et al. "Hybrid quantum-classical algorithms and quantum error mitigation."*).

Motivation

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Q: Can we unify the elimination of barren plateaus and the mitigation of the quantum errors in **a single problem**?

Can we unify the elimination of barren plateaus and the mitigation of the quantum errors in **a single problem**?

Yes

Intuition

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The expressive power of $U(\boldsymbol{\theta})$ is improved;
The barren plateaus' phenomenon is serious;
The accumulated noise becomes larger;
The optimizated result $\boldsymbol{\theta}^{(T)}$ is far way from $\boldsymbol{\theta}^{*}$

Decreased circuit depth

Increased circuit depth

The expressive power of $U(\boldsymbol{\theta})$ is decreased;
The barren plateaus' phenomenon is negligible;
The accumulated noise is negligible;
The optimizated result $\boldsymbol{\theta}^{(T)}$ is far away to $\boldsymbol{\theta}^{*}$

Intuition

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The expressive power of $U(\boldsymbol{\theta})$ is improved;
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The expressive power of $U(\boldsymbol{\theta})$ is decreased;
The barren plateaus' phenomenon is negligible;
The accumulated noise is negligible;
The optimizated result $\boldsymbol{\theta}^{(T)}$ is far away to $\boldsymbol{\theta}^*$

Target point

Increased circuit depth

The expressive power of $U(\boldsymbol{\theta})$ is sufficient;
The accumulated noise is tolerable;
The optimizated result $\boldsymbol{\theta}^{(T)}$ is close to $\boldsymbol{\theta}^*$

Intuition

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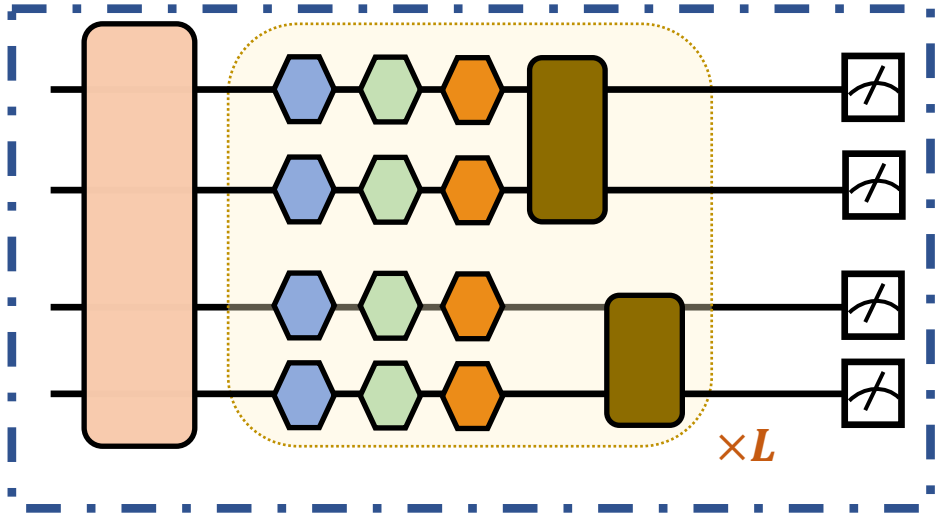
The elimination of barren plateaus and the suppression of quantum noise amount to seeking an appropriate circuit architecture of $U(\boldsymbol{\theta})$ satisfying the following requirements:

- a good expressive power to cover the target result $\boldsymbol{\theta}^*$;
- using few number of quantum gates and shallow circuit depth;
- adapting to different connectiveity constraints of various quantum processors.



Problem setup

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Considering the circuit architecture information and the related noise, the objective of QNN is rewritten as

$$(\boldsymbol{\theta}^*, \boldsymbol{a}^*) = \arg\min_{\theta \in \boldsymbol{C}, \mathbf{a} \in \mathcal{S}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}})$$

$\mathcal{S}$: the set that contains all possible circuit to build $U(\boldsymbol{\theta})$;

$\mathcal{E}_{\boldsymbol{a}}$: the quantum channel that simulates the quantum system noise induced by $\mathbf{a} \in \mathcal{S}$

Remarks

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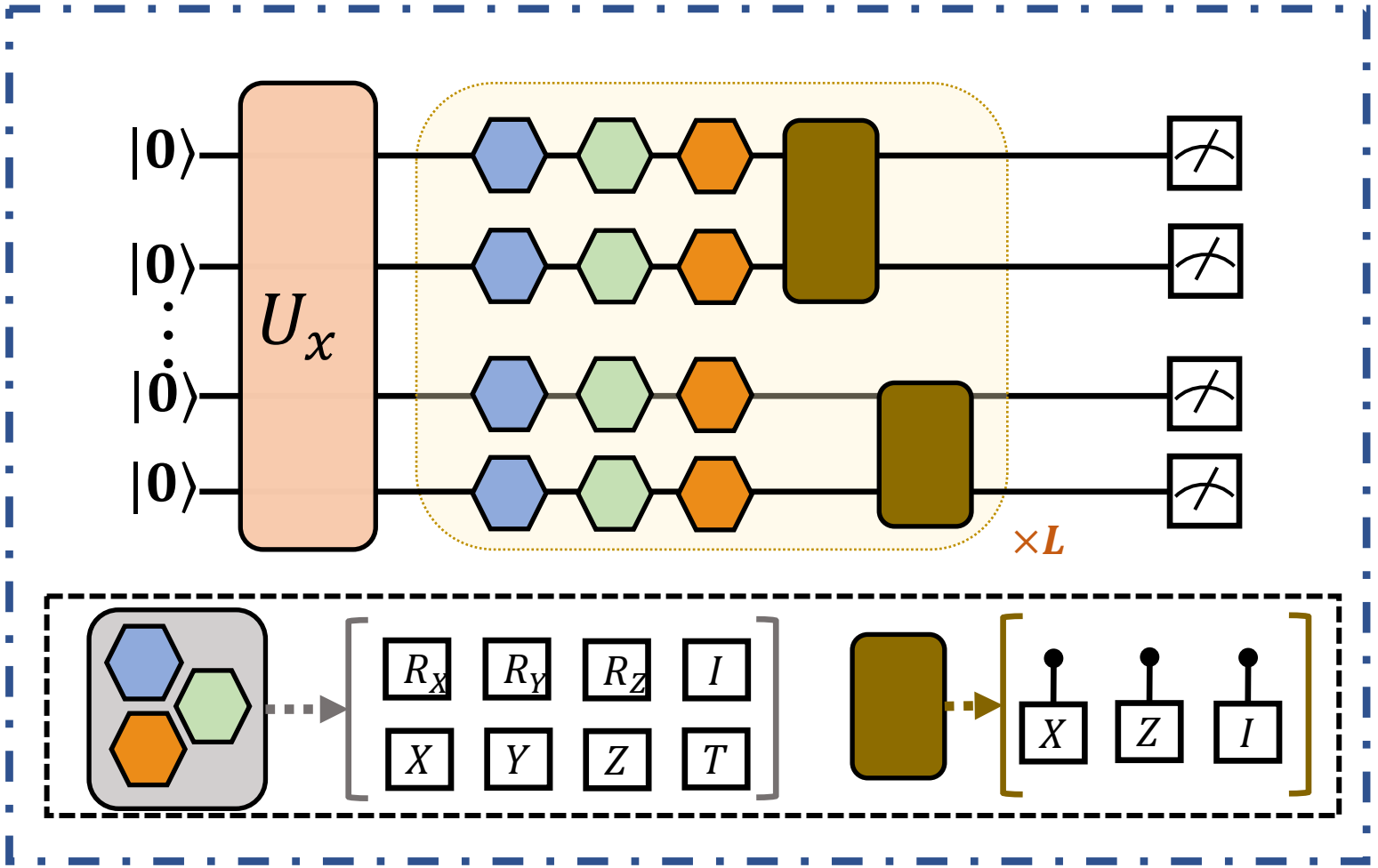
The brute-force searching is infeasible, since the total number of circuit achitectures $|\mathcal{S}|$ **exponentially scales** with the qubits count N and the circuit depth L.

$$\mathrm{O}((8^{3N}\times 3^{N})^{L})$$



Classical analog

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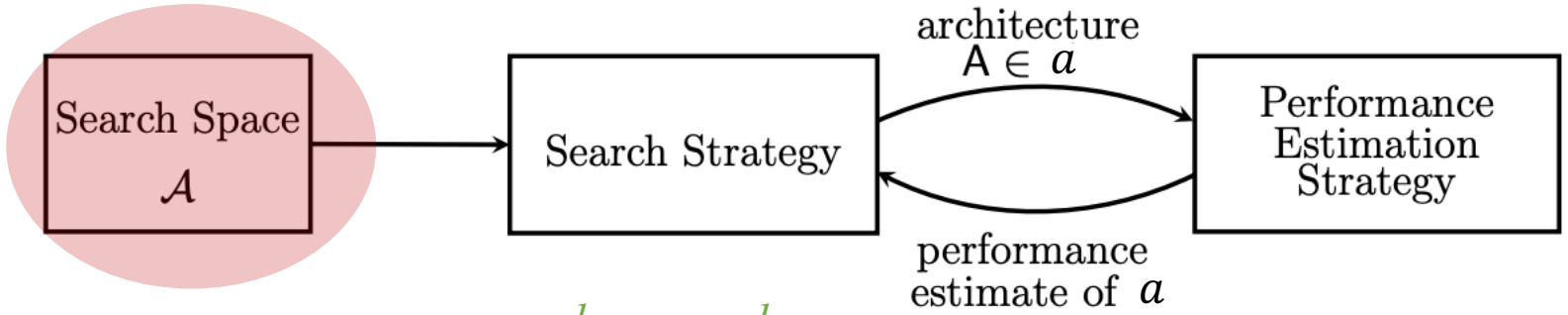
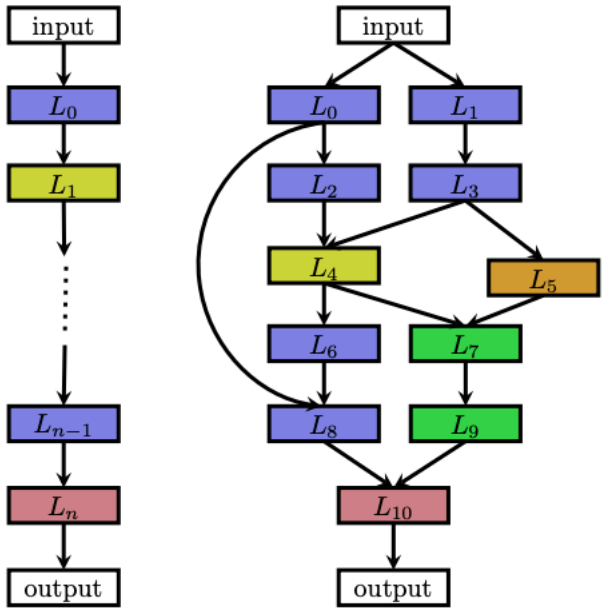
AutoML: Neural network architecture search (NAS)



random search;
Bayesian;
evolutionary, RL, GD, ...

Different architecture spaces to search



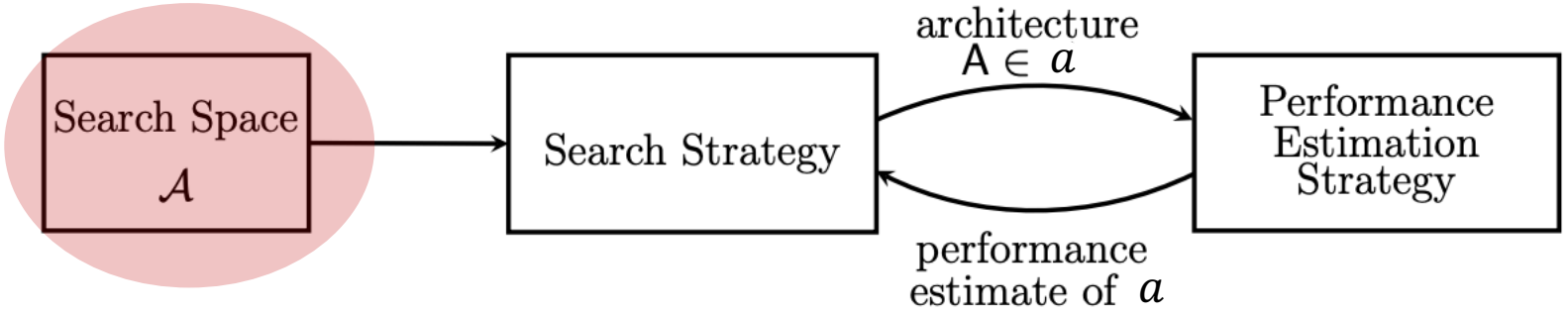
$$w_a = \underset{w}{\operatorname{argmin}}\, \mathcal{L}_{\text{train}}\left(\mathcal{N}(a, w)\right)$$

$$a^* = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \mathrm{ACC}_{\text{val}}\left(\mathcal{N}(a, w_a)\right)$$

Elsken, Thomas, Jan Hendrik Metzen, and Frank Hutter. "Neural Architecture Search: A Survey." Journal of Machine Learning Research 20 (2019): 1-21.

Classical analog

Exponentially large



$$w_a = \arg\min_{w} \mathcal{L}_{\text{train}}\left(\mathcal{N}(a, w)\right)$$

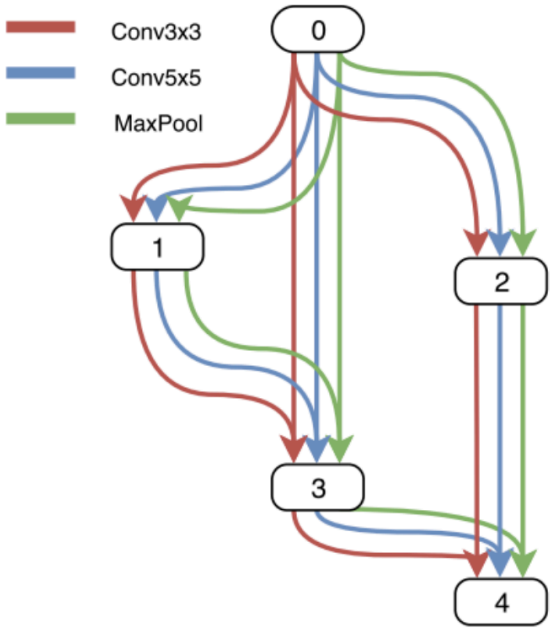
$$a^* = \arg\max_{a \in \mathcal{A}} \text{ACC}_{\text{val}}\left(\mathcal{N}(a, w_a)\right)$$

A strategy to avoid exponential overheard: Weight Sharing

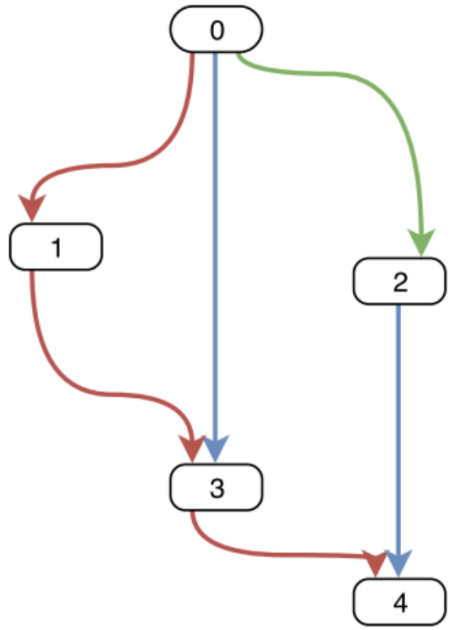
Optimization of NAS

$$W_{\mathcal{A}} = \arg\min_{W} \mathcal{L}_{\text{train}}\left(\mathcal{N}(\mathcal{A}, W)\right)$$

$$a^* = \arg\max_{a \in \mathcal{A}} \text{ACC}_{\text{val}}\left(\mathcal{N}(a, W_{\mathcal{A}}(a))\right)$$



Supergraph / supernet $\mathcal{A}$



subgraph / subnet a

Quantum circuit architecture search (QAS)

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Here we propose the quantum circuit architecture search scheme (QAS) to tackle

$$(\boldsymbol{\theta}^*, \boldsymbol{a}^*) = \arg\min_{\theta \in \boldsymbol{C}, \mathbf{a} \in \mathcal{S}} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}}).$$

- The output of QAS avoids barren plateaus and suppresses errors;
- The runtime cost of QAS is almost same with conventional QNN-based algorithms.

