Low Rank Approximation in Simulations of Quantum Algorithms

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Background

General quantum algorithms are hard to simulate

- Algorithm expressed by a unitary transformation of a quantum state $U|\psi\rangle$
- n qubits state described by 2^n complex numbers: $|\psi\rangle \in \mathbb{C}^{2^n}$
- Direct representation $\Longrightarrow$ Exponential cost (not scalable)

Input/output state and U tend to have low-rank structures

- Input state: usually are rank-1, e.g. $|0\rangle^n, |+\rangle^n$
- Output state: amplitude amplification feature $\Longrightarrow$ few elements with large amplitudes
- $U = U^{(1)}U^{(2)}\cdots U^{(D)}$, each $U^{(i)}$ is a 1-qubit/2-qubit gate

Low rank representation of quantum states

- Tensor network representation $\Longrightarrow$ model quantum many-body systems
- **This work**: canonical polyadic (CP) decomposition representation

Our Contributions

Introduce low-rank CP decomposition for the simulation of quantum algorithms

- Simple, fast, easy to program
- Convenient for quantum entanglement analysis

	Computational cost	Memory cost	Fidelity
QFT w/ standard basis input	$\mathcal{O}(n^2)$	$\mathcal{O}(n)$	1.0
Phase estimation	$\mathcal{O}(n^3/\epsilon^2 + n^2/\epsilon^3)$	$\mathcal{O}(n/\epsilon + 1/\epsilon^2)$	$> 1 - \epsilon$
Grover's Algorithm	$\mathcal{O}(a^3 n)$	$\mathcal{O}(a^2 n)$	1.0
Quantum walk w/ complete graph with loops	$\mathcal{O}(n)$	$\mathcal{O}(n)$	1.0
Quantum walk w/ complete bipartite graph	$\mathcal{O}(n)$	$\mathcal{O}(n)$	1.0
General algorithms with depth D and rank s	$\mathcal{O}(Ds^2n^2 + Ds^3n)$	$\mathcal{O}(sn + s^2)$	/

CP Representation for Quantum Circuits

Represent each state and gate as sum of Kronecker products

$$|\psi\rangle = \sum_{j=1}^{R} a_j^{(1)} \otimes a_j^{(2)} \cdots \otimes a_j^{(n)}, \quad U = \sum_{j=1}^{R} V_j^{(1)} \otimes V_j^{(2)} \cdots \otimes V_j^{(n)}, \quad \text{R is the CP rank}$$

- When U is a 1-qubit gate, $R = 1$, when U is a 2-qubit gate, $R = 2$

$$\text{Controlled-U} : \begin{bmatrix} I & O \\ O & U \end{bmatrix} = E_1 \otimes I + E_2 \otimes U, \quad \text{where} \quad E_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, E_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

- Applying 1-qubit gate won't affect the CP rank of the state
- Applying 2-qubit gate will at most double the CP rank the state

$$\text{example} : (E_1 \otimes I + E_2 \otimes U)(a_1 \otimes a_2) = E_1 a_1 \otimes a_2 + E_2 a_1 \otimes U a_2$$

Simulation Algorithm with Low-rank Approximation

Simulation with low-rank approximation

Input: Input state $|\psi\rangle$, gates $U = U^{(1)}U^{(2)}\dots U^{(D)}$, maximum CP rank allowed $r_{\max}$
Output: Approximation to $U|\psi\rangle$
For $k \in \{1, 2, ..., D\}$ **do**
  Compute $|\phi\rangle = U^{(k)}|\psi\rangle$
  If the rank of $|\phi\rangle$ exceeds $r_{\max}$ **then**
    $|\phi\rangle \leftarrow$ **Rank-reduction**$(|\phi\rangle, r_{\max})$
  Endif
  $|\psi\rangle \leftarrow |\phi\rangle$;
Endfor
Return $|\phi\rangle$

- Accuracy of rank reduction is dependent on the algorithm
- Two rank reduction techniques:
  - Alternating least squares (ALS)
  - Direct elimination of scalar multiples

Rank Reduction Techniques

Alternating least squares (ALS)

Solving a sequence of linear least squares sub-problems in each iteration:

$$\min_{a_1^{(1)},\ldots,a_R^{(1)}} \left\| |\psi\rangle - \sum_{j=1}^{R} a_j^{(1)} \otimes a_j^{(2)} \cdots \otimes a_j^{(n)} \right\|_F^2$$

- $|\psi\rangle$ represented in CP format with rank $s > R$
- Costs $\mathcal{O}(t(Rsn^2 + R^3 n))$ with t iterations
- ALS **doesn't guarantee** best low-rank approximation

