A review of simulation techniques of quantum computing

Bartłomiej Bukowski

Kraków Quantum Informatics Seminar (KQIS)
AGH University of Science and Technology, Kraków

bartlomiejbukowski.b@gmail.com

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Agenda

Quantum bits - Qubits

State vector

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$\alpha, \beta \in \mathbb{C}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

basis states in Dirac notation

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Multiple Qubits

Tensor product

$$|\phi\rangle = |\psi_1\rangle \bigotimes |\psi_2\rangle \bigotimes \cdots \bigotimes |\psi_n\rangle$$

$$|\psi_1\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$$

$$|\psi_2\rangle = \beta_0|0\rangle + \beta_1|1\rangle$$

$$|\psi_1\rangle \bigotimes |\psi_2\rangle = \begin{bmatrix}\alpha_0 \\ \alpha_1\end{bmatrix} \bigotimes \begin{bmatrix}\beta_0 \\ \beta_1\end{bmatrix} = \begin{bmatrix}\alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_0 \\ \alpha_1\beta_1\end{bmatrix} =$$

$$\alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle$$

Quantum register

n-qubit system state

$$|\phi\rangle = \sum_{j=0}^{2^n-1} \alpha_j |j\rangle_n = \alpha_0|0\rangle_n + \alpha_1|1\rangle_n + \cdots + \alpha_{2^n-1}|2^n-1\rangle_n$$

$$\alpha_j \in \mathbb{C}$$

$$\sum_{j=0}^{2^n-1} |a_j|^2 = 1$$

Quantum operations

Unitary operator

Any operation on a quantum system can be represented by a unitary matrix U which operates on its state vector.
The matrix U is unitary, when $UU^\dagger = U^\dagger U = I$. $U^\dagger$ is a Hermitian conjugate of U and $U^\dagger = (\overline{U})^T = \overline{U^T}$, where $\overline{U}$ denotes a complex conjugate of matrix U and U^T denotes the matrix transposition.

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

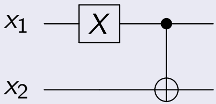
$$|\psi'\rangle = U|\psi\rangle = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} a\alpha + b\beta \\ c\alpha + d\beta \end{bmatrix}$$

Quantum gates

Name	Symbol	Matrix
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$
Pauli-Y	Y	$\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$
Square Root of Not	$\sqrt{X}$	$\frac{1}{2}\begin{bmatrix}1-i & 1+i\\ 1+i & 1-i\end{bmatrix}$
Phase Scale (by angle γ)	θ	$\begin{bmatrix}e^{i\gamma} & 0\\ 0 & e^{i\gamma}\end{bmatrix}$
Rotation Z	R_z	$\begin{bmatrix}e^{-i\frac{\gamma}{2}} & 0\\ 0 & e^{i\frac{\gamma}{2}}\end{bmatrix}$

Quantum circuits

Example quantum circuit



Matrix representation of presented circuit

$$C_{01}(X \otimes I) = \left(\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \right) \left(\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \right)$$

$$= \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Simulating Quantum Physics with Computers

It is impossible to represent the results of quantum mechanics with a classical universal device. [1]

Our only hope is that we're going to simulate probabilities. [1]

Problems with Simulation of Quantum Processes

Naive vector-matrix representation memory consumption

Qubit Number	5	10	20	21
State vector	512 B	16 kB	16 MB	32 MB
Operation matrix	16 kB	16 MB	16 TB	64 TB

Memory needed to represent state vector: $O(2^n)$.

Memory needed to represent unitary matrix: $O(2^{2n})$.

Modifying quantum state time complexity

Complexity of matrix-vector multiplication requires $O(2^n)$ operations for very sparse matrices, but even $O(2^{2n})$ for others.

Complexity of matrix-matrix multiplication ranges from $O(2^{2n})$ to $O(2^{3n})$ depending on algorithm and matrix features.

