Error analysis in Quantum Krylov algorithms

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Motivation and outline

Goal: estimate ground state energy of quantum Hamiltonian.

Classically challenging due to exponential Hilbert space dimension*.

Outline of this talk:

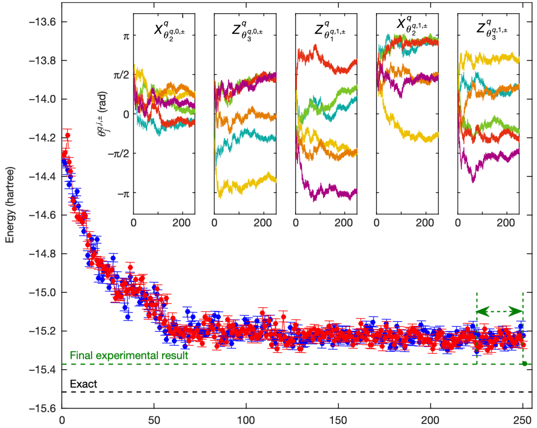
1. Overview of quantum Krylov algorithm

2. Overview of error bound results

*Assuming general, hard case: sufficiently entangled, supported on exponentially-many basis states, etc.

Example applications:

- Condensed matter physics
- Nuclear physics
- High-energy physics
- Quantum chemistry



A. Kandala *et al.*, Nature 549, 242 (2017).

Lanczos/Arnoldi method

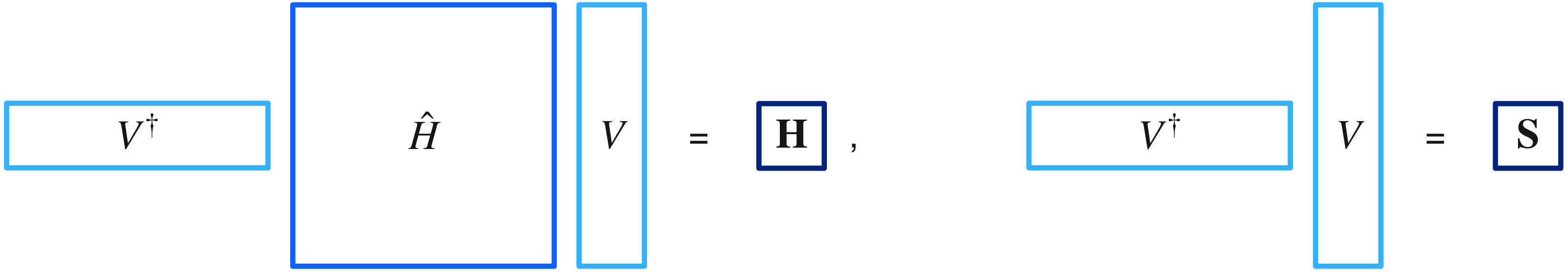
= classical method for approximating lowest eigenvalues.

(Very) high-level idea:

Krylov space

1. Initial guess $|\psi_0\rangle \quad \Rightarrow \quad \hat{H}|\psi_0\rangle \quad \Rightarrow \cdots \Rightarrow \quad \hat{H}^{D-1}|\psi_0\rangle$

2. $(\mathbf{H}, \mathbf{S})$ = project H onto span$\underbrace{[|\psi_0\rangle, \hat{H}|\psi_0\rangle, \hat{H}^2|\psi_0\rangle, \ldots, \hat{H}^{D-1}|\psi_0\rangle]}_{V}$



3. Lowest eigenvalue of $(\mathbf{H}, \mathbf{S})$ i.e., of $\mathbf{H}\mathbf{v} = \lambda \mathbf{S}\mathbf{v}$, approximates lowest eigenvalue of $\hat{H}$

Lanczos/Arnoldi method

Advantage: converges exponentially with D (in ∞ precision arithmetic).

Disadvantage: classically, requires storing entire statevectors $\hat{H}^i|\psi_0\rangle$ ⇒ exponential overhead.

Can we construct a quantum version that mitigates statevector overhead while keeping fast convergence?[1]

Recent review! ↓

[1] Parrish and McMahon, https://arxiv.org/abs/1909.08925; Motta *et al.*, https://arxiv.org/abs/2312.00178; and many more!

