Simulation of Quantum Systems with Time-Evolving Block Decimation

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/final_project

Quantum Information and Computing
AA 2022–23

James Chryssanthacopoulos
with collaboration with David Lange
8 April 2023

Università degli Studi di Padova

Outline

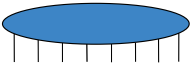
- To study a quantum system, one has to solve Schrodinger equation

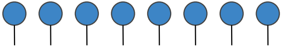
$$\hat{H}\left|\Psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle$$

- One solution involves direct numerical integration, where initial state is updated using time evolution operator

$$\left|\Psi(t+\Delta t)\right\rangle = e^{-i\hat{H}\Delta t}\left|\Psi(t)\right\rangle$$

- This requires solving system of equations at each time step that scales with system size, but in many-body problems, system size is **exponential** in number of sites, N
- In tensor network notation, general N-body system is shown on left. Mean-field ansatz on right greatly simplifies computation, but it ignores entanglement

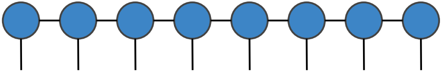




How does one **preserve entanglement** while remaining **computationally tractable**?

Matrix Product States

- Matrix product states generalize mean-field ansatz to allow for entanglement between sites. Graphically



where bond between states has fixed **bond dimension** χ

- Wavefunction is given by

$$|\Psi\rangle = A_1^{\mu_1} A_{\mu_1,2}^{\mu_2} \cdots A_{\mu_{N-2},N-1}^{\mu_{N-1}} A_{\mu_{N-1},N} |1\,2 \cdots N\rangle$$

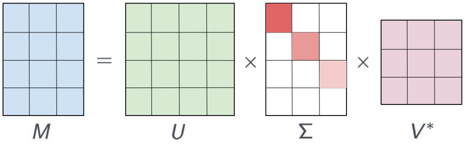
where $A_{\mu_{i-1},i}^{\mu_i}$ tensors have physical dimension $i \in \{1, \dots, N\}$ and **auxiliary dimension** $\mu_i \in \{1, \dots, \chi\}$

- Number of states scales like $Nd\chi^2$, which is **polynomial** in N

How does one evolve MPS in time without **breaking structure**?

Factoring Quantum State into MPS

- An arbitrary quantum state can be factored as an MPS using matrix factorization technique called **singular value decomposition**
- SVD generalizes eigendecomposition to any $m \times n$ matrix. It finds two orthonormal bases and singular values such that matrix is factorized into $M = U\Sigma V^*$, where U, V are unitary matrices



- SVD is driver behind simulating quantum systems with MPS's, allowing MPS structure to be preserved at each iteration

Time-Evolving Block Decimation

- Method for evolving quantum system while efficiently truncating exponentially-large Hilbert space

Suzuki-Trotter Decomposition

MatrixProductState class

Ground State Energy