List of available simulation techniques

- Numerical Linear Algebra Methods
- Qubit-wise multiplication [11]
- P-blocked state representation
- Hash Table State Representation
- Decision Diagrams
- Quantum Multi-Valued Decision Diagrams [20] [19]

Overview of Quantum Computer Simulators

- Simulation Libraries
  - libquantum [12]
  - Quantum++ [12]
  - Qlib for MatLab [13]
- Quantum Programming Languages
  - OpenQASM [14]
  - QML
- Frameworks
  - Q# [15]
  - Qiskit [16]
  - ProjectQ [4]
- GUI Simulators
  - QuIDE [17]
  - quirk [18]

Qubit-wise Multiplication

Split the operation on 2^n-element vector into smaller matrices

Unitary operation on n-qubit system can be expressed as composition of simple, one- or two-qubit elementary gates [11]

Example

$$A = I \otimes I \otimes H \otimes I \otimes I$$

$$\psi = |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle$$

$$\psi' = |0\rangle \otimes |0\rangle \otimes H|0\rangle \otimes |0\rangle \otimes |0\rangle$$

- Memory usage reduction from $O(2^{2n})$ to $O(2^n)$.
- Avoiding operations on big matrices.

P-blocked State Representation

$p - \textit{blocked}$ state [21]

$\rho = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_k$

- ρ_i is the state of at most p qubits
- each p_i state is represented as density matrix $2^p \times 2^p$
- complexity reduction from $O(2^n)$ to $O(k2^{2p})$ (for best case $p = 1 \longrightarrow O(4k)$)

Drawbacks

- no entanglements in $p + 1$ qubits
- qubit entanglement tracking algorithm
- for the worst case $p = n$ operations on state vector require $O(2^{2n})$ memory alongside with complications of performed operations because of entanglement tracking algorithm
- Bell states or any m-qubit GHZ state cannot be represented using this technique

Hash Table State Representation

Improvement over Qubit-wise Multiplication

- State vector is very sparse
- Store only non-zero complex values that represent probability of collapsing to certain quantum state

$$\psi = \begin{array}{c} 000 \\ 001 \\ 010 \\ 011 \\ 100 \\ 101 \\ 110 \\ 111 \end{array} \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ 0 \\ \frac{1}{2} \\ 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$$

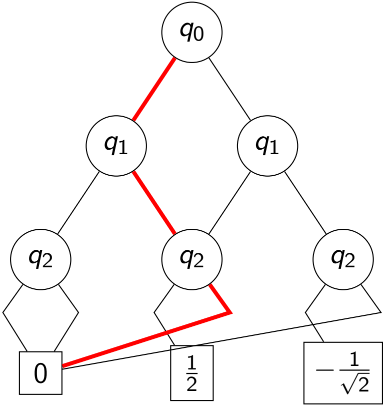
Keys	Values
2	$\frac{1}{2}$
4	$\frac{1}{2}$
6	$-\frac{1}{\sqrt{2}}$

Binary Decision Diagrams

Observation

- State vector and operation matrices repeat themselves.

$$\psi = \begin{array}{c} 000 \\ 001 \\ 010 \\ 011 \\ 100 \\ 101 \\ 110 \\ 111 \end{array} \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \mathbf{0} \\ \frac{1}{2} \\ 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$$



QMDDs as an enhancement over Decision Diagrams

- Elementary quantum operations typically affect only a small number of the qubits of a quantum system.
- The transformation matrix/state vector for the whole system often contains the same pattern repeatedly throughout the matrix.
- Transformation matrices/state vectors are often sparse with many zero entries frequently appearing in blocks.
- Every modification of quantum system, that is represented by $2^n \times 2^n$ matrix can be partitioned into 4 sub-matrices of dimension $2^{n-1} \times 2^{n-1}$ as follows:

$$U = \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix}$$

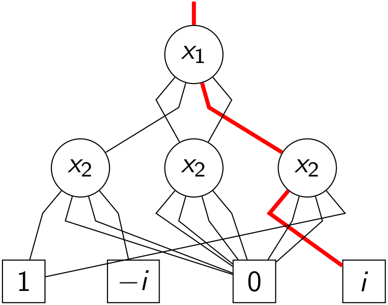
- Every state of quantum system can be represented by vector of size 2^n that can be partitioned into 2 sub-vectors of size 2^{n-1}:

$$\psi = \begin{bmatrix} \psi_0 & \psi_1 \end{bmatrix}$$

QMDDs as an enhancement over Decision Diagrams

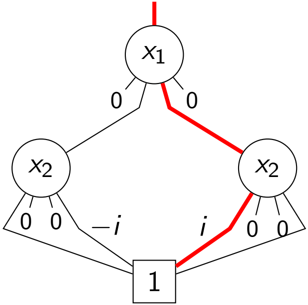
$x_1 \backslash x_2$	00	01	10	11
00	0	0	1	0
01	0	0	0	$-i$
10	**i**	0	0	0
11	0	1	0	0

a) Transformation matrix

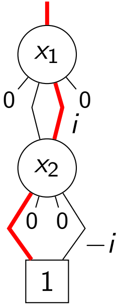


b) Decision Diagram with multiple terminal nodes

QMDDs as an enhancement over Decision Diagrams



c) Decision Diagram with edge weights



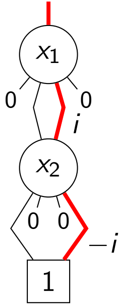
d) Quantum Multiple-Valued Decision Diagram