Quantum “Lanczos method” = “Quantum Krylov”

Options for generating Krylov space: multiply $|\psi_0\rangle$ by…

- Powers of $\hat{H}$ — same as original Lanczos ⇒ nontrivial on quantum but possible in principle.[1]
- $e^{-\hat{H}k\,dt}$ — this version claimed “Qlanczos.”[2]
- $T_k(\hat{H})$ — arises naturally from block encoding.[3]
- $e^{i\hat{H}k\,dt}$ — many good options e.g. Trotterization, qubitization, etc.

Will focus on last version in this talk.

[1]Seki and Yunoki, PRX Quantum 2, 010333 (2021); [2]Motta *et al.*, Nat. Phys. 16, 205–210 (2020); [3]Kirby *et al.*, Quantum 7, 1018 (2023).

Quantum Krylov with real time-evolutions

Majority of works have focused on Krylov states generated by real time-evolution:

$$V = [\,|\psi_0\rangle, \quad \hat{U}\,|\psi_0\rangle, \quad \hat{U}^2\,|\psi_0\rangle, \ldots, \hat{U}^{D-1}\,|\psi_0\rangle] \text{ for } \hat{U} = e^{i\hat{H}\,dt}$$

Need to estimate on quantum computer

$$\mathbf{H_{jk}} = \langle\psi_0\,|\,(\hat{U}^j)^\dagger \hat{H}\hat{U}^k\,|\,\psi_0\rangle,$$

$$\mathbf{S_{jk}} = \langle\psi_0\,|\,(\hat{U}^j)^\dagger \hat{U}^k\,|\,\psi_0\rangle$$

for each $j, k = 0,1,...,D-1,$

then classically calculate lowest eigenvalue of $\mathbf{Hv} = \lambda\mathbf{Sv} \quad \Rightarrow$ output.

Real-time quantum Krylov with errors

$$\text{Ideal } (\mathbf{H}, \mathbf{S}) \xrightarrow{\text{errors}} (\mathbf{H}', \mathbf{S}')$$

Worry #1: ill-conditioning.

- $\mathbf{S}$ has exponentially-growing condition number with D
- $\Rightarrow$ $\mathbf{S}'$ may not even be positive semidefinite.

Resolution: regularization.[1]

- Project $(\mathbf{H}', \mathbf{S}')$ onto eigenspaces of $\mathbf{S}'$ with eigenvalues above threshold $\epsilon > 0$.
- Epperly *et al.* showed this step introduces energy error linear in ϵ.

- Epperly *et al.* also bounded total error in lowest energy estimate in presence of noise η…
- **Goal:** but bound is sublinear in η. Can we improve to linear?

[1] Epperly, Lin, Nakatsukasa, SIMAX 43(3), 1263-1290 (2022).

Real-time quantum Krylov with errors

$$\text{Ideal } (\mathbf{H}, \mathbf{S}) \xrightarrow{\text{errors}} (\mathbf{H}', \mathbf{S}')$$

Inspiration: common "folklore" claim in quantum computing community…

"The reason quantum Krylov algorithms are robust to errors is that the errors just perturb the subspace, and then you still find the lowest energy in the subspace."

In other words, for $\mathbf{H} = \mathbf{V}^\dagger \hat{H} \mathbf{V}$, $\mathbf{S} = \mathbf{V}^\dagger \mathbf{V}$, errors cause $\mathbf{V} \to \mathbf{V}'$.

<u>This is not true in general!</u>

We show that

- generic error-ful $(\mathbf{H}', \mathbf{S}')$ after regularization can be expressed as $(\mathbf{V}'^\dagger \hat{H}' \mathbf{V}', \mathbf{V}'^\dagger \mathbf{V}')$, such that
    1. we can bound $||\hat{H}' - \hat{H}||$ in terms of the error rate
    2. span $\mathbf{V}'$ contains a perturbed approximate ground state of $\hat{H}$

Main ideas for lower bound

Idea #1: work with regularized pair $(\mathbf{H}'', \mathbf{S}'') = (\Pi' \mathbf{H}' \Pi', \Pi' \mathbf{S}' \Pi')$

- $\Pi' =$ projector onto eigenspaces of $\mathbf{S}'$ with eigenvalues above $\epsilon > 0$
- $(\mathbf{H}'', \mathbf{S}'') =$ matrix pair we actually solve to get approximate energies (removing the "projected out" dim'ns)