Direct elimination of scalar multiples

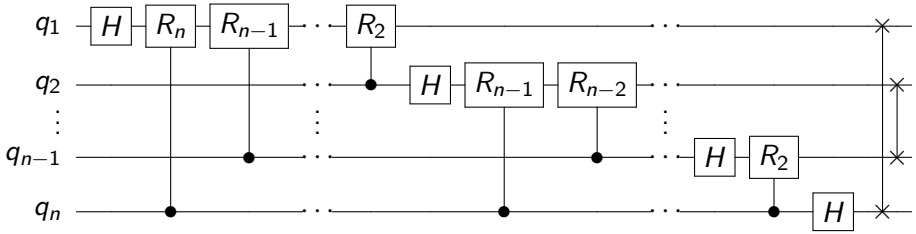
$$|\psi\rangle = \sum_{j=1}^{s} \alpha_j |\psi_j\rangle$$

- Each $|\psi_j\rangle$ is a rank-1 tensor
- Directly check whether two rank-1 tensors are in the same direction

$$\cos(\theta_{p,q}) = \frac{\langle\psi_p|\psi_q\rangle}{\|\psi_p\| \cdot \|\psi_q\|}$$

- If $|\cos(\theta_{p,q})| = 1.0$, just combine them
- Efficient for Grover's algorithm and some quantum walks

Quantum Fourier Transform



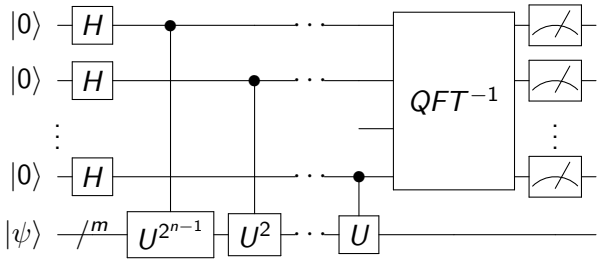
All the intermediate states are rank 1 if the input is a standard basis (e.g. $|0\rangle^n$, $|1\rangle^n$)

- Input factor to each controlling qubit is always either $|0\rangle$ or $|1\rangle$
- example: $(E_1 \otimes I + E_2 \otimes R_n)(|1\rangle \otimes |\alpha\rangle) = |1\rangle \otimes R\,|\alpha\rangle$
- When the input is the linear combination of s standard basis, all the intermediate states are rank s

Circuit with general rank-1 inputs cannot be low-rank approximated

Phase Estimation

Estimate θ where $U|\psi\rangle = e^{i2\pi\theta}|\psi\rangle$



When $|\psi\rangle$ is the eigenvector of U:

- all the intermediate states on the first register before the QFT^{-1} operator can be represented by a rank-1 state
- all the intermediate states in the QFT^{-1} operator can be approximated by rank-$R = \mathcal{O}(1/\epsilon)$ states, and the fidelity is at least $(1-\epsilon)$

Input to QFT^{-1}: $\frac{1}{2^{n/2}}\left(|0\rangle + e^{i2\pi 2^{n-1}\theta}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + e^{i2\pi 2^{1}\theta}|1\rangle\right) \otimes \left(|0\rangle + e^{i2\pi 2^{0}\theta}|1\rangle\right)$

Grover's Algorithm

Search one marked item

- Goal is to find a particular item x^* from a set X of $N = 2^n$ items that contains x^*
- Applying the operator $U^{(g)}$ for $\mathcal{O}(\sqrt{N})$ times
- All the intermediate states are in the subspace spanned by $|x^*\rangle$ and $|+\rangle^n \implies R \leq 2$

Search multiple marked items

- Find an arbitrary element in the marked subset A from the set X
- All the intermediate states are in the subspace spanned by $|A\rangle := \frac{1}{\sqrt{|A|}} \sum_{x \in A} |x\rangle$ and $|+\rangle^n$
- Intermediate state has ranks bounded by $|A| + 1$

Quantum Walks based Search

Quantum walks: quantum analog of classical random walks, with quadratic speed-up

$$\text{Markov chain stochastic matrix: } P_{ij} = \begin{cases} 1/\text{outdeg}(j) & \text{if } ij \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Random walks based search

Start at a random vertex u
Repeat $T = \mathcal{O}(N)$ times:
  $u \leftarrow$ sample one vertex from Pu
  Check if u is the marked vertex
  If marked, output

Quantum walks based search

Start at superposition of all edge states $|u\rangle$
Repeat $T = \mathcal{O}(\sqrt{N})$ times:
  $|u\rangle \leftarrow U^{(w)}|u\rangle$
  $|u\rangle \leftarrow U^{(o)}|u\rangle$
Measure $|u\rangle$

Quantum Walks based Search

Search on a complete graph with self-loops

- $P = \frac{1}{N} e_N e_N^T$, $e_N \in \mathbb{R}^N$ is an all-ones vector
- Similar to Grover's algorithm, $R \leq 2$ **for all intermediate states**

Search on a complete bipartite graph

- If $|V_1| = |V_2| = N/2$, $P = X \otimes (\frac{2}{N} e_{N/2} e_{N/2}^T)$, $\quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
- $R \leq 4$ **for all intermediate states**