The paradigm of QAS

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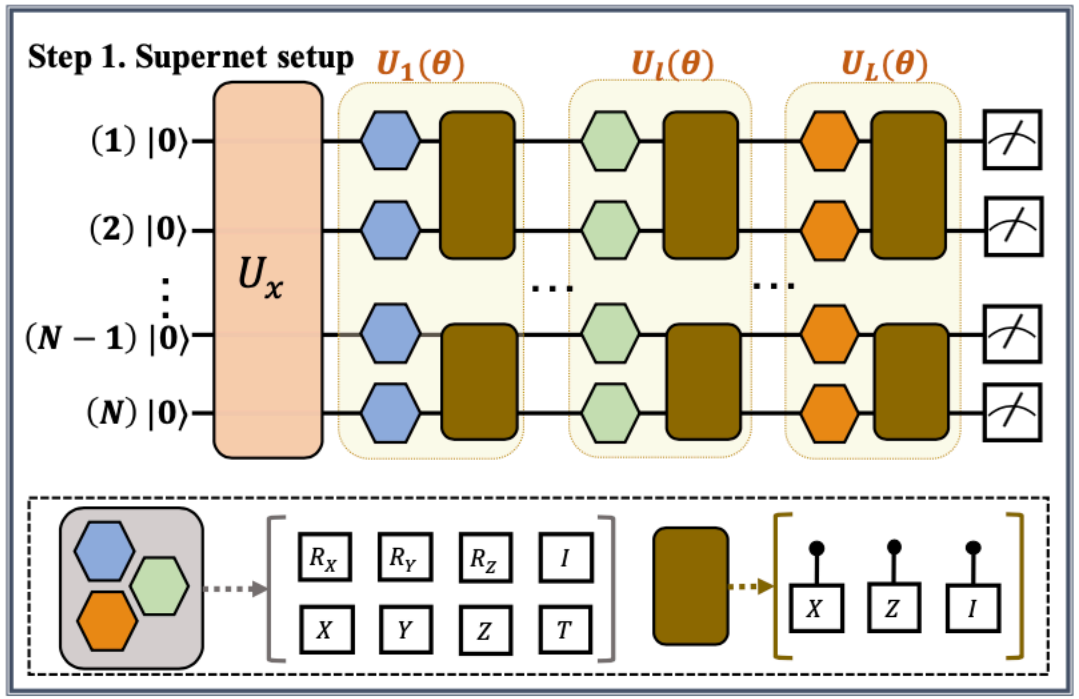

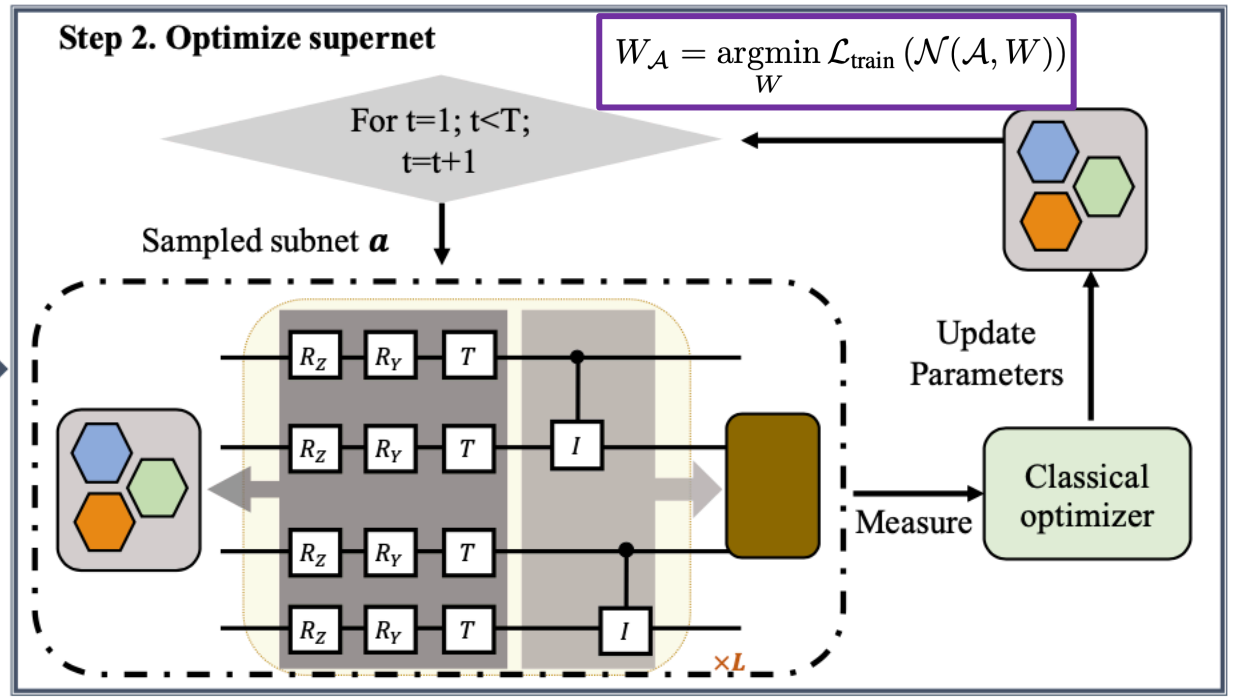

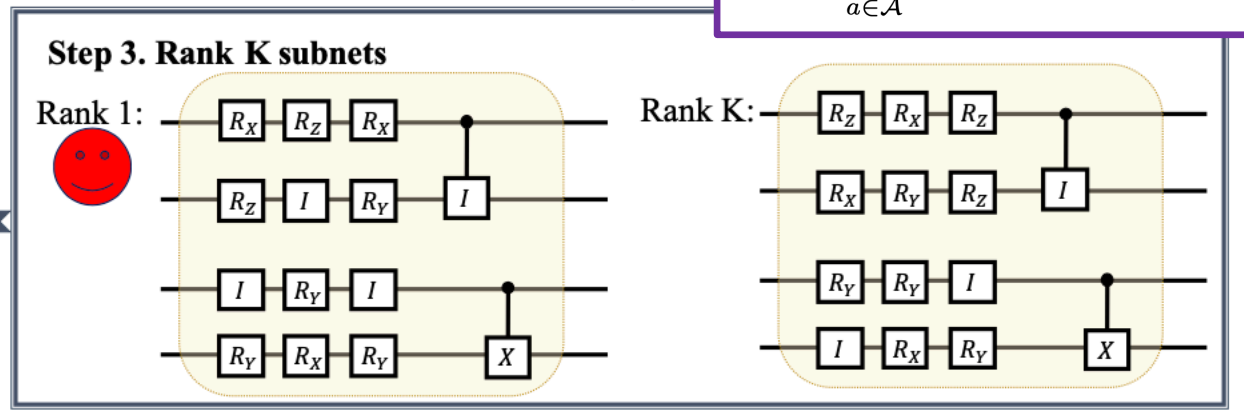

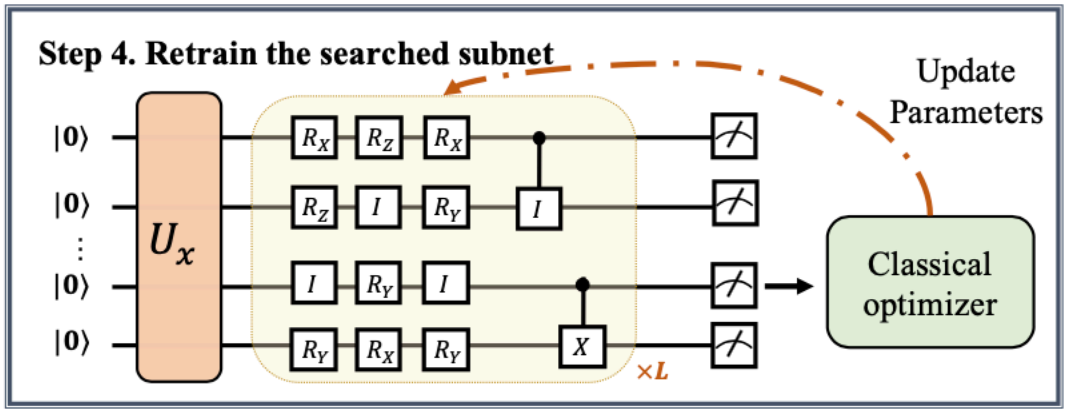

Step 1 of QAS: supernet setup + weight sharing strategy

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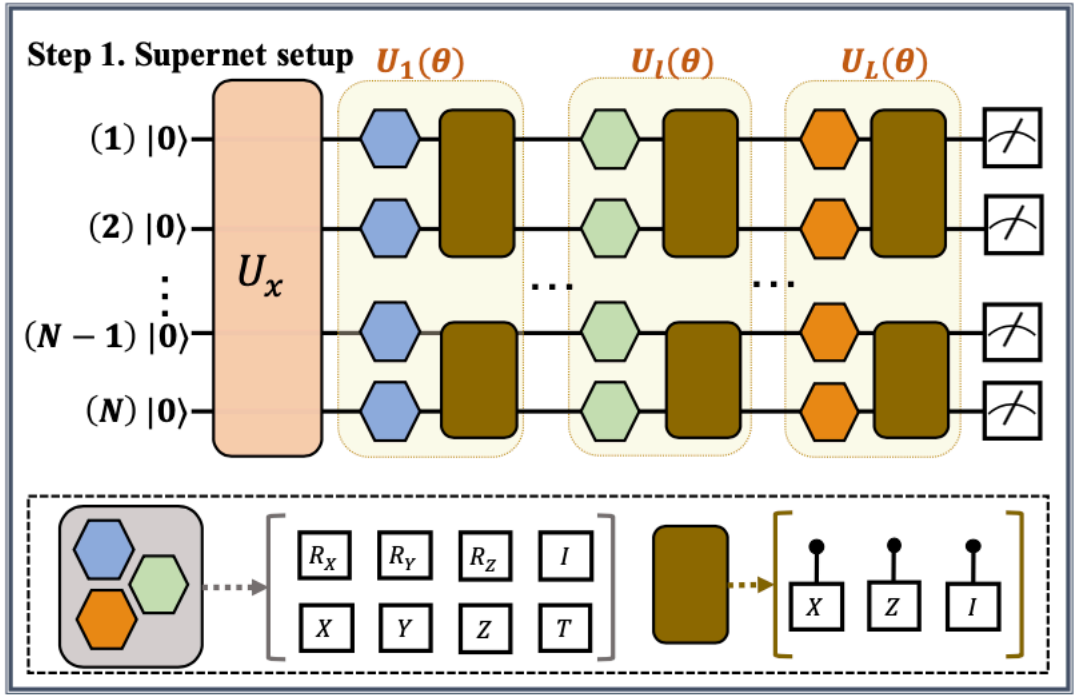
The aim of the supernet in QAS is **manipulating all possible variational quantum circuit architectures** of $U(\boldsymbol{\theta})$.



Step 1 of QAS: supernet setup + weight sharing strategy

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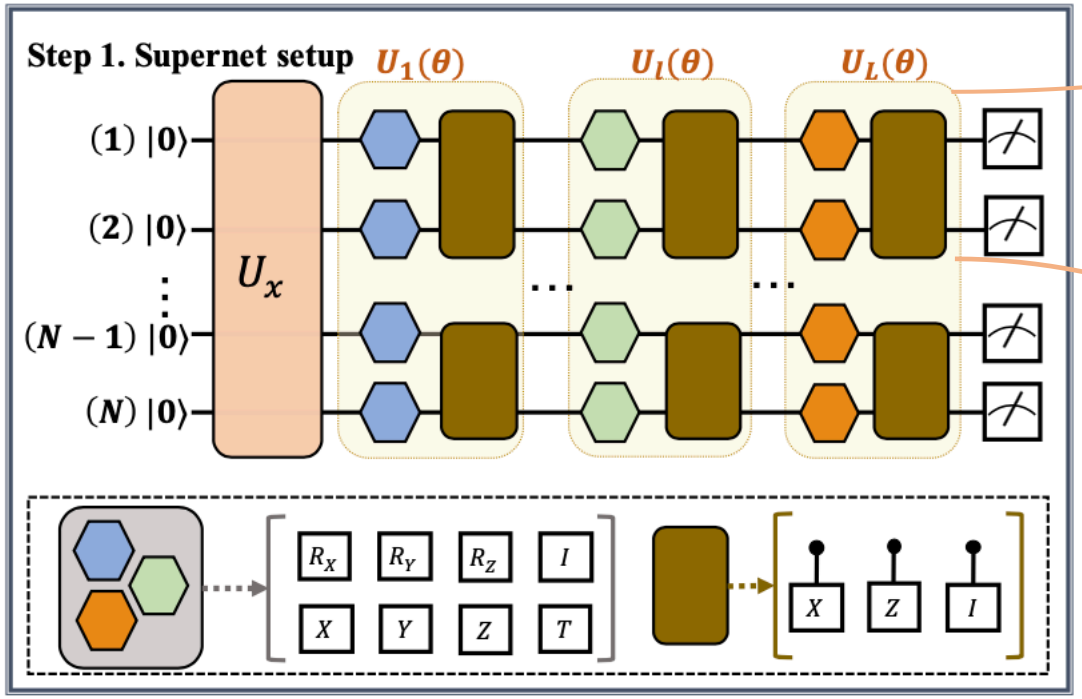
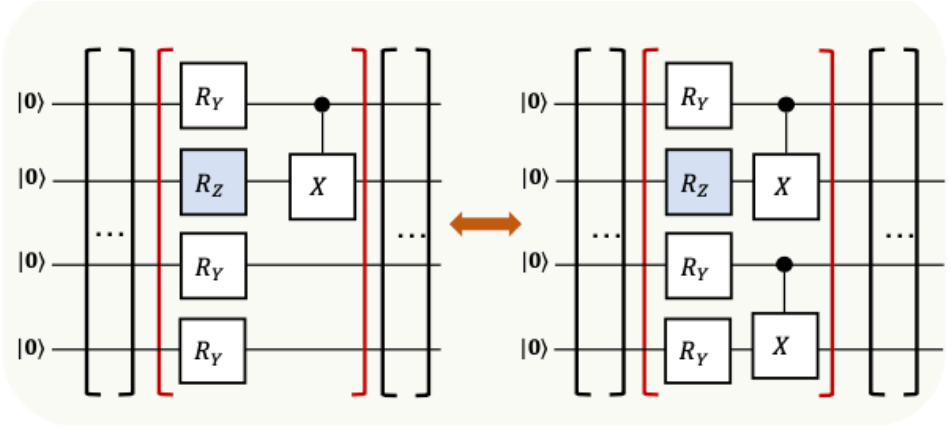
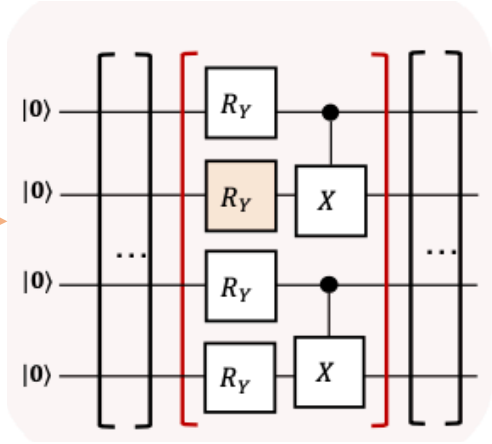
The weight sharing strategy: the weights in the supernet are shared across different architectures under the block level.







