On Convergence and Efficiency of Quantum Imaginary Time Evolution

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Variational Quantum Simulations

VQS Objective

Find a quantum state $|\psi\rangle$ that minimizes a given cost function Cost.

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Example

Let H be a Hamiltonian. Find the ground state $|\psi_{\text{gs}}\rangle$ minimizing the energy

$$\text{Cost}(|\psi\rangle) := \langle\psi| H |\psi\rangle .$$

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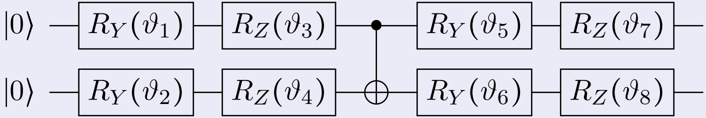
- Some of these gates are depend on a parameter ϑ_k $(1 \leq k \leq N \leq N_G)$, e.g.,



where $R_G(\vartheta_k) = \exp\left(-\frac{i}{2}\vartheta_k G\right)$ is a rotation gate.

VQS Algorithm (aka the abstract compiler)

- A *Parametric Quantum Circuit* C (for us) is the map

$$C: \text{ parameter space } \mathcal{P} \to \text{unitaries on quantum device Hilbert space } U(\mathcal{H}),$$

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- *VQS quantum part:* use quantum device to measure cost function $\mathrm{Cost}(C(\vartheta)\,|\mathrm{init}\rangle)$ at a given parameter set ϑ.
- *VQS classical part:* use classical feedback loop optimizer to solve

$$\vartheta \mapsto \mathrm{Cost}(C(\vartheta)\,|\mathrm{init}\rangle) \to \min .$$

common compilation obstacles

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Quantum Imaginary Time Evolution

- convergence guarantees
- efficient compilation for bounded order systems

Convergence

- consider Hamiltonian H with eigenvalues $\lambda_0 = \ldots = \lambda_{\mu-1} < \lambda_\mu \leq \ldots \leq \lambda_N$ and corresponding eigenbasis $|\psi_0\rangle, \ldots, |\psi_N\rangle$ with $N = 2^Q - 1$ for a Q-qubit system

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- aim to implement

$$|\psi(t)\rangle = \frac{e^{-tH}|\psi(0)\rangle}{\|e^{-tH}|\psi(0)\rangle\|_2}$$

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- for $|\psi(t)\rangle = \sum_{j=0}^{N} \alpha_j(t)|\psi_j\rangle$ and assuming[1] $\exists j < \mu : \alpha_j(0) \neq 0$:

$$\alpha_j(t) = \frac{\alpha_j(0)}{\sqrt{\sum_{k=0}^{N} |\alpha_k(0)|^2 e^{-2t(\lambda_k - \lambda_j)}}} \to \begin{cases} \frac{\alpha_j(0)}{\sqrt{\sum_{k=0}^{\mu-1} |\alpha_k(0)|^2}} & , \ j < \mu, \\ 0 & , \ j \geq \mu. \end{cases}$$

[1] This is true with probability 1 assuming non-zero hardware noise.

Absence of critical slowing down

- let $\mathrm{pr}_{T_{|\psi(t)\rangle}\partial B_{\mathcal{H}}(0,1)}$ be the orthoprojector onto the tangent space of the unit sphere $\partial B_{\mathcal{H}}(0,1)$ at the state $|\psi(t)\rangle$, then

$$\frac{d}{dt}|\psi(t)\rangle = \langle\psi(t)|H|\psi(t)\rangle|\psi(t)\rangle - H|\psi(t)\rangle = -\mathrm{pr}_{T_{|\psi(t)\rangle}\partial B_{\mathcal{H}}(0,1)} H|\psi(t)\rangle$$

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- hence with $E(t) := \langle\psi(t)| H |\psi(t)\rangle$: $E'(t) = -2\left\|\mathrm{pr}_{T_{|\psi(t)\rangle}\partial B(0,1)} H |\psi(t)\rangle\right\|_2^2 \leq 0$

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- critical slowing down requires $E'(t) \approx 0$, but then $|\psi(t)\rangle \approx$ eigenstate of H, and by monotonicity of $\alpha_j(t)$ this can only happen if the evolution is (almost) converged

Rate of convergence

- let $\Delta := \lambda_\mu - \lambda_0$ be the energy gap, then for $t \gg 0$

$$\left\| |\psi(t)\rangle - \lim_{\tau\to\infty} |\psi(\tau)\rangle \right\|_2^2 \leq \frac{e^{-2t\Delta}}{\left(\sum_{j=0}^{\mu-1} |\alpha_j(0)|^2\right)^3} |1 + \mathcal{O}(e^{-2t\Delta})|^2$$

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- if $f(0) \propto 2^{-Q}$ can be achieved, then critical evolution time $t_f \in \mathcal{O}(Q/\Delta)$

Combinatorial optimization

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- $p(t) \geq \varepsilon$ guaranteed for

$$t \geq \frac{Q\ln 2 - \ln\mu + \ln\varepsilon - \ln(1-\varepsilon)}{2\Delta} \in \mathcal{O}(Q/\Delta)$$

Bounded order systems

- express H as Pauli sum $\sum_j a_j S_j$ with $a_j \in \mathbb{R}$ and S_j tensor product of single-qubit Paulis (X, Y, Z, I)
- Hamiltonian of order B: each S_j has at most B non-trivial factors
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  - realistic combinatorial optimization: many real-world problems have super-polynomial order scaling ✓/✗
  - factoring: order 4 but doesn't have polynomial coefficient scaling ✗

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Trotterization

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- Trotterize with time-step δ

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Compilation Task

Find circuits $C_{j,\tau}(\vartheta_{j,\tau})$ that act like the corresponding $e^{-\delta a_j S_j}$ including normalization.

$$|\psi(t)\rangle = \frac{e^{-tH}|\psi(0)\rangle}{\|e^{-tH}|\psi(0)\rangle\|_2} = \frac{\prod_{\tau=1}^{t/\delta}\prod_j e^{-\delta a_j S_j}|\psi(0)\rangle}{\|e^{-tH}|\psi(0)\rangle\|_2} = \prod_{\tau=1}^{t/\delta}\prod_j C_{j,\tau}(\vartheta_{j,\tau})|\psi(0)\rangle$$

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- minimum viable stepsize δ guaranteed by a determinant being non-zero $\Rightarrow$ polynomial scaling in B
- total compilation time polynomial in Q/Δ and acceptible noise ε
  - $\mathcal{O}(\mathrm{poly}(Q/\Delta))$ time-steps with individual compilation cost $\mathcal{O}(Q^B \varepsilon^{-2})$

What have we got? [arXiv:2506.03014]

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What do we need?

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Future ideas?

- approximate imaginary time evolution for some “bad” systems
- any other conditions on systems that allow us to conclude whether they can or cannot be solved efficiently