QMDDs as an enhancement over Decision Diagrams

Columns ($x_1 x_2$): 00, 01, 10, 11; rows ($x_1 x_2$): 00, 01, 10, 11

$$\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 \end{bmatrix}$$

a) Transformation matrix



d) Quantum Multiple-Valued Decision Diagram

Quantum Multi-Valued Decision Diagrams - definition

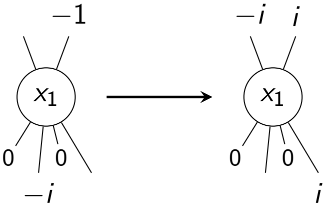
- Representation of an $r^n \times r^n$ complex matrix as a rooted directed acyclic graph.
- It has two types of vertices: single terminal vertex and zero or more non-terminal vertices.
- Each non-terminal vertex denotes the partitioning of a matrix by the application of following equation:

$$U = \begin{bmatrix} N(U_{00}) & N(U_{01}) \\ N(U_{10}) & N(U_{11}) \end{bmatrix} * \begin{bmatrix} \widehat{U}_{00} & \widehat{U}_{01} \\ \widehat{U}_{10} & \widehat{U}_{11} \end{bmatrix}$$

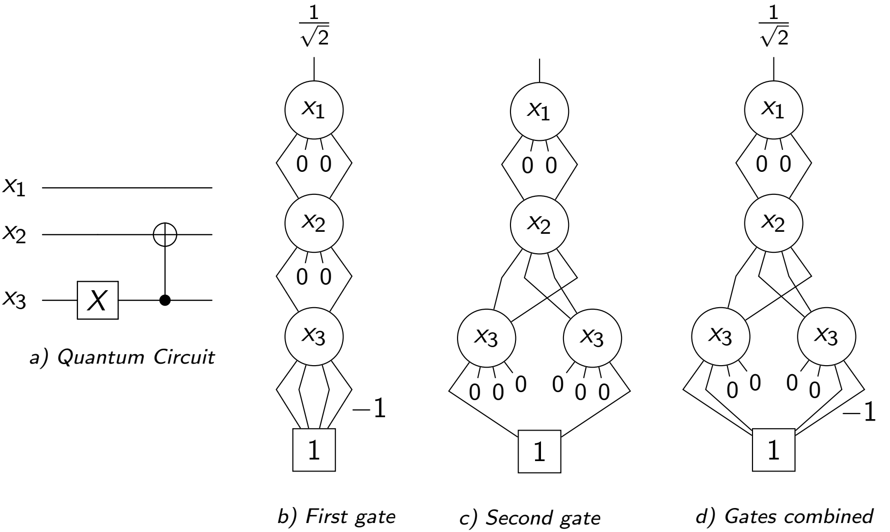
- There is an initial edge pointing to the root vertex with complex weight representing the QMDD normalization factor.
- QMDD is reduced:
  - No duplicated edges.
  - All vertices are unique.
- Above points are also applicable to states vectors.

QMDDs - normalization

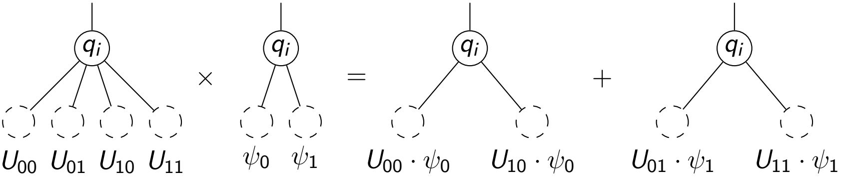
- QMDDs are built and normalized bottom-up.
- The non-terminal vertex v is normalized if $w(e_j) = 1$ for the lowest j for which $w(e_j) \neq 0$ for j being the outgoing edge's index.