Step 2 of QAS: optimize supernet

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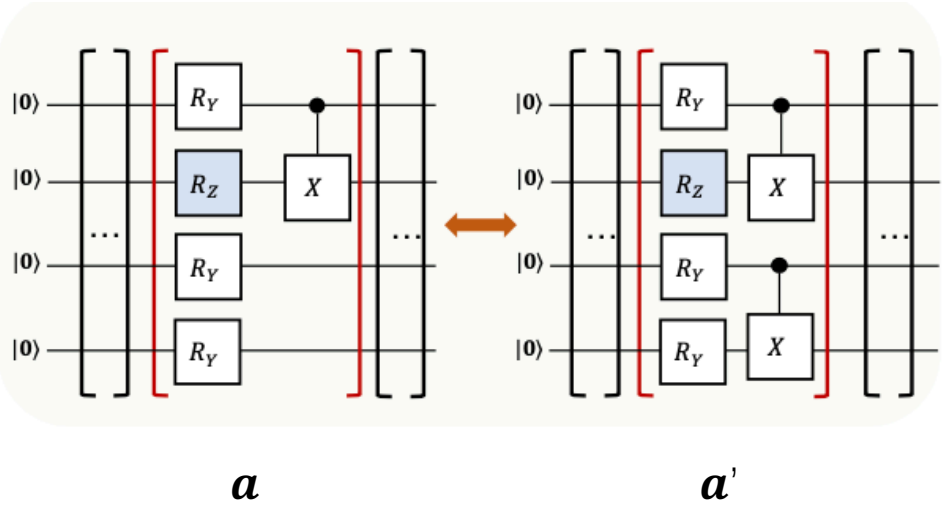
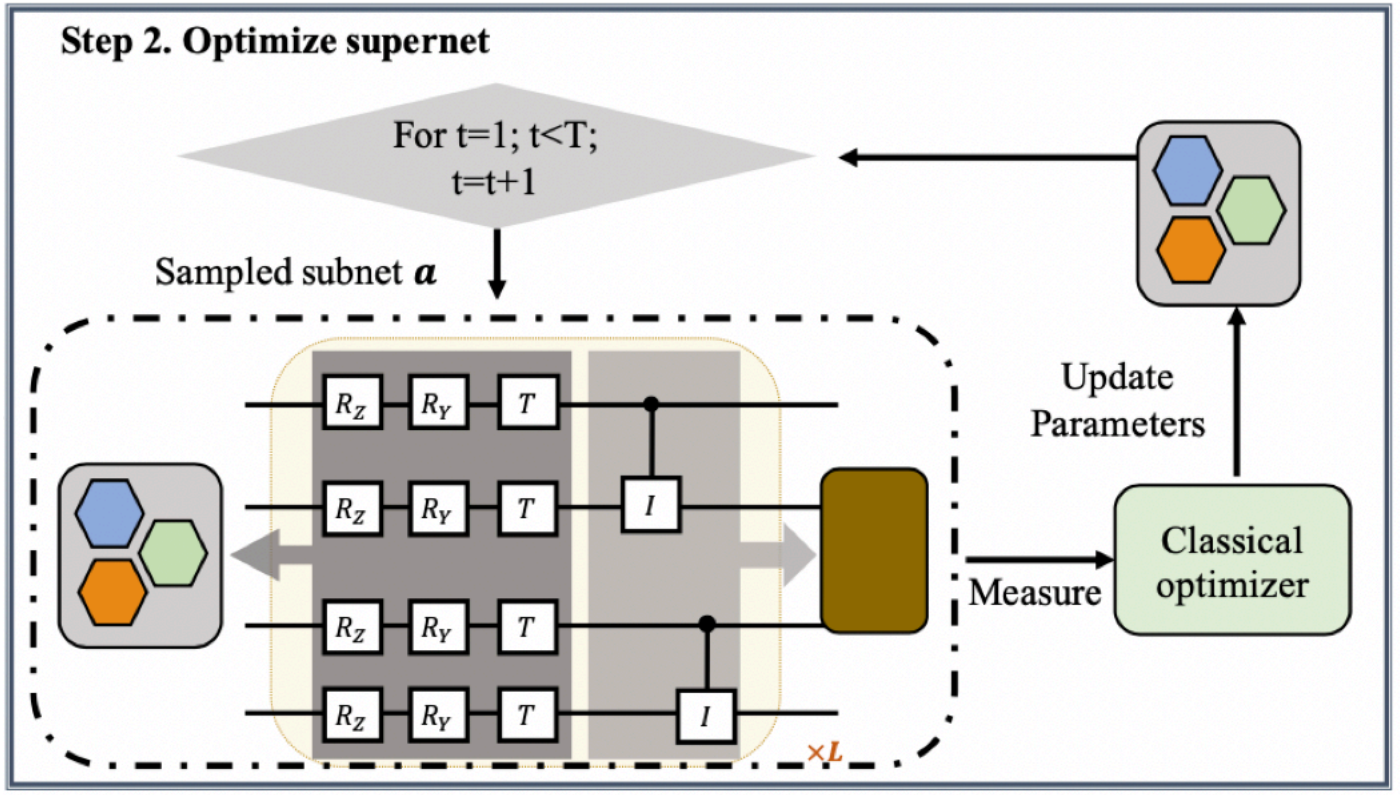
At the t-th iteration, QAS uniformly samples a subnet $\mathbf{a}^{(t)} \in \mathcal{S}$ to minimize $\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}})$, i.e., the parameters of the supernet relating to $\mathbf{a}^{(t)}$ is updated to

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + \eta \frac{\partial \mathcal{L}(\boldsymbol{\theta}^{(t)}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}})}{\partial \boldsymbol{\theta}^{(t)}},$$

where η is the learning rate.



$\boldsymbol{a}$ $\boldsymbol{a}'$



Step 3 of QAS: Rank K subnet

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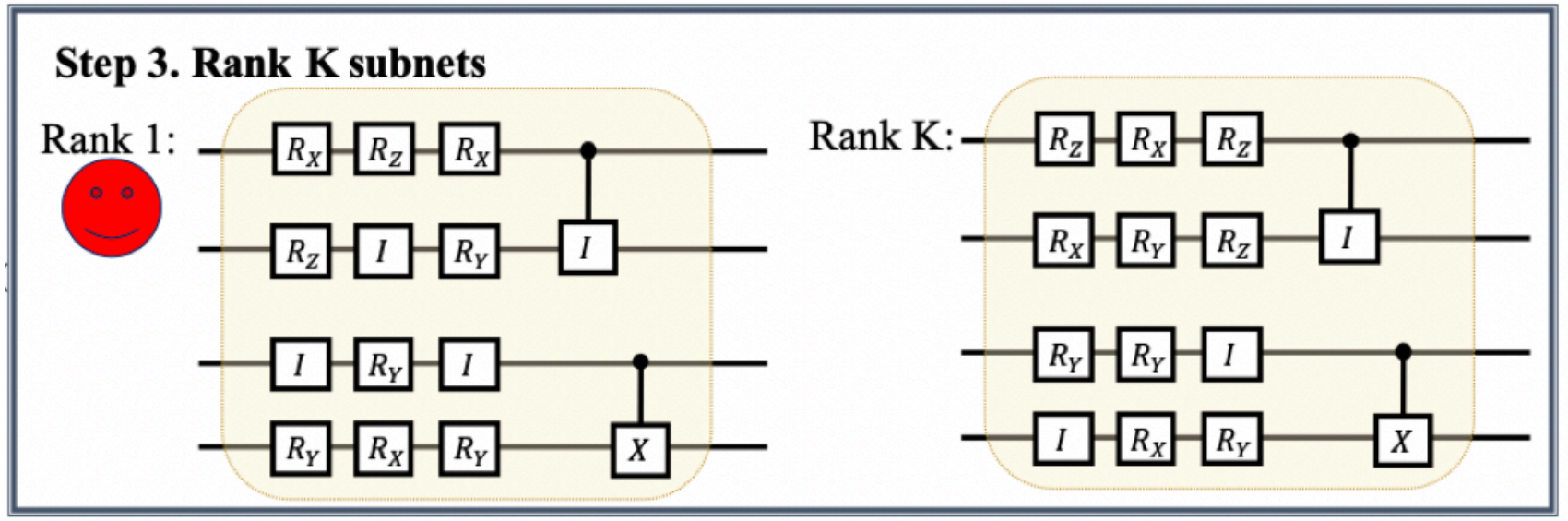
QAS uniformly samples K subnets, then ranks their performances, and assigns the subnet with the best performance as the output to approximate $\mathbf{a}^*$.



Step 4 of QAS: Rank K subnet

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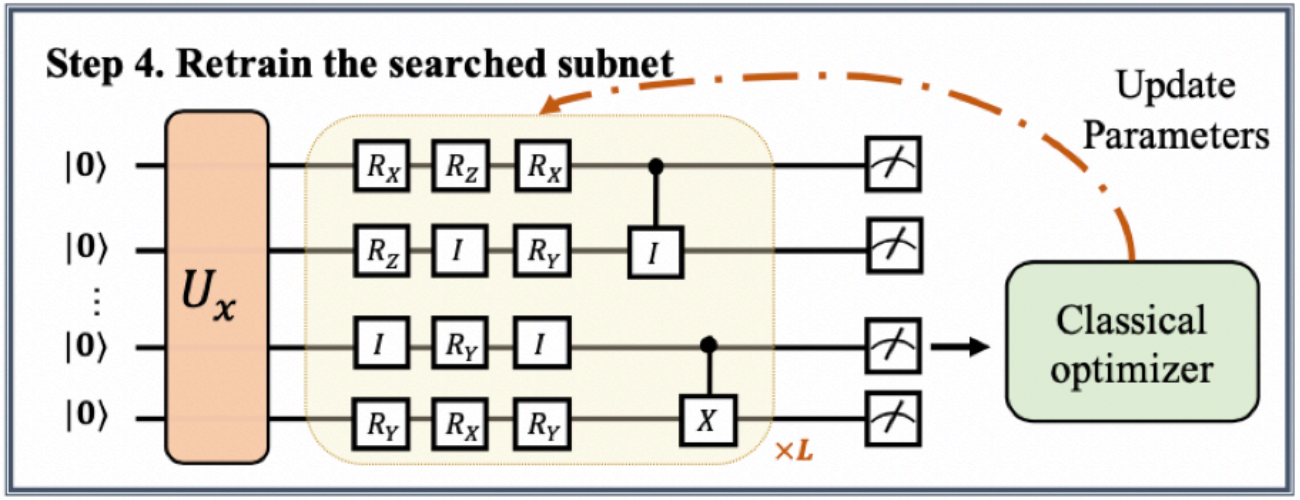
QAS retrain the searched subnet to approximate the optimal parameters.



The fierce competition phenomenon of QAS

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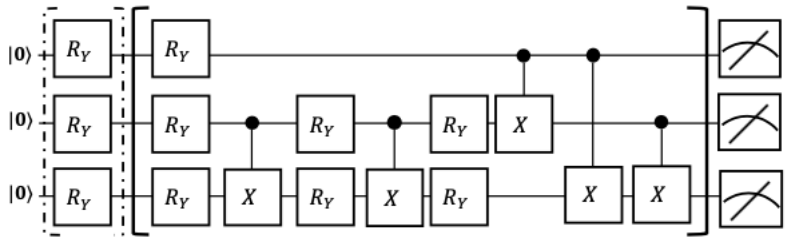
Fierce competition in QAS: the performance of a specified subnet may be largely varied by independently training and QAS.