Search on general graphs cannot be low-rank approximated

Experimental Results

Quantum Fourier transform (with CP-ALS)

- Can easily perform simulation on **up to 60 qubits** when the input state is a standard basis
- With random rank-1 inputs: entanglement increases quickly

Number of qubits	16	20	24	28	40	**40**
Rank limit (r_{max})	256	256	256	256	1024	**2048**
Fidelity estimation	0.998	0.975	0.918	0.788	0.534	**0.580**

Phase estimation (with CP-ALS)

- Can easily perform simulation on **up to 60 qubits** when the second register input is the eigenvector of the oracle gate

Number of qubits	20	24	28	32	40	**60**
Rank limit (r_{max})	20	20	20	20	20	**20**
Fidelity estimation	0.9997	0.9998	0.9993	0.9997	0.9972	**0.9994**

Experimental Results

Grover's algorithm ($r_{max} = 2$)

- CP-ALS can be inaccurate for large circuits

Number of qubits	8	10	12	14	16	16
Number of ALS initializations	3	3	3	3	**3**	**10**
Amplitude on x^*	1.	0.999	1.0	1.0	**0.0**	**1.0**

- Direct elimination of scalar multiples is faster and more stable

Number of qubits	10	15	20	25	30
Amplitude on x^*	0.999	1.0	1.0	1.0	1.0

Quantum walks based search

- Can easily perform simulation on **up to 36 qubits** on complete graphs with self-loops and complete bipartite graphs
- On general cyclic graphs, low-rank approximation can be inaccurate

Conclusion

Introduce low-rank CP decomposition for the simulation of quantum algorithms

- Simple, fast, easy to program
- Convenient for quantum entanglement analysis

Several famous quantum algorithms with specific inputs/structure can be efficiently simulated

- **QFT**: all the intermediate states have rank 1 when the input state is a standard basis
- **Phase estimation**: all the intermediate states are low-rank tensor when the second register input is an eigenvector of the oracle gate
- **Grover's algorithms**: states are low-rank when the marked set size is $\mathcal{O}(1)$
- **Quantum walks based search**: states are low-rank only on specific structured graphs

Results consistent with literature on dequantization/quantum speed-ups

- QFT with specific inputs can be dequantized (A. Abbott, Applied Mathematics and Computation, 2012)
- Grover's algorithm relies on interference, rather than entanglement, to provide speedups (S. Lloyd, Physical Review A, 1999)

- Implementations are publicly available at https://github.com/LinjianMa/koala
- Paper will be released soon

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Measure $|u\rangle$

- Quantum walks defined on a Hilbert space $\mathcal{H}^{N^2} = \mathcal{H}^N \otimes \mathcal{H}^N$
- Each edge (x, y) is represented by the state $|x\rangle \otimes |y\rangle$
- Weighted superposition of the edges starting from x: $|\psi^{(x)}\rangle := |x\rangle \otimes \sum_{y \in V} \sqrt{P_{yx}} |y\rangle$
- $S = \sum_{x,y \in V} |y, x\rangle \langle x, y|, \quad U^{(d)} = 2 \sum_{x \in V} |\psi^{(x)}\rangle \langle \psi^{(x)}| - I$
- $U^{(w)} = S U^{(d)} S U^{(d)}, \quad U^{(o)} = I - 2 \sum_{y \in V} |x^*, y\rangle \langle x^*, y|$

Quantum Walks based Search

Search on a complete graph with self-loops

- $P = \frac{1}{N} e_N e_N^T$, $e_N \in \mathbb{R}^N$ is an all-ones vector
- $U^{(o)} = \left(I - 2 \left| x^* \right\rangle \left\langle x^* \right| \right) \otimes I$
- $U^{(w)} = \left(2 \left| + \right\rangle^n \left\langle + \right|^n - I \right) \otimes \left(2 \left| + \right\rangle^n \left\langle + \right|^n - I \right)$
- Similar to Grover's algorithm, $R \leq 2$ **for all intermediate states**

Search on a complete bipartite graph

- If $|V_1| = |V_2| = N/2$, $P = X \otimes (\frac{2}{N} e_{N/2} e_{N/2}^T)$, $\quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
- $R \leq 4$ **for all intermediate states**

Search on general graphs cannot be low-rank approximated

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- Goal is to find a particular item x^* from a set X of $N = 2^n$ items that contains x^*
- Applying the operator $U^{(g)} = U^{(o)}U^{(d)}$ for $\mathcal{O}(\sqrt{N})$ times.

$$\text{Oracle operator} : U^{(o)}|x\rangle = (-1)^{f(x)}|x\rangle, \quad \text{where} \quad f(x) = \begin{cases} 1 & \text{if } x = x^*, \\ 0 & \text{otherwise.} \end{cases}$$

$$\text{Diffusion operator} : U^{(d)} = 2|+\rangle^n \langle +|^n - I$$

- All the intermediate states are in the subspace spanned by $|x^*\rangle$ and $|+\rangle^n \implies R \leq 2$

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