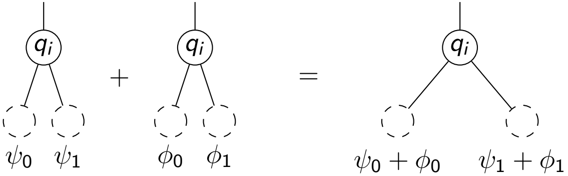


QMDDs - matrices creation and multiplication



QMDDs - multiplication matrix and state vector





QMDDs - complexity

Memory

- State vector worst case (full binary tree):
  - nodes: $|v| = 1 + \sum_{i=0}^{i=0} 2^i = 2^n$
  - complex values on edges: $2 \cdot (2^n - 1) + 1 = 2^{n+1} - 1$
  - approximately twice as many than in array-based solution
  - only if no redundancies are found
- Unitary matrix worst case (full quad-tree):
  - nodes: $|v| = 1 + \sum_{i=0}^{n-1} 4^i = 1 + \frac{4^n - 1}{3}$
- Elementary quantum gates targeting single qubit and arbitrary number of control qubits require only linear number of nodes

Operations time complexity

- Kronecker product: $O(|v|)$
- Multiplying matrices/state vectors: $O(n \cdot |v|)$
- Measuring state vector: $O(|v| + n)$

QMDDs - experimental results

Computation	#Qubits	LiqUI [2]		QX [3]		ProjectQ [4]		QuiDDPro [5]			QMDD		
		Time[s]	Memory[MB]	Time[s]	Memory[MB]	Time[s]	Memory[MB]	Time[s]	Memory[MB]	#Nodes	Time[s]	Memory[MB]	#Nodes
Entanglemnet	22	3.53	193.33	0.42	200.47	1.08	152.41	0.04	14.93	45	<0.01	48.02	43
	23	4.09	248.25	0.80	396.94	0.49	248.01	0.04	14.92	47	<0.01	48.03	45
	31							0.04	14.93	63	<0.01	48.11	61
	100							0.14	15.98	201	<0.01	49.32	199
QFT	18	3.02	192.91	0.27	16.56	0.87	57.82	24.21	192.77	65535	0.01	48.47	18
	21	6.46	192.83	3.63	102.75	0.66	100.75	10208.06	2511.26	4194303	0.01	48.78	21
	31										0.03	50.53	31
	64										0.09	68.00	64
Grover	16	97.78	195.11	55.90	57.28	6.65	51.88	6.93	16.29	39	0.14	50.54	130
	18	770.26	193.42	583.45	144.41	16.37	58.12	23.49	17.24	44	0.33	50.78	148
	20	8494.59	198.22	6394.54	382.51	77.95	77.17	85.86	19.05	39	0.78	50.80	166
	21	>18000.00		>18000.00		229.45	101.27	168.07	20.60		0.97	50.91	175
	27			>18000.00		>18000.00		>18000.00			14.65	51.26	238
	30					>18000.00		>18000.00			37.23	51.32	256
	40					>18000.00		>18000.00			1239.96	52.01	346
Shor	13	76.75	65.88			0.40	47.56	1665.28	92.03	16375	0.21	52.65	40
	15	298.59	62.72			9.30	51.43	16236.14	365.22	65535	0.54	55.09	72
	17	343.83	128.81			19.25	55.10	>18000.00			0.76	57.63	66
	31							>18000.00			44.60	97.91	305
	33							>18000.00			1019.55	156.12	6517
	37							>18000.00			5585.64	259.96	20917

All simulations have been conducted on a regular Desktop computer, i.e. a 64-bit machine with 4 cores (8 threads) running at a clock frequency of 3.8 GHz and 32 GB of memory running Linux 4.4 (source: [19])

Ryoshi IDE

Motivation

- Migration *QuIDE* to web environment
- Comparison *Hash Table State Vector Representation* with *QMDDs*

Simulator features

- Text editor supporting (de facto standard) OpenQASM
- Graphical circuit designer
- Step evaluator with vector state snooping

Summary

- *QMDDs* as promising replacement for *array-based* representation of quantum states and unitary matrices.
- Taking advantage of specific domain observations - redundancies.
- Approach that seemed more complex brings better results at the end - Decision Diagrams.
- Quantiki - leading social portal for everyone involved in quantum information science (https://quantiki.org [22]).
- Institute for Integrated Circuits, Johannes Kepler University Linz, Austria, (http://iic.jku.at/eda [23]).

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Qunatiki
Leading social portal for everyone involved in quantum information science.
URL https://www.quantiki.org/

Institute for Integrated Circuits
Johannes Kepler University Linz, Austria
URL http://iic.jku.at/eda

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