1st subnet $\boldsymbol{a}_1$



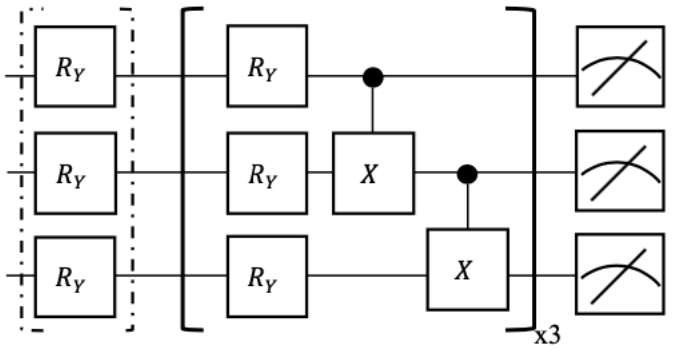
Independent training

99% acc | 94% acc

QAS with the weight sharing

91% acc | 93% acc

2cd subnet $\boldsymbol{a}_2$



Solution to the fierce competition phenomenon of QAS

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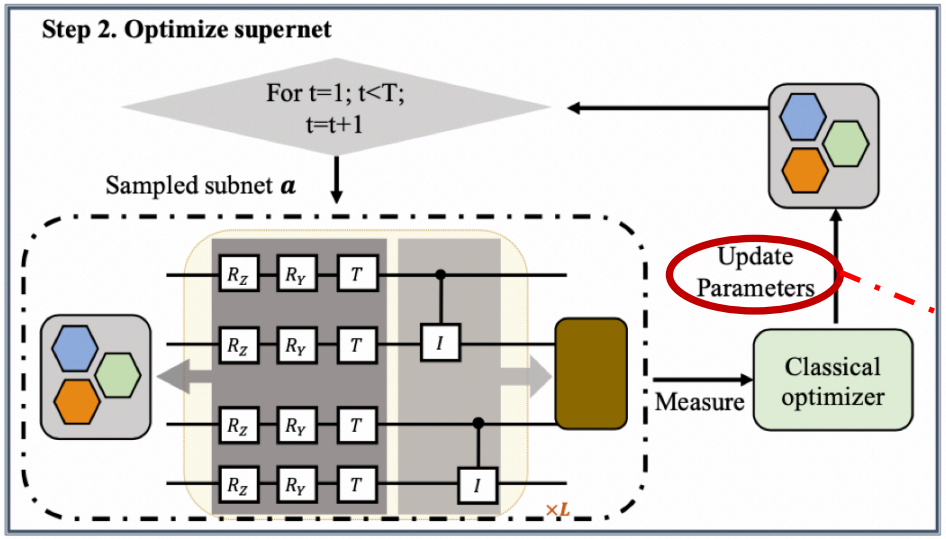
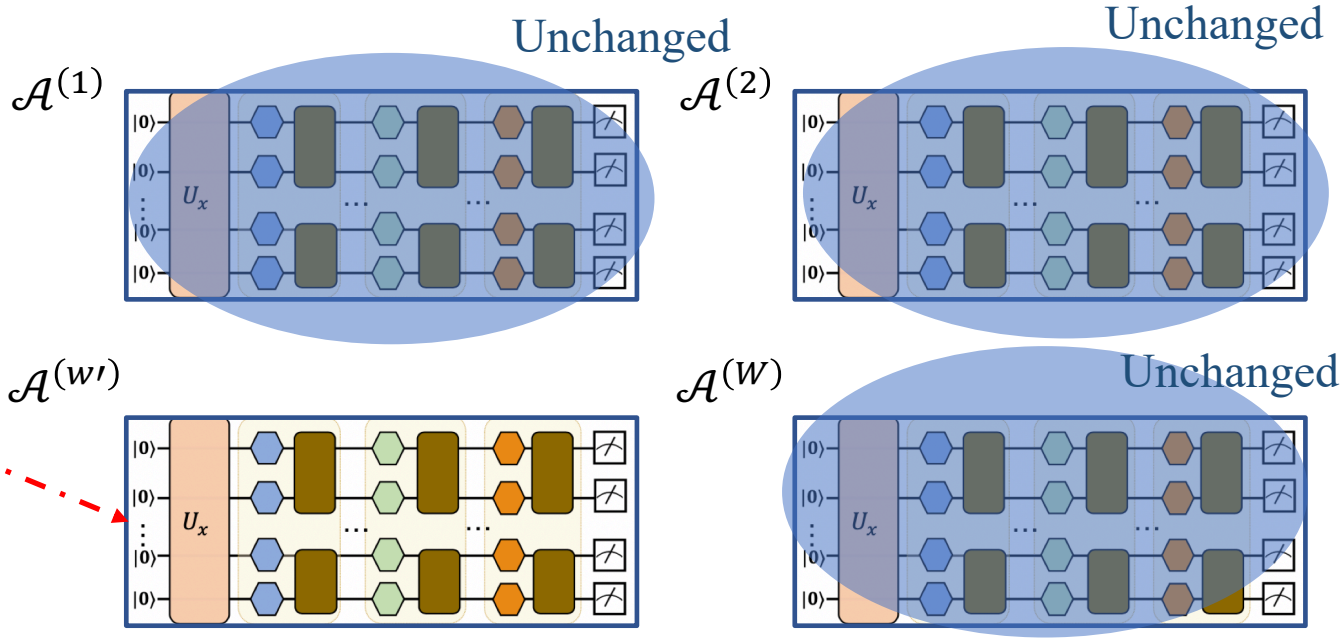
Solution: Employ multiple supernets $\{\mathcal{A}^{(w)}\}_{w=1}^{W}$ and optimize them independently. In the stages II-III, the sampled subnet $\boldsymbol{a}^{(t)}$ is categorized into the w′-th supernet when

$$w' = \arg\min_{w\in[W]} \mathcal{L}\left(\boldsymbol{\theta}^{(t,w)}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}}\right).$$





Relationship with the adversarial bandit problems

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Theorem 1. Let W and T be the number of supernets and iterations, respectively. Suppose that the subnet $\boldsymbol{a}^{(t)}$ is assigned to the $I_w^{(t)}$-th supernet $\mathcal{A}^{\left(I_w^{(t)}\right)}$ with $I_w^{(t)} \in [W]$ at the t-th iteration, where the corresponding objective function is $\mathcal{L}\left(\boldsymbol{\theta}^{(t,I_w^{(t)})}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}}\right) \in [0,1]$. Define the regret as

$$R_T = \sum_{t=1}^{T} \mathcal{L}\left(\boldsymbol{\theta}^{(t,I_w^{(t)})}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}}\right) - \min_{\{w_t\}_{t=1}^{T}} \sum_{t=1}^{T} \mathcal{L}\left(\boldsymbol{\theta}^{\left(t,I_w^{(t)}\right)}, \boldsymbol{z}, \boldsymbol{a}, \mathcal{E}_{\boldsymbol{a}}\right).$$

The method used in QAS to determine $\{I_w^{(t)}\}$ promises the regret $R_T \leq 0$, while the regret for the best bandit algorithms is lower bounded by $R_T = \Omega(T)$.

Summary: The proposed strategy outperforms all bandit learning algorithms in the measure of the regret.

Experiment results for classification tasks

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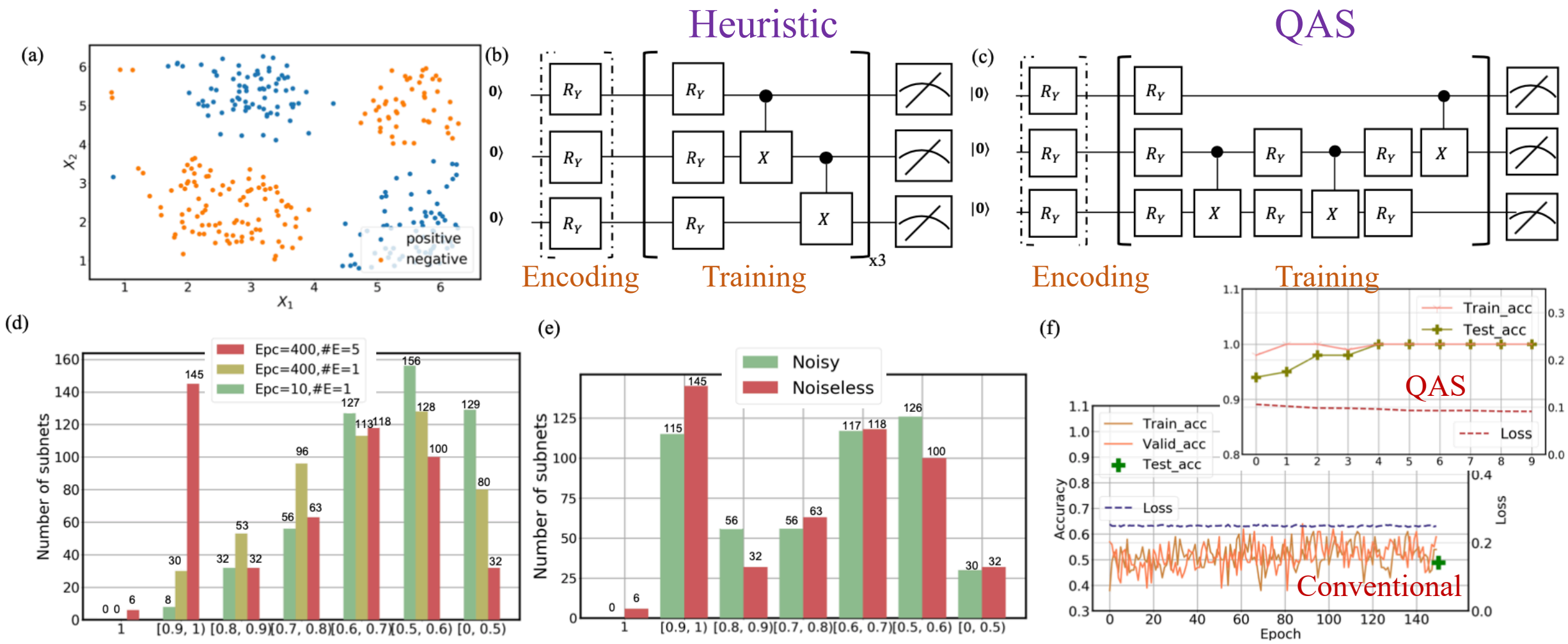

Experiment results for the ground state energy estimation

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The molecular hydrogen Hamiltonian is formulated as

$$H_h = \mathrm{g} + \sum_{i=1}^{3} g_i Z_i + \sum_{i=1,k=1,i<k}^{3} g_{i,k} Z_i Z_k + g_a Y_0 X_1 X_2 Y_3 + g_b Y_0 Y_1 X_2 X_3 + g_c X_0 X_1 Y_2 Y_3 + g_d X_0 Y_1 Y_2 X_3,$$

where $\{X_i, Y_i, Z_i\}$ denote the Pauli matrices acting on the i-th qubit and the real scalars g with or without subscripts are efficiently computable functions of the hydrogen-hydrogen bond length.

Experiment results for the ground state energy estimation

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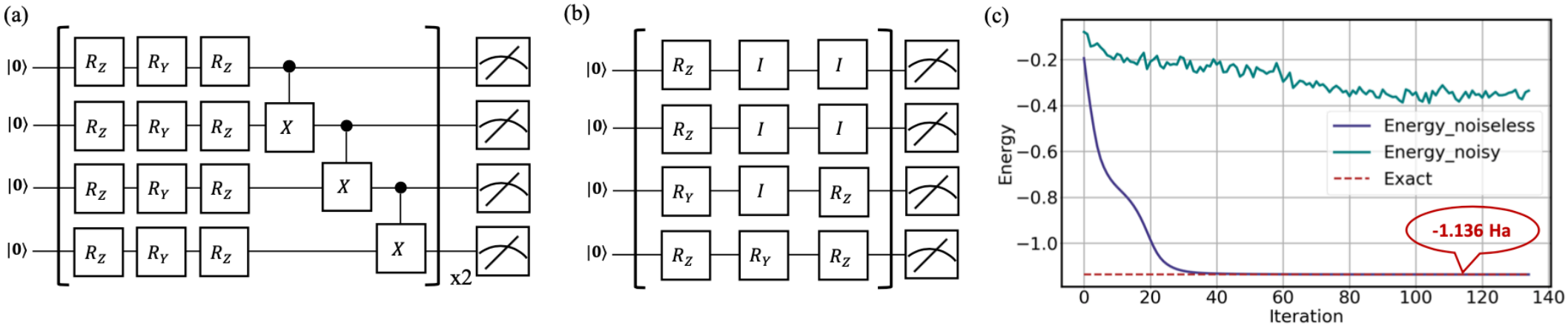
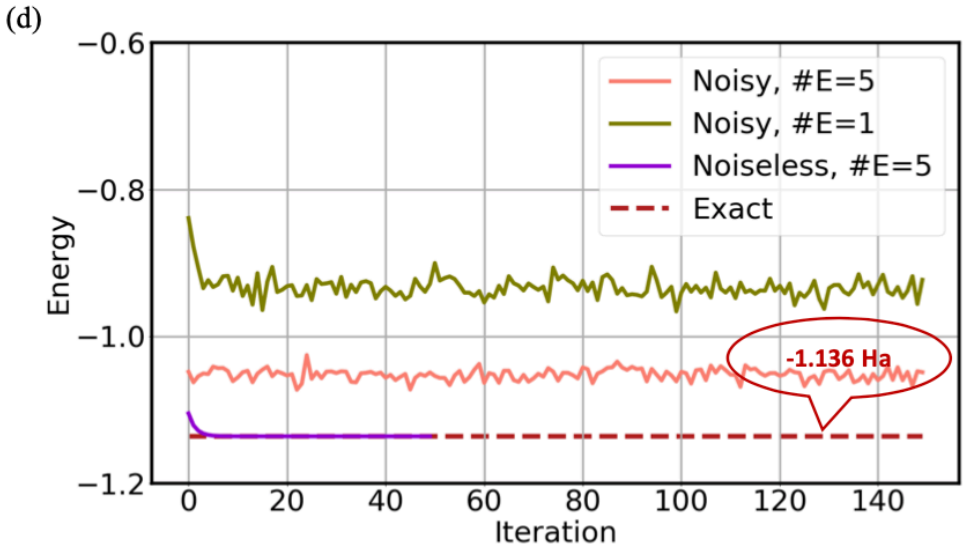
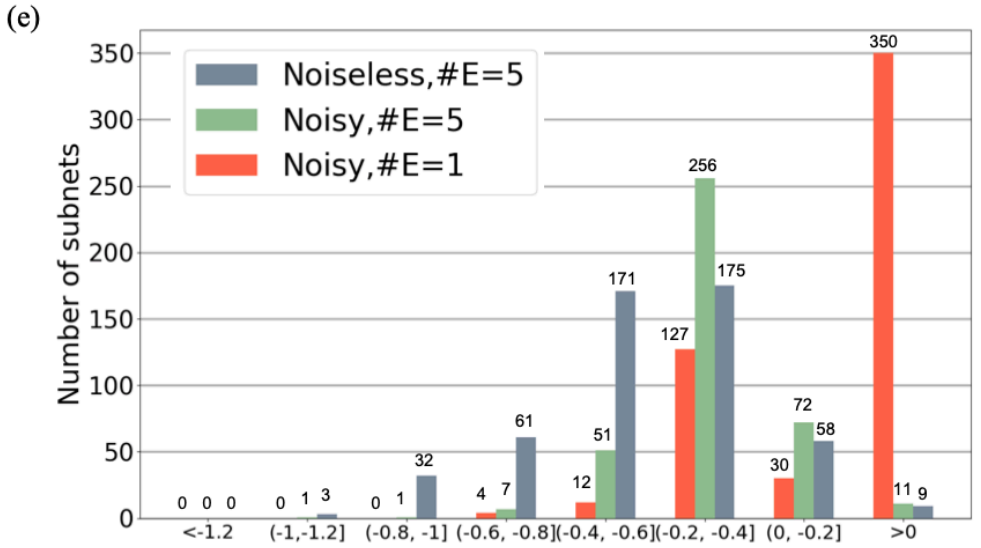
Heuristic

