Lanczos Algorithm for Qiskit Dynamics

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$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$

Qiskit

Why Lanczos

Qiskit

- Local Hamiltonians describing qubit systems are sparse

$$H = \begin{pmatrix} 0 & 0 & \alpha & \beta \\ 0 & d_0 & 0 & 0 \\ \alpha^* & 0 & 0 & 0 \\ \beta^* & 0 & 0 & d_1 \end{pmatrix}$$

- Calculating time evolution requires exponentiating the Hamiltonian

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

- This can be done by diagonalizing H

$$e^{-iHt} = S^\dagger e^{-iDt} S$$

Why Lanczos

- Time evolution requires only sparse matrix – vector multiplication

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

$$= \sum_n \frac{(-it)^n}{n!} H^n |\psi_0\rangle$$

$$= \sum_n \frac{(-it)^n}{n!} |u_n\rangle$$

- $|u_0\rangle = |\psi\rangle \quad |u_1\rangle = H|u_0\rangle \quad |u_2\rangle = H|u_1\rangle \ \ldots.$

Why Lanczos (Krylov Subspace)

- $K_r = \{|\psi\rangle,\ A|\psi\rangle, A^2|\psi\rangle, A^3|\psi\rangle \ldots A^k|\psi\rangle\}$ Is the krylov subspace for a given matrix A and vector $|\psi\rangle$ of order k
- One can construct a basis $\{|\phi_i\rangle\}$ for this subspace using Gram-Schmidt

$$\left|\widetilde{\phi}_{k-1}\right\rangle = |u_{k-1}\rangle - \sum_i \langle\phi_i|u_{k-1}\rangle\,|\phi_i\rangle$$

$$|\phi_{k-1}\rangle = \frac{\left|\widetilde{\phi}_{k-1}\right\rangle}{\left\langle\widetilde{\phi}_{k-1}\middle|\widetilde{\phi}_{k-1}\right\rangle}$$

Why Lanczos (Krylov Subspace)

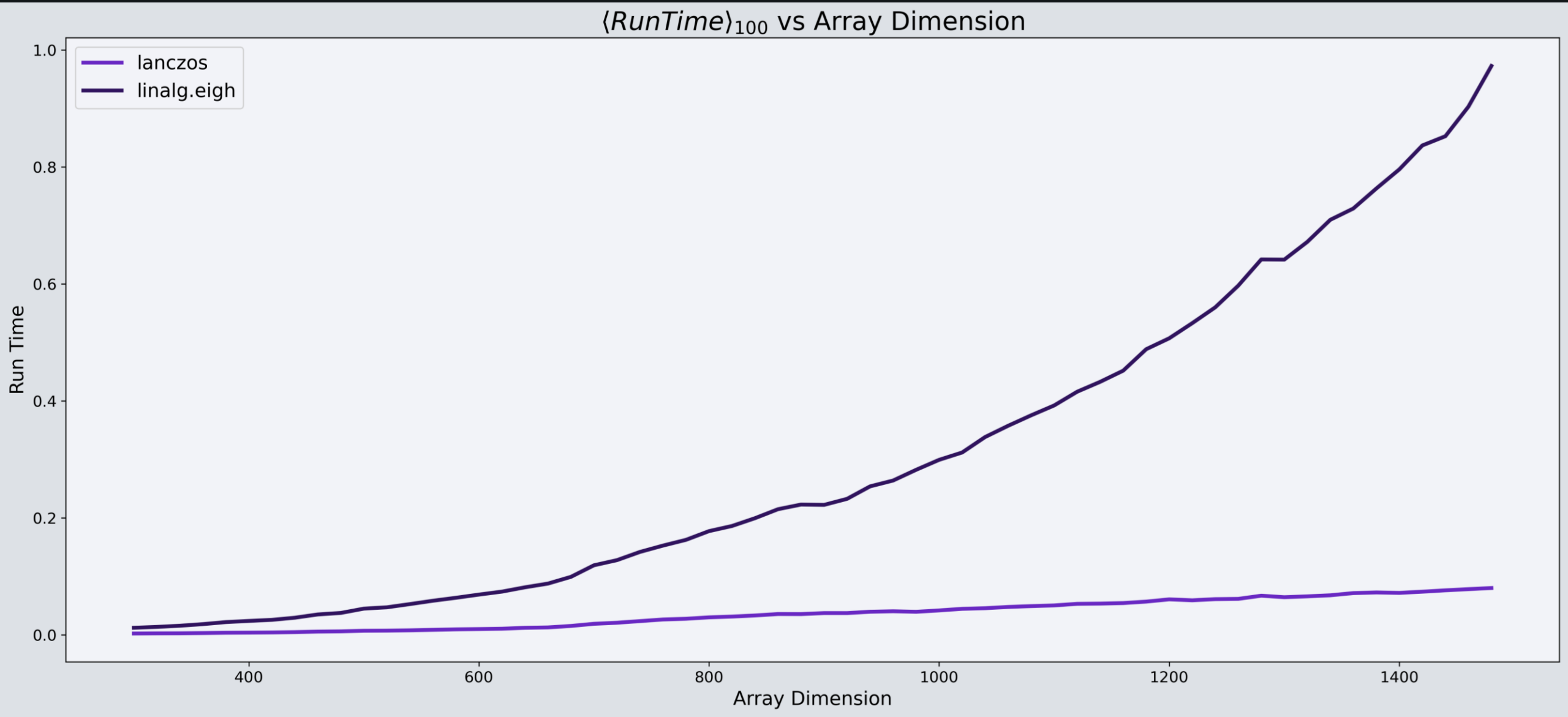
- One can construct an orthogonal matrix $Q_{n,k}$ With $|\phi_i\rangle$ as the columns such that

$$T_{k,k} = Q_{k,n}^{\dagger} H_n Q_{n,k}$$

- Where T is a Tridiagonal matrix
- $\therefore e^{-Ht} = e^{-iQTQ^{\dagger}t} = Qe^{-iTt}Q^{\dagger} = QVe^{-i\mathbf{diag}(T)t}V^{\dagger}Q^{\dagger}$
- Diagonalizing a Tridiagonal matrix is a lot faster since typically, $k \ll n$

Lanczos vs NumPy

(ground state calculation)



Thank You

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GitHub: github.com/rupeshknn/lanczos-QD