Main ideas for lower bound

Idea #2: choose a convenient $\mathbf{V}'$ such that $\mathbf{V}'^{\dagger}\mathbf{V}' = \mathbf{S}''$

- Let $\mathbf{V} = F\sqrt{\mathbf{S}}$ be polar decomposition of $\mathbf{V}$, so F is $2^n \times D$ with orthonormal columns
- Let $\mathbf{V}' = FG\sqrt{\mathbf{S}''}$, with G any $D \times D$ unitary $\Rightarrow \mathbf{V}'^{\dagger}\mathbf{V}' = \sqrt{\mathbf{S}''}G^{\dagger}F^{\dagger}FG\sqrt{\mathbf{S}''} = \mathbf{S}''$

Main ideas for lower bound

Idea #3: choose $\hat{H}'$ such that $\mathbf{V}'^{\dagger}\hat{H}'\mathbf{V}' = \mathbf{H}''$, and $\hat{H}' = \hat{H}$ everywhere else (outside span$(\mathbf{V}')$)

- Corresponding expression: $\hat{H}' = \hat{H} + \mathbf{V}'\mathbf{S}''^{+}\left(\mathbf{H}' - \mathbf{V}'^{\dagger}\hat{H}\mathbf{V}'\right)\mathbf{S}''^{+}\mathbf{V}'^{\dagger}$
- Use freedom in G to minimize $||\hat{H}' - \hat{H}||$
- Good choice turns out to be such that $G\sqrt{\Pi'\mathbf{S}\Pi'}$ = polar decomp of $\sqrt{\mathbf{S}}\Pi'$

Aside for anyone actually trying to follow the above: $\mathbf{S}''^{+}\mathbf{V}'^{\dagger} \cdot \mathbf{V}' = \mathbf{S}''^{+}\mathbf{S}'' = \Pi'$ and $\Pi'\mathbf{H}'\Pi' = \mathbf{H}''$

Main ideas for lower bound

Proof of lower bound proceeds from

$$\|\hat{H}' - \hat{H}\| = \|\mathbf{V}'\mathbf{S}''^{+}\left(\mathbf{H}' - \mathbf{V}'^{\dagger}\hat{H}\mathbf{V}'\right)\mathbf{S}''^{+}\mathbf{V}'^{\dagger}\| = \|\sqrt{\mathbf{S}''^{+}}\left(\mathbf{H}' - \mathbf{V}'^{\dagger}\hat{H}\mathbf{V}'\right)\sqrt{\mathbf{S}''^{+}}\|$$

$$\leq \|\sqrt{\mathbf{S}''^{+}}\left(\mathbf{H}' - \mathbf{H}\right)\sqrt{\mathbf{S}''^{+}}\| + \|\sqrt{\mathbf{S}''^{+}}\mathbf{V}^{\dagger}\hat{H}\left(\mathbf{V} - \mathbf{V}'\right)\sqrt{\mathbf{S}''^{+}}\| + \|\sqrt{\mathbf{S}''^{+}}\left(\mathbf{V}^{\dagger} - \mathbf{V}'^{\dagger}\right)\hat{H}\mathbf{V}'\sqrt{\mathbf{S}''^{+}}\|$$

Bounding each term yields

$$\|\hat{H}' - \hat{H}\| \leq \frac{\|\mathbf{H}' - \mathbf{H}\| + (\sqrt{2} + 1)\|\mathbf{S}' - \mathbf{S}\|\,\|\hat{H}\|}{\epsilon}$$

Choice of “free” unitary G only matters in second term.

Main ideas for lower bound

$$\|\hat{H}' - \hat{H}\| \leq \frac{\|\mathbf{H}' - \mathbf{H}\| + (\sqrt{2}+1)\|\mathbf{S}' - \mathbf{S}\|\,\|\hat{H}\|}{\epsilon}$$

- Weyl's theorem ⇒ above upper bounds difference between lowest eigenvalues E_0' and E_0 of $\hat{H}'$ and $\hat{H}$
- Rayleigh-Ritz ⇒ E_0' lower bounds lowest eigenvalue of $(\mathbf{H}'', \mathbf{S}'') = (\mathbf{V}'^{\dagger}\hat{H}'\mathbf{V}', \mathbf{V}'^{\dagger}\mathbf{V}')$
- Combine: $-\|\hat{H}' - \hat{H}\|$ lower bounds ground state energy error of noisy, regularized matrix pair $(\mathbf{H}'', \mathbf{S}'')$ with respect to E_0, which we are trying to estimate