QAS







Experiment results for the ground state energy estimation

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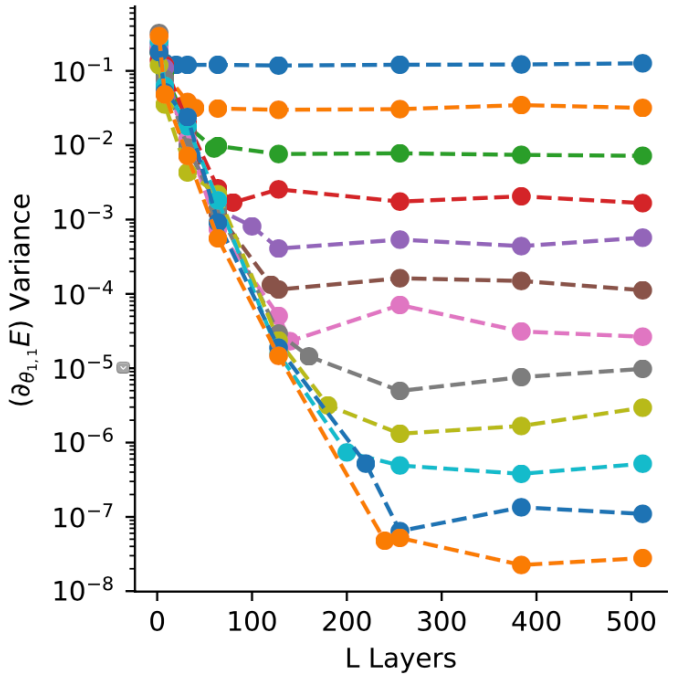
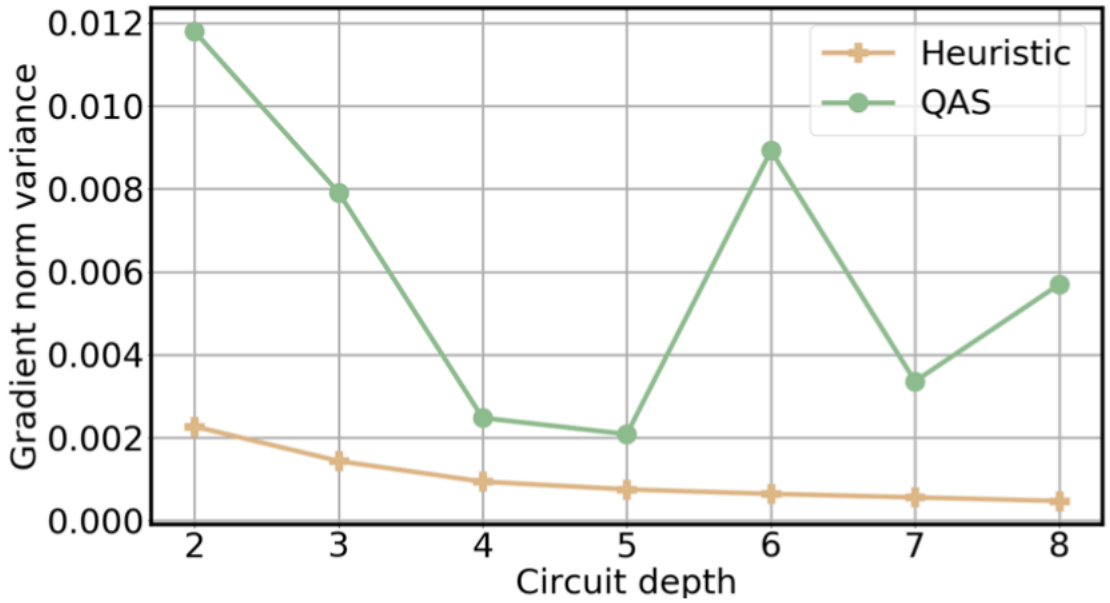
QAS contributes to the alleviation of barren plateaus.





Experiment results for the ground state energy estimation

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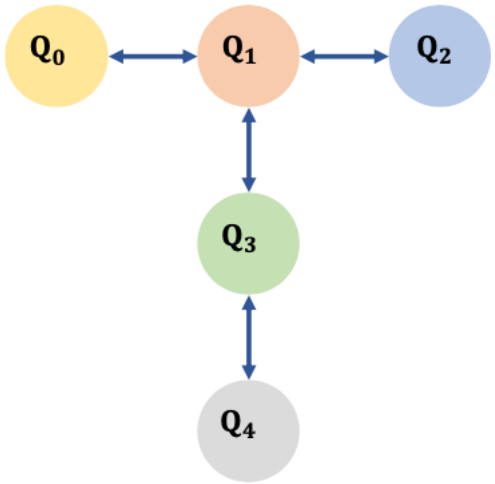
We last carry out QAS and the conventional VQE on IBM's 5-qubit quantum machine, i.e., 'Ibmq_ourense', to accomplish the ground state energy estimation of H_h.



Qubit	T1(μs)	T2(μs)	Readout error	Single-qubit U2 error gate	CNOT error rate
Q0	75.75	50.81	1.65E-2	5.22E-4	cx0-1: 9.55E-3
Q1	78.47	27.56	2.38E-2	4.14E-4	cx1-0: 9.55E-3 cx1-2: 9.44E-3 cx1-3: 1.25E-2
Q2	101.51	107.00	1.57E-2	1.83E-4	cx2-1: 9.44E-3
Q3	79.54	78.38	3.95E-2	4.30E-4	cx3-1: 1.25E-2 cx3-4: 8.34E-3
Q4	74.27	30.00	4.74E-2	4.20E-4	cx4-3: 8.34E-3

Experiment results for the ground state energy estimation

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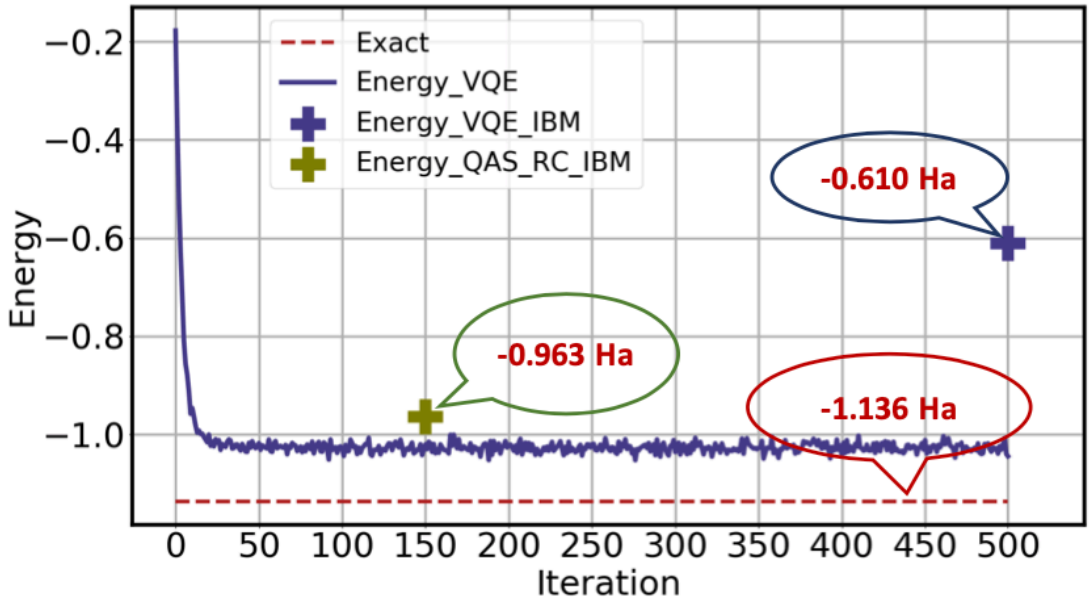
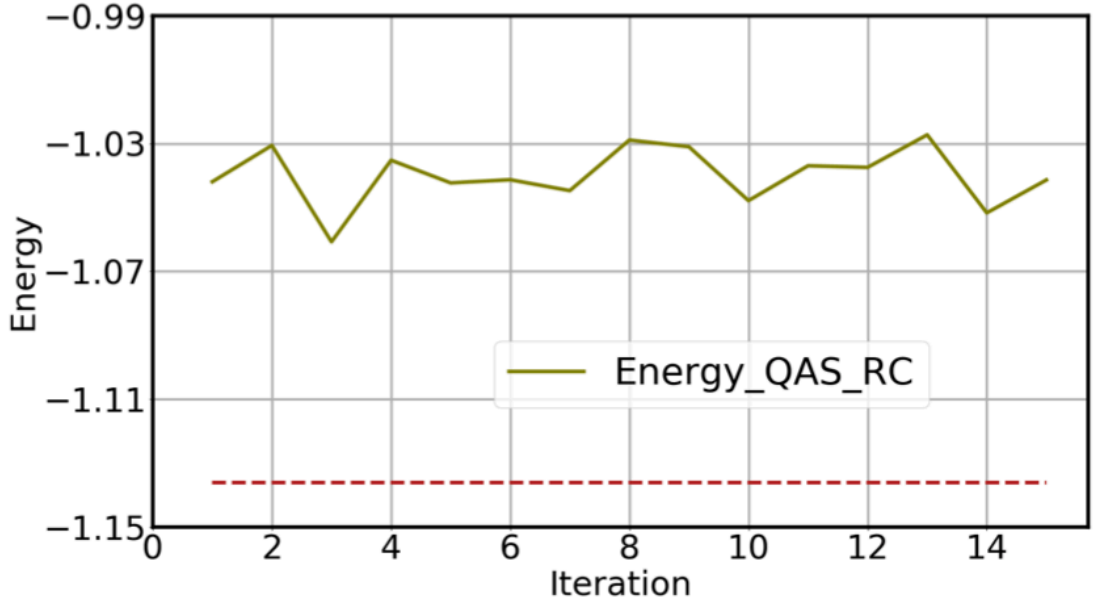
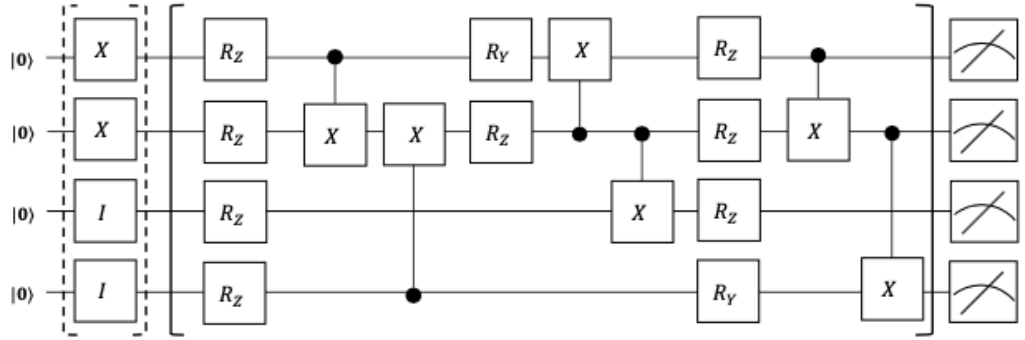
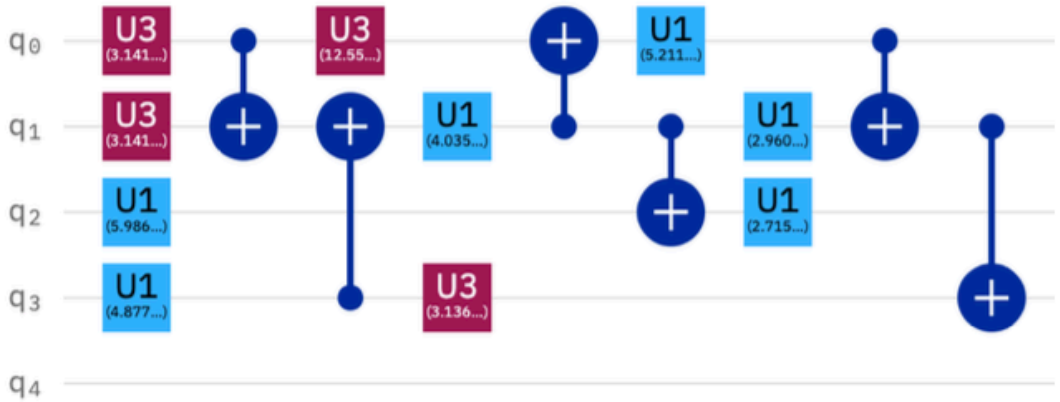
Experiment results of the ground state energy estimation of VQE and QAS.





The searched circuit architecture by QAS





Improvements

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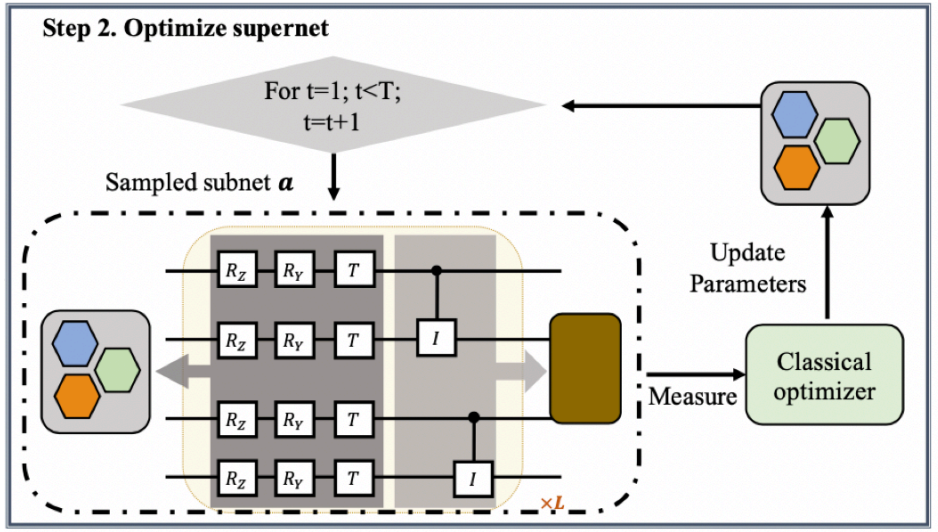
- Improving the ranking stage of QAS, i.e., replacing the uniformly sampling by evolutionary algorithms or reinforcement learning algorithms.



- Employing the adversarial bandit learning algorithms to train multiple supernets. Benefits: reduce the runtime cost. Disadvantages: inducing a relatively large regret bound.

III. The power of quantum kernels in the NISQ era

Kernel methods

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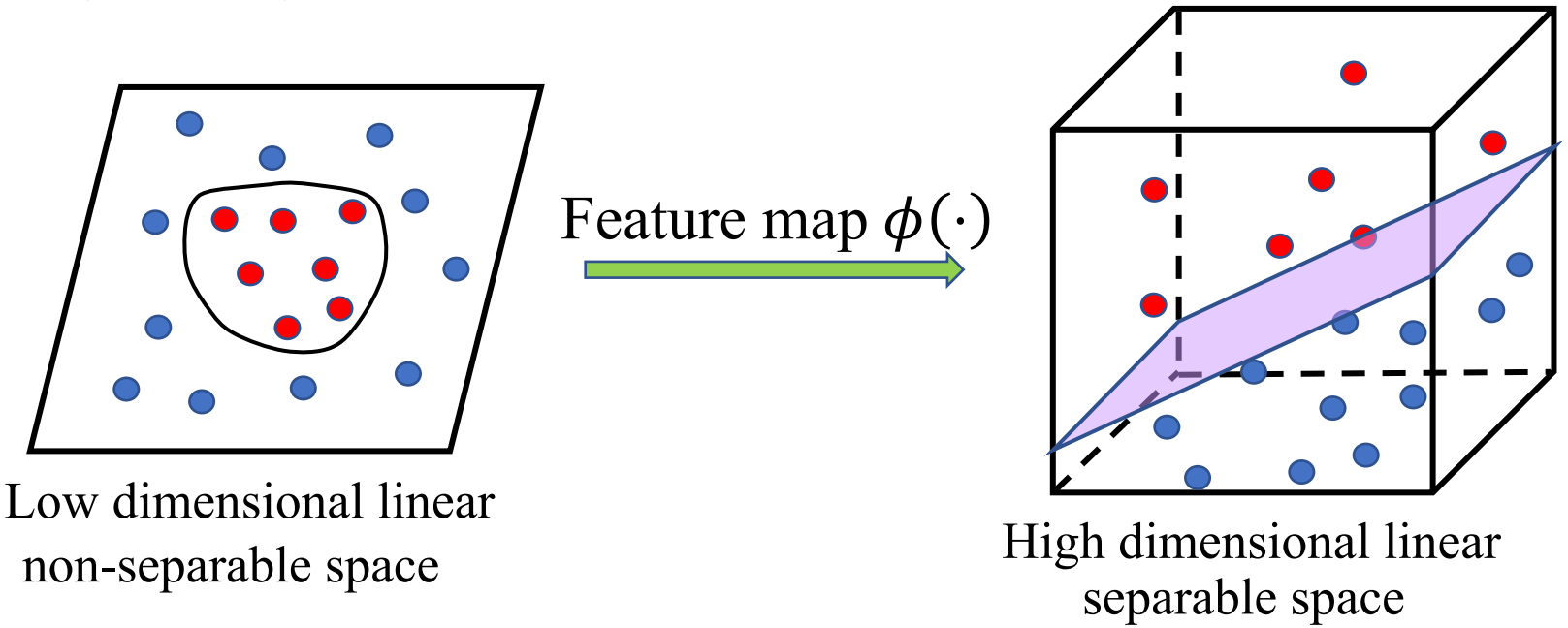
Core idea:

- Mapping the given input $x^{(i)} \in \mathbb{R}^d$ into a high-dimensional feature space, i.e., $\phi(\cdot)$: $\mathbb{R}^d \rightarrow \mathbb{R}^q$ $(q \gg d)$.
- Constructing a kernel function $\kappa(x^{(i)}, x^{(j)}) = \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$ and the corresponding kernel matrix $\mathrm{K}_{ij} = \kappa(x^{(i)}, x^{(j)})$



Typical kernels: the radial basis function kernel, Gaussian kernel, and polynomial kernel.

Kernel methods

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Core idea:

For efficient optimization of w, we consider minimization of the following loss function

$$\min_{w} \lambda\langle w, w\rangle + \sum_{i=1}^{N} \left(\langle w, \phi(x)\rangle - \mathrm{Tr}(U^{\dagger}OU\rho(x_i))\right)^2,$$

$h(x_i)$ y_i

The optimal ω can be written down explicitly as

$$w = \sum_{i=1}^{N}\sum_{j=1}^{N} \phi(x_i)((K + \lambda I)^{-1})_{ij}\,\mathrm{Tr}(U^{\dagger}OU\rho(x_j)).$$

Quantum kernel methods

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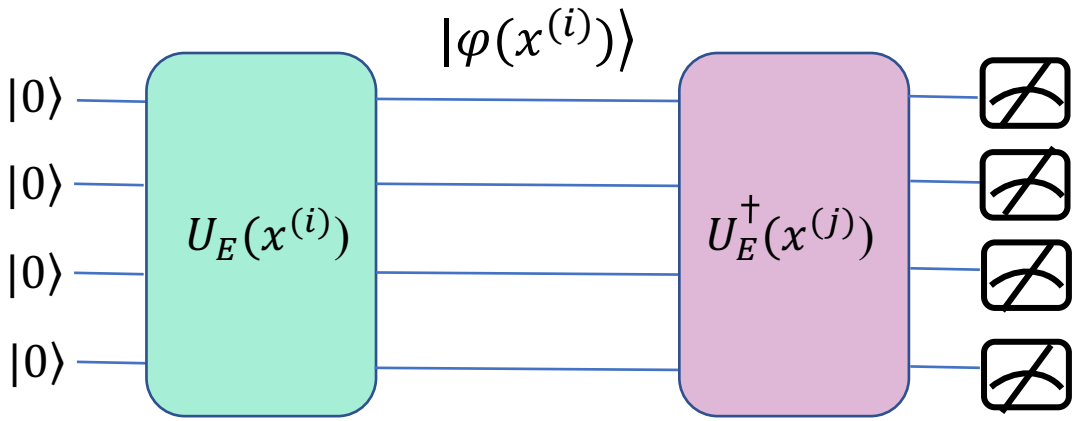
- Replacing classical feature map $\phi(\cdot)$ with a variational quantum circuit $U_E(\cdot)$.
- Mapping the give classical data $x^{(i)} \in \mathbb{R}^d$ to exponentially large feature space, i.e., $|\phi(x^{(i)})\rangle = U_E(x^{(i)})\,|0^d\rangle \in \mathbb{R}^{2^d}$. Denote N as the number of qubits, then $N = d$.
- The result of kernel function $\kappa(\cdot,\cdot)$ coincides with applying measurements on the prepared. quantum states, then the (i,j)-th element in kernel matrix is $\mathbf{W}_{ij} = |\langle\varphi(\boldsymbol{x}^{(j)})|\varphi(\boldsymbol{x}^{(i)})\rangle|^2$



Overview

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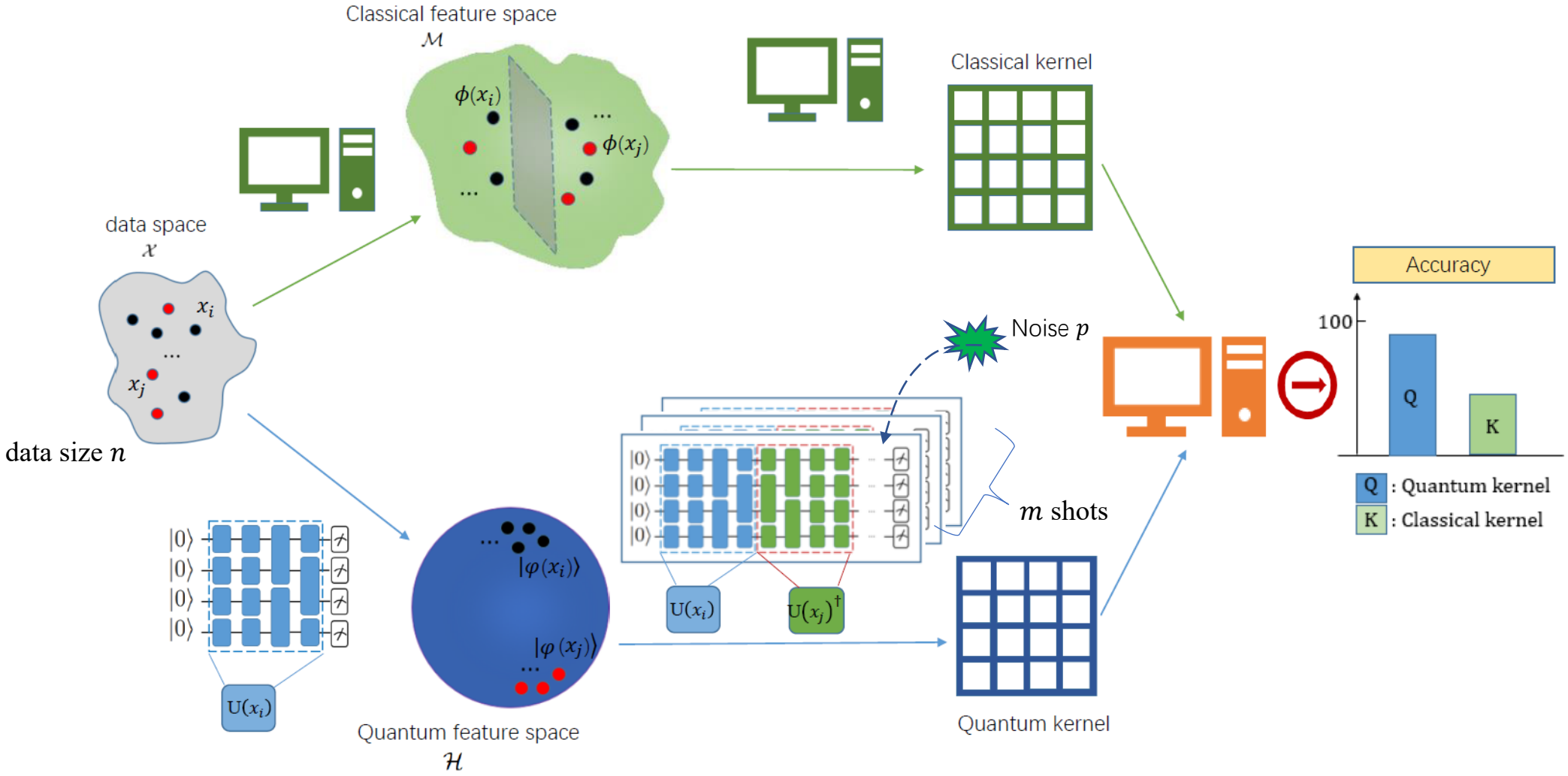

The power of quantum kernels

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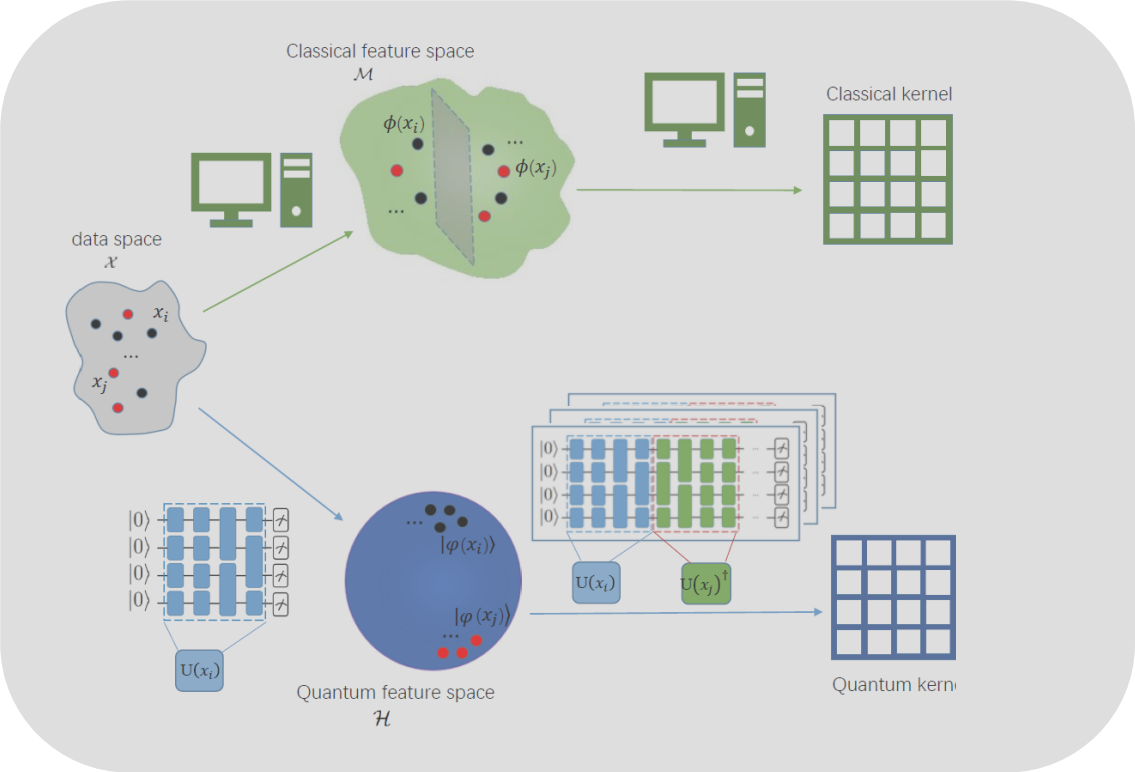

How quantum kernel methods outperform classical kernel methods in predicting the unseen data ?

The power of data in quantum kernels

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Problem setup.

Each data pair $(x^{(i)}, y^{(i)})$ is constructed by $y^{(i)} = f\left(x^{(i)}\right) = \mathrm{Tr}\left(OU(\boldsymbol{\theta}^*)\rho\left(x^{(i)}\right)U(\boldsymbol{\theta}^*)^\dagger\right)$, where $U(\boldsymbol{\theta}^*)$ a specified unitary evolution applied on the encoded quantum example $\rho\left(x^{(i)}\right)$, and O is a certain measurement operator.

Given N examples, the goal of a learning model is to infer a map $h(\cdot)$ such that $y^{(i)} = h\left(x^{(i)}\right)$.

The power of data in quantum kernels

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Results.

Huang et al. [arXiv:2011.01938] present a generalization error bound under **the ideal scenario,** i.e., given n examples, the generalization error of classical kernels follows

$$\mathbb{E}_{x\sim\mathcal{D}}|h(x)-f(x)| \leq c\sqrt{\frac{s_K(n)}{n}}$$

where $s_K(n)$ refers to the model complexity with

$$s_K(n) = \sum_{i=1}^{n}\sum_{j=1}^{n}(K^{-1})_{ij}\,\mathrm{Tr}(O^U\rho(x_i))\,\mathrm{Tr}(O^U\rho(x_j)).$$

The power of data in quantum Kernels

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$$\mathbb{E}_{x\sim\mathcal{D}}|h(x)-f(x)| \leq c\sqrt{\frac{s_K(n)}{n}} \qquad s_K(n) = \sum_{i=1}^{n}\sum_{j=1}^{n}(K^{-1})_{ij}\,\mathrm{Tr}(O^U\rho(x_i))\,\mathrm{Tr}(O^U\rho(x_j)).$$

Two insights

- Given the same sample size, a small $\frac{Y^\top \mathrm{W}^{-1} Y}{Y^\top \mathrm{K}^{-1} Y}$ leads to a large quantum advantage over the classical kernel methods.

- Under the same kernel method, a large n leads to a better prediction performance.

How about power of quantum kernels in the NISQ era?