Upper bound rough ideas

Similar scheme to lower bound:

- work with $(\mathbf{H}'', \mathbf{S}'')$
- Now will use particular point c' in Krylov space to upper bound lowest energy:
  - so, choose convenient $\mathbf{V}', \hat{H}'$ such that $c'^{\dagger}\mathbf{V}'^{\dagger}\mathbf{V}'c' = c'^{\dagger}\mathbf{S}''c', \; c'^{\dagger}\mathbf{V}'^{\dagger}\hat{H}'\mathbf{V}'c' = c'^{\dagger}\mathbf{H}''c'$
- Prove bound on $\|\hat{H}' - \hat{H}\|$ and also show that $\mathbf{V}'c'$ is an approximate ground state
  - Use similar method to Epperly, Lin, and Nakatsukasa (2022).
- Result:

$$E_0' - E_0 \;\leq \frac{12\|\hat{H}\|}{|\gamma_0'|^2}\left[\left(D + \frac{\|\hat{H}\|}{\Delta'} + \frac{1}{12}\right)\eta + D\epsilon + 4\left(1 + \frac{\pi\Delta'}{4\|\hat{H}\|}\right)^{-2D}\right]$$

for $\eta = \max\left(\|\mathbf{S}' - \mathbf{S}\|, \dfrac{\|\mathbf{H}' - \mathbf{H}\|}{\|\hat{H}\|}\right)$, $\gamma_0' \approx$ ampl. of ground state in init state, $\Delta' \approx$ spectral gap

Final thoughts

- You *can* think of errors in quantum Krylov as perturbing the Krylov space, as long as you let them perturb the Hamiltonian as well!
- You can use this to get lower and upper bounds that both look linear in η…
- BUT lower bound is $O\left(\frac{\eta}{\epsilon}\right)$ and upper bound is $O\left(\eta + \epsilon\right)$.
    - Quantifies idea that threshold is trading off between upper and lower bounds.
- In practice $\epsilon = O(\eta)$ is often found to yield good convergence, leading to open questions:
    - How generally true is that?
    - Is there a tighter lower bound? (Since mine is $O(1)$ in that case!)

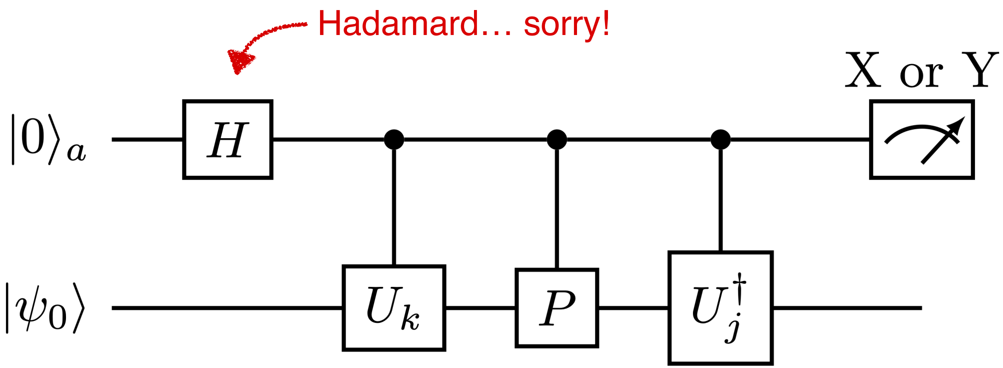
Thank you! Questions?

https://arxiv.org/abs/2401.01246

Extra: estimating matrix elements (simple version)

Targets: $\mathbf{H_{jk}} = \langle\psi_0|(\hat{U}^j)^\dagger \hat{H}\hat{U}^k|\psi_0\rangle, \quad \mathbf{S_{jk}} = \langle\psi_0|(\hat{U}^j)^\dagger \hat{U}^k|\psi_0\rangle$.

Can approach using Hadamard test:



Yields $\langle X\rangle_a = Re\left[\langle\psi_0|(U^j)^\dagger P U^k|\psi_0\rangle\right], \quad \langle Y\rangle_a = Im\left[\langle\psi_0|(U^j)^\dagger P U^k|\psi_0\rangle\right]$