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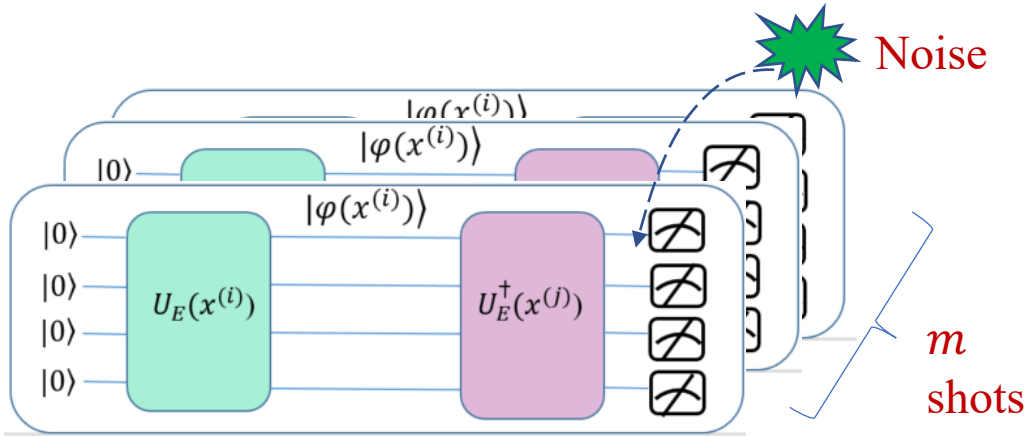
In the NISQ era, quantum kernels are affected by the system noise and finite shots.



- Consider the depolarization channel $\mathcal{N}_p(\rho(\boldsymbol{x}^{(i)})) = (1-p)\rho(\boldsymbol{x}^{(i)}) + \frac{p\mathbb{I}_{2^N}}{2^N}$, where p is the depolarization rate. Then the quantum kernel can be written as

$$\widetilde{\mathrm{W}} = (1-p)\,\mathrm{W} + \frac{p\mathbb{I}_{2^N}}{2^N}$$

- Consider the finite measurements, the estimated element of quantum kernels yields

$$\widehat{\mathrm{W}}_{ij} = \frac{1}{m}\sum_{k=1}^{m} V_k, \qquad V_k \sim \mathrm{Ber}(\widetilde{\mathrm{W}}_{ij})$$

The power of quantum kernels under the NISQ setting

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Under the NISQ setting, we give a generalization error bound for the estimate kernel $\widehat{\mathrm{W}}$.

Theorem 3. *Let the size of training dataset be n and the number of measurements is m. Define $Y = [y_1, \cdots, y_n]^\top$ as the label vector and $c_{\mathrm{W}} = \| \mathrm{W}^{-1} \|_2$. Suppose the system noise is modeled by $\mathcal{N}_p$. With probability at least $1-\delta$, the noisy quantum kernel $\widehat{W}$ can be used to infer a hypothesis $h(\boldsymbol{x})$ with generalization error*

$$\mathbb{E}_{\boldsymbol{x},\widehat{\mathrm{W}}} |h(\boldsymbol{x}) - f(\boldsymbol{x})| \leq \tilde{O}\left(\sqrt{\frac{c_1}{n}} + \sqrt{\frac{1}{c_2}\frac{n}{\sqrt{m}}}\right) \tag{D10}$$

where $c_1 = Y^\top \mathrm{W}^{-1} Y$ *and* $c_2 = \max(c_{\mathrm{W}}^{-2}((\frac{1}{2}\log(\frac{4n^2}{\delta}))^{\frac{1}{2}} + m^{\frac{1}{2}} p\left(1 + \frac{1}{2^{N+1}}\right))^{-1} - \frac{n}{\sqrt{m}} c_{\mathrm{W}}^{-1}, 0)$.

An additional term $\sqrt{n/(c_2\sqrt{m})}$ compared to the bound of Huang et al. has following implications:

- $n/\sqrt{m}$ suggests that an increased number of data n will result in a higher generalization error.
- The performance of quantum kernels in the NISQ era are heavily depends on the number of measurements.
- The term c_2 indicates the negative role of the system noise. Moreover, the generalization error bound would be infinite once $p > 1/(nc_{\mathrm{W}}(1 + 1/2^{N+1}))$.

The power of quantum kernels under the NISQ setting

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Under the NISQ setting, we give a generalization error bound for the estimate kernel $\widehat{\mathrm{W}}$.

$$\mathbb{E}_{\boldsymbol{x},\widehat{\mathrm{W}}} |h(\boldsymbol{x}) - f(\boldsymbol{x})| \leq \tilde{O}\left(\sqrt{\frac{c_1}{n}} + \sqrt{\frac{1}{c_2}\frac{n}{\sqrt{m}}}\right) \tag{D10}$$

where $c_1 = Y^\top \mathrm{W}^{-1} Y$ *and* $c_2 = \max(c_{\mathrm{W}}^{-2}((\frac{1}{2}\log(\frac{4n^2}{\delta}))^{\frac{1}{2}} + m^{\frac{1}{2}} p\left(1 + \frac{1}{2^{N+1}}\right))^{-1} - \frac{n}{\sqrt{m}} c_{\mathrm{W}}^{-1}, 0)$.

An additional term $\sqrt{n/(c_2\sqrt{m})}$ compared to the bound of Huang et al. has following implications:

- $n/\sqrt{m}$ suggests that an increased number of data n will result in a higher generalization error;
- The performance of noisy quantum kernels heavily depends on shots m;
- The term c_2 indicates the negative role of the system noise. Moreover, the generalization error bound would be infinite once $p > 1/(nc_{\mathrm{W}}(1 + 1/2^{N+1}))$.

Proof Sketches of Theorem 1

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Following the result of Huang et al., with probability $1-\delta/2$, the generalization error of $\widehat{\mathrm{W}}$ yields

$$\mathbb{E}_{\boldsymbol{x},\widehat{\mathrm{W}}}\left|f(\boldsymbol{x})-h(\boldsymbol{x})\right| \leq \widetilde{O}\left(\sqrt{\frac{Y^{\top}\widehat{\mathrm{W}}^{-1}Y}{n}}\right)$$

Note that $\sqrt{Y^{\top}\widehat{\mathrm{W}}^{-1}Y}=\sqrt{Y^{\top}\left(\widehat{\mathrm{W}}^{-1}-\mathrm{W}^{-1}\right)Y+Y^{\top}\mathrm{W}^{-1}Y} \leq \sqrt{\left\|\widehat{\mathrm{W}}^{-1}-\mathrm{W}^{-1}\right\|_2 Y^{\top}Y}+\sqrt{Y^{\top}\mathrm{W}^{-1}Y}$ (3)

and the connection of $\left\|\widehat{\mathrm{W}}^{-1}-\mathrm{W}^{-1}\right\|_2$ and $\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2$, that is

$$\left\|\mathrm{W}^{-1}-\widehat{\mathrm{W}}^{-1}\right\|_2 \leq \frac{c_{\mathrm{W}}^2\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2}{1-c_{\mathrm{W}}\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2} \quad .\left(c_{\mathrm{W}}=\left\|\mathrm{W}^{-1}\right\|_2\right) \tag{4}$$

To achieve $\|\mathrm{W}^{-1}-\widehat{\mathrm{W}}^{-1}\|_2 \leq \delta$, it is sufficient to show $\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2 \leq \frac{\delta}{c_{\mathrm{W}}(\delta+c_{\mathrm{W}})}$.

Meanwhile, utilizing the Chernoff-Hoeffding bound and the equation $\widetilde{\mathrm{W}}=(1-p)\,\mathrm{W}+\frac{p\mathbb{I}_{2^N}}{2^N}$ yields

$$\Pr\left(\left|\mathrm{W}_{ij}-\widehat{\mathrm{W}}_{ij}\right| \geq p\left(1+\frac{1}{2^{N+1}}\right)+\frac{\delta}{2}\right) \leq 2\exp\left(\frac{-\delta^2 m}{2}\right). \tag{5}$$

Proof Sketches of Theorem 1

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Then a similar concentration inequality in term of the norm $\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2$ can be written as

$$\Pr\left(\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2 \geq \delta'\right) \leq \Pr\left(\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_{\mathrm{F}} \geq \delta'\right) \qquad \left(\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2 \leq \left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_{\mathrm{F}}\right)$$

$$= \Pr\left(\sum_{i=1}^{n}\sum_{j=1}^{n}\left|\mathrm{W}_{ij}-\widehat{\mathrm{W}}_{ij}\right|^2 \geq \delta'^2\right)$$

$$\leq \Pr\left(\bigcup_{i=1}^{n}\bigcup_{j=1}^{n}\left|\mathrm{W}_{ij}-\widehat{\mathrm{W}}_{ij}\right|^2 \geq \frac{\delta'^2}{n^2}\right) \qquad \text{(union bound)}$$

$$\leq 2n^2\exp\left(-2\left(\frac{\delta'}{n}-p\left(1+\frac{1}{2^{N+1}}\right)\right)^2 m\right) \qquad \text{(using Eqn. (4) and requiring } \delta' > np\left(1+\frac{1}{2^{N+1}}\right)\text{)}$$

Combing this inequality with Eqn. (4), we have

$$\Pr\left(\left\|\mathrm{W}^{-1}-\widehat{\mathrm{W}}^{-1}\right\|_2 \geq \delta\right) \leq \Pr\left(\left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_2 \geq \frac{\delta}{c_{\mathrm{W}}(\delta+c_{\mathrm{W}})}\right) \leq 2n^2\exp\left(-2\left(\frac{\delta}{nc_{\mathrm{W}}(\delta+c_{\mathrm{W}})}-p\left(1+\frac{1}{2^{N+1}}\right)\right)^2 m\right). \qquad (6)$$

Setting the right term in Eqn. (6) as $\delta'/2$ we can get that with probability at least $1-\delta'/2$, (needs to meet non-negative)

$$\left\|\mathrm{W}^{-1}-\widehat{\mathrm{W}}^{-1}\right\|_2 \leq \max\left(c_{\mathrm{W}}^{-2}\left(\left(\frac{1}{2}\log\left(\frac{4n^2}{\delta}\right)\right)^{\frac{1}{2}}+m^{\frac{1}{2}}p\left(1+\frac{1}{2^{N+1}}\right)\right)^{-1}-\frac{n}{\sqrt{m}}c_{\mathrm{W}}^{-1},0\right).$$

Note that this bound can meet all needed conditions. And this complete the proof.

Numerical evidence

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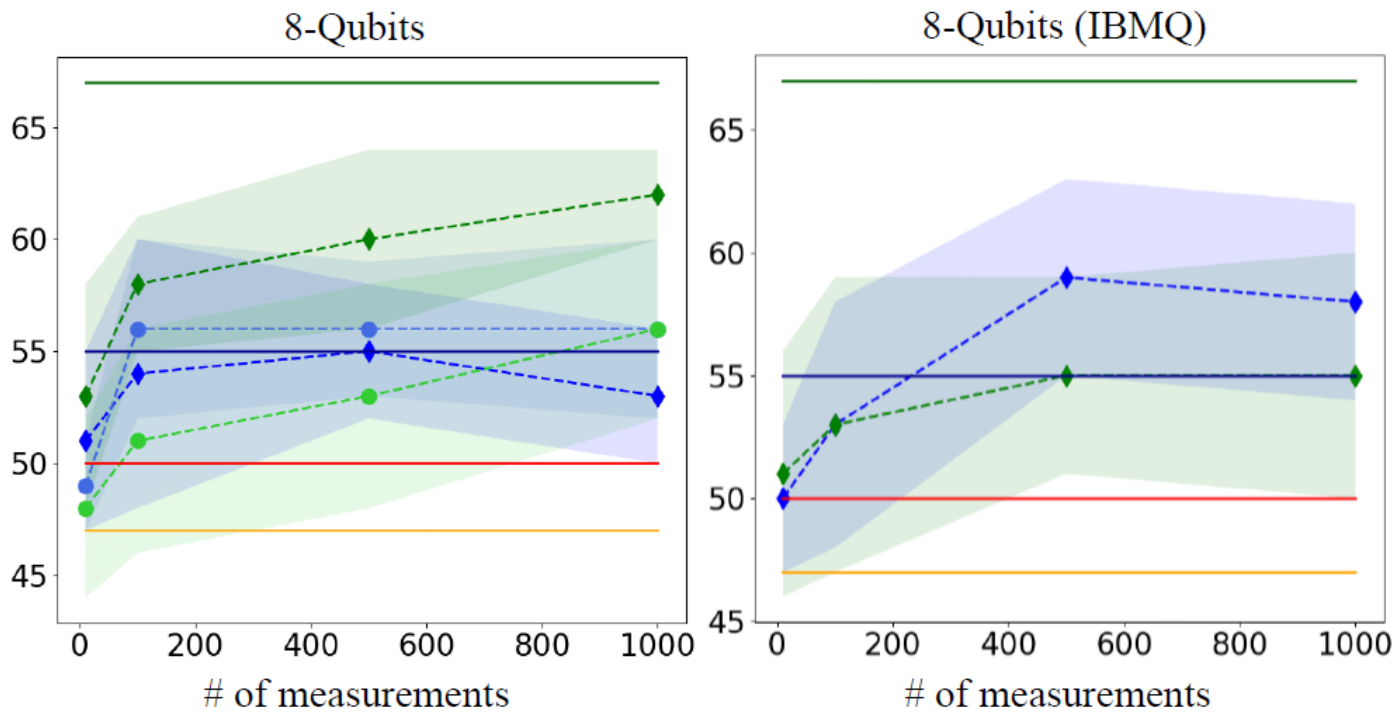
The numerical simulations conducted on the Fashion-Mnist dataset accord with our theoretical results.



Enhance Performance of Noise Quantum Kernels

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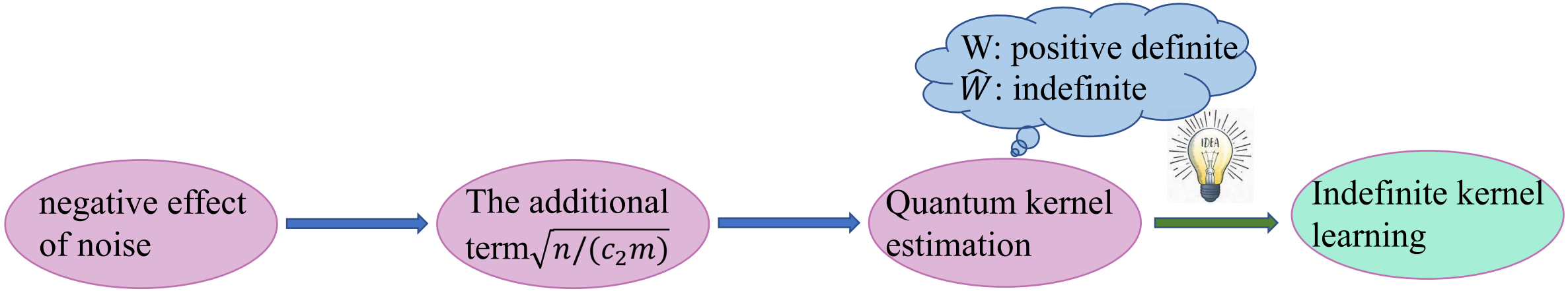
how to preserve the superiority of quantum kernels carried on NISQ machines?

- Slimming the size of training data;
- Suppressing the effects of noise (HOW?)

Tracing back the source of such negative effect can get that



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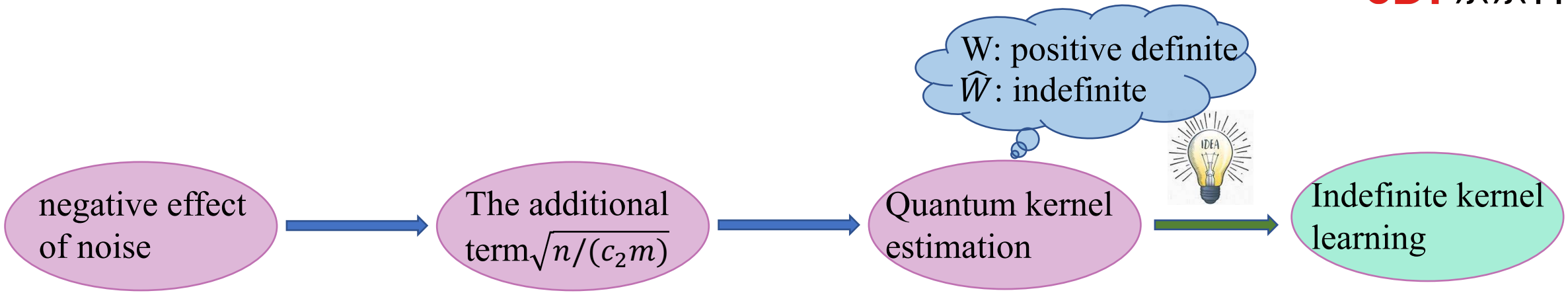

Denote the eigenvalues of $\widehat{\mathrm{W}}$ as $\widehat{\lambda}_i$ ($\widehat{\lambda}_1 \geq \cdots \geq \widehat{\lambda}_r \geq 0 \geq \cdots \geq \widehat{\lambda}_n$) and the eigenvectors as $\boldsymbol{u}_i$.

Three advanced spectral transformation techniques:

Clip: clipping all negative eigenvalues to zero, i.e., $\widehat{\mathrm{W}}_{\mathrm{c}} = \sum_{i=1}^{r} \widehat{\lambda}_i \boldsymbol{u}_i \boldsymbol{u}_i^{\top}$.

Flip: flipping the sigh of negative eigenvalues, i.e., $\widehat{\mathrm{W}}_{\mathrm{f}} = \sum_{i=1}^{r} \widehat{\lambda}_i \boldsymbol{u}_i \boldsymbol{u}_i^{\top} - \sum_{i=1}^{r} \widehat{\lambda}_i \boldsymbol{u}_i \boldsymbol{u}_i^{\top}$.

Shift: shifting all eigenvalues by a positive constant, i.e., $\widehat{\mathrm{W}}_s = \sum_{i=1}^{n} (\widehat{\lambda}_i - \widehat{\lambda}_n) \boldsymbol{u}_i \boldsymbol{u}_i^{\top}$.

Note that our goal is to shirk the distance between noiseless and noisy quantum kernels.

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Lemma 1. *Let* W *and* $\widehat{\mathrm{W}}$ *be the ideal and noisy quantum kernel, respectively. Applying the spectral transformation techniques to* $\widehat{\mathrm{W}}$*, the obtained kernel* $\widehat{\mathrm{W}}_\diamond \in \left\{\widehat{\mathrm{W}}_\mathrm{c}, \widehat{\mathrm{W}}_\mathrm{f}, \widehat{\mathrm{W}}_\mathrm{s}\right\}$ *yields*

$$\left\|\mathrm{W}-\widehat{\mathrm{W}}_\diamond\right\|_\mathrm{F} \leq \left\|\mathrm{W}-\widehat{\mathrm{W}}\right\|_\mathrm{F}, \tag{7}$$

where $\|\cdot\|_\mathrm{F}$ *refers to the Frobenius norm.*

Proof sketches: We give a brief proof for the clipping case and the other cases are similar.

Denote $\mathrm{W}=\sum_{i=1}^{n}\lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top$, where λ_i refer to the eigenvalues a$\boldsymbol{v}_i$ are the corresponding eigenvectors.

Supported by the definition of the Frobenius norm, an equivalent of achieving Eqn. (6) is

$$\mathrm{Tr}\left(\left(\mathrm{W}-\widehat{\mathrm{W}}_\mathrm{c}\right)^2\right) \leq \mathrm{Tr}\left(\left(\mathrm{W}-\widehat{\mathrm{W}}\right)^2\right) \Longleftrightarrow \mathrm{Tr}\left(\widehat{\mathrm{W}}_\mathrm{c}^2\right)-2\,\mathrm{Tr}\left(\mathrm{W}\widehat{\mathrm{W}}_\mathrm{c}\right) \leq \mathrm{Tr}\left(\widehat{\mathrm{W}}^2\right)-2\,\mathrm{Tr}\left(\mathrm{W}\widehat{\mathrm{W}}\right)$$

Considering $\mathrm{Tr}(\widehat{\mathrm{W}}^2)$, $\mathrm{Tr}(\widehat{\mathrm{W}}^2)=\sum_{i=1}^{n}\hat{\lambda}_i^2 \geq \sum_{i=1}^{r}\hat{\lambda}_i^2 = \mathrm{Tr}(\widehat{\mathrm{W}}_\mathrm{c}^2)$. (8)

Considering $\mathrm{Tr}(\mathrm{W}\,\widehat{\mathrm{W}})$,

$$\mathrm{Tr}(\mathrm{W}\,\widehat{\mathrm{W}}) = \mathrm{Tr}\left(\left(\sum_{i=1}^{n}\lambda_i\boldsymbol{v}_i\boldsymbol{v}_i^\top\right)\left(\sum_{j=1}^{r}\hat{\lambda}_j\boldsymbol{u}_j\boldsymbol{u}_j^\top+\sum_{j=r+1}^{n}\hat{\lambda}_j\boldsymbol{u}_j\boldsymbol{u}_j^\top\right)\right) = \mathrm{Tr}\left(\mathrm{W}\,\widehat{\mathrm{W}}_\mathrm{c}\right)+\sum_{i=1}^{n}\sum_{j=r+1}^{n}\lambda_i\hat{\lambda}_j\left(\boldsymbol{u}_j^\top\boldsymbol{v}_i\right)^2 \leq \mathrm{Tr}\left(\mathrm{W}\,\widehat{\mathrm{W}}_\mathrm{c}\right). \tag{9}$$

In conjunction with Eqn. (8) and (9), we can achieve Eqn (7).

The power of noisy quantum kernels

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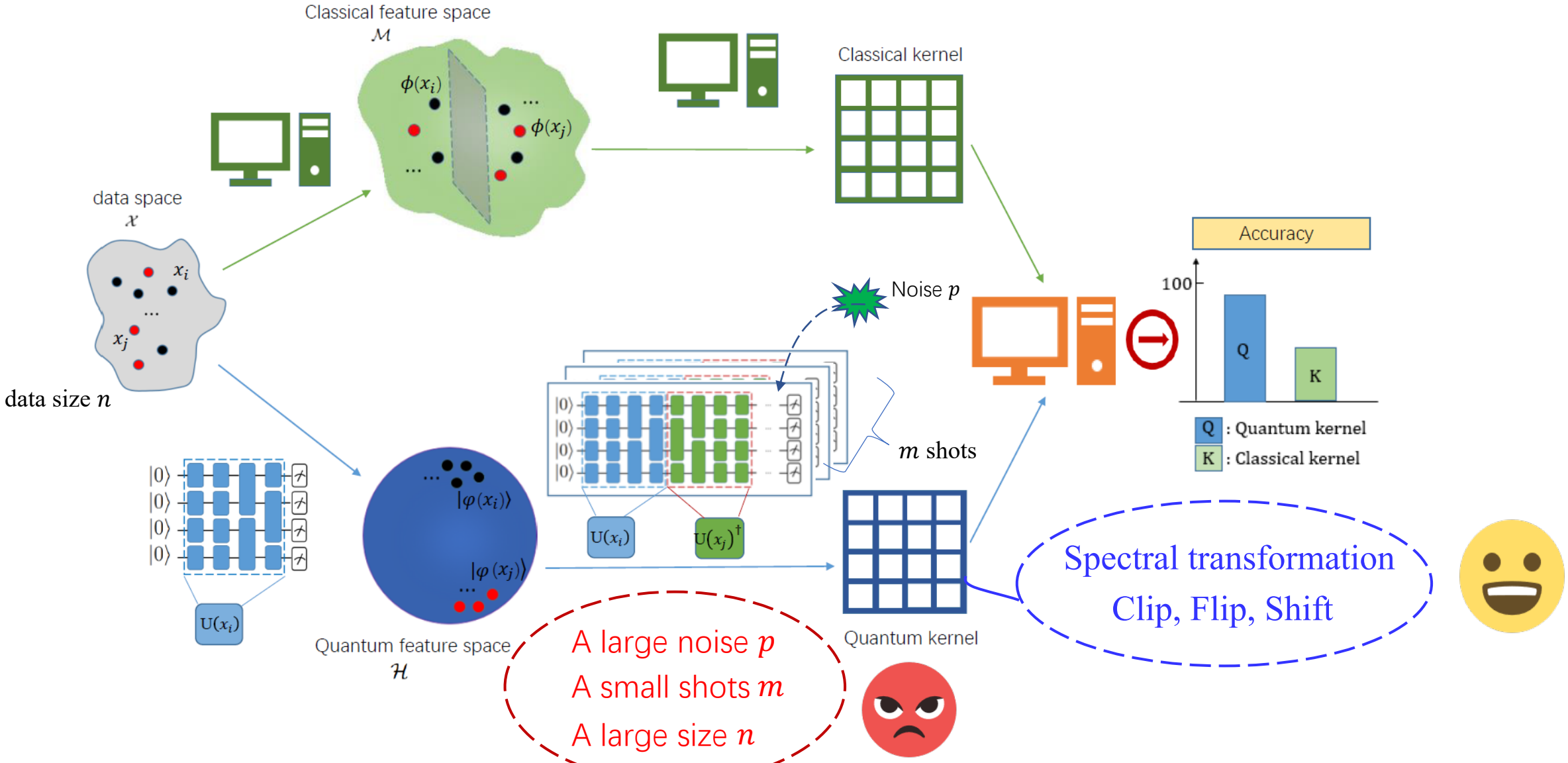

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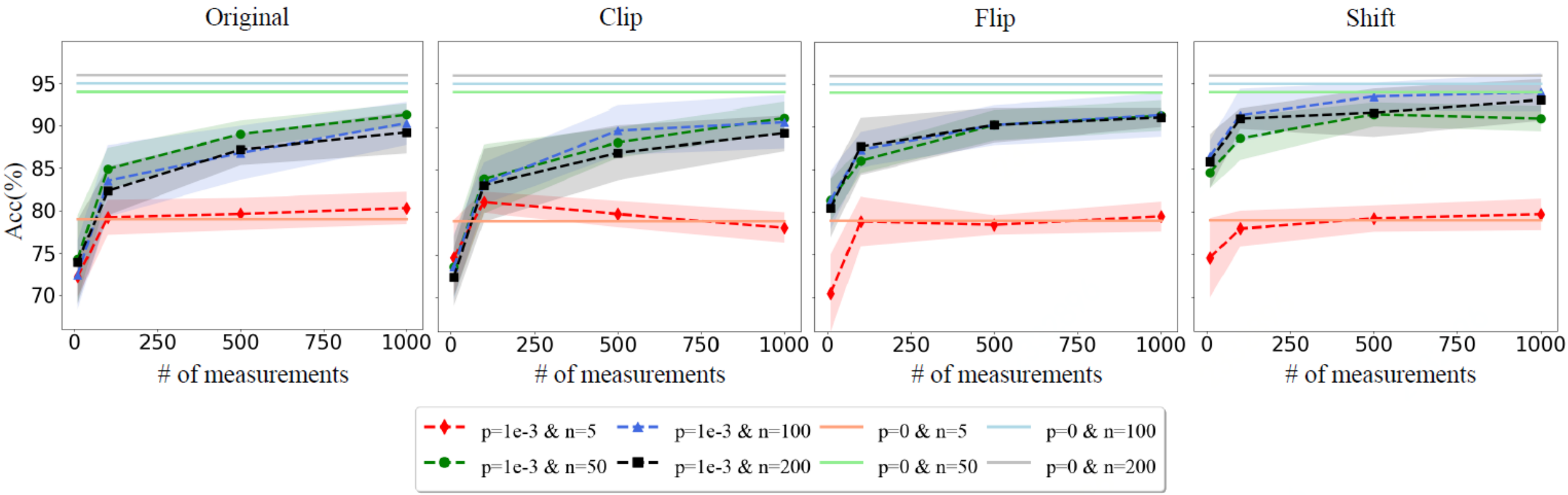
Numerical simulations achieved with the depolarization noise model



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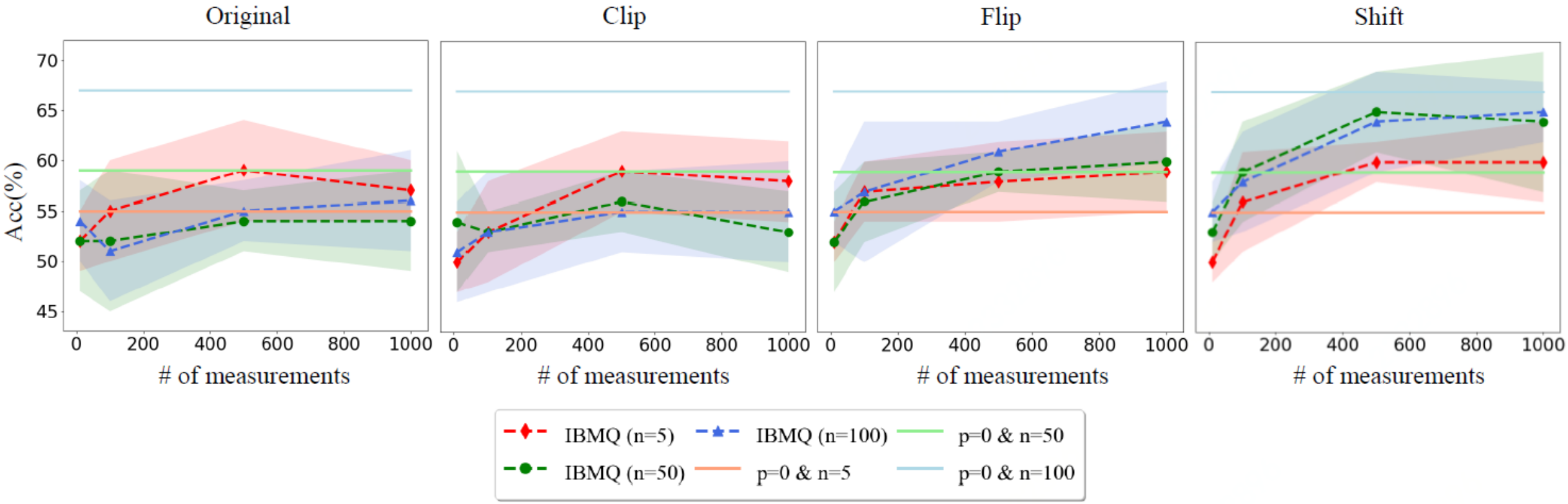
Numerical simulations achieved on IBMQ-Melbourne's noisy settings.



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Thank You!