Optimizing Decision Diagrams for Measurements of Quantum Circuits

Ryosuke Matsuo[1], Rudy Raymond[2,3,4], Shigeru Yamashita[5], Shin-ichi Minato[6]

1. Osaka University
2. IBM Research Tokyo
3. The University of Tokyo
4. Keio University
5. Ritsumeikan University
6. Kyoto University

Background

Variational quantum algorithm (VQA):
•Promising application of near-term quantum computers
•Require measurement methods that efficiently extract information from quantum state

Shallow-circuit quantum measurement:
•Estimate quantum state by measuring each qubit
•Measurement based on single-qubit gate such as Pauli operations X, Y, Z
•Robust to noise of quantum computers

Classical Shadow:
•Obtain the estimator by polynomial number of measurements
•There are several methods for increasing accuracy of estimator
•Decision Diagram (DD)-based method [Hillmich et al. 2021]: High accuracy

Shallow-circuit quantum measurements

Consider n-qubit Hamiltonian H represented by following equation

$$H = \sum_{P \in \{I,X,Y,Z\}^n} \alpha_P P$$

Shallow-circuit quantum measurement problem:
Given quantum state $\rho \in \mathbb{C}^{2^n}$, we estimate $\mathrm{Tr}(H\rho)$ with small variance
by single qubit pauli-operation and measurement on computational basis ($|0\rangle, |1\rangle$)

⇩ Reduced

Optimization of probability distribution β over measurement basis $\mathcal{P}^n (\mathcal{P} = \{X, Y, Z\})$

Variance of estimator

$$\mathrm{Var}(\nu) = \frac{1}{S}\left(\left(\sum_{P,Q} \alpha_P \alpha_Q g(P,Q,\beta)\mathrm{Tr}(PQ\rho)\right) - \left(\mathrm{Tr}(H\rho)\right)^2\right)$$

This is small when # of measurement basis covering P, Q is small

⇒ Reduces the variance

Explanation of terminology "cover":

$\mathrm{Cover}(P) \coloneqq \{B \in \mathcal{P}^n | B_i = P_i \text{ whenever } P \neq I\}$

B covers P. $\Longrightarrow \mathrm{Tr}(P\rho)$ can be estimated by measurement on B.

e.g.) $XXXX$ covers $XIXI$

Existing decision diagram (DD)-based method [Hillmich, et al. 2021]:

- Extract measurement basis from DD representing Hamiltonian
- Demonstrate high accuracy compared with other classical shadow methods

Extract measurement basis from DD

DD for quantum measurements:
Rooted directed acyclic multi-graph $G = (V, E)$
Date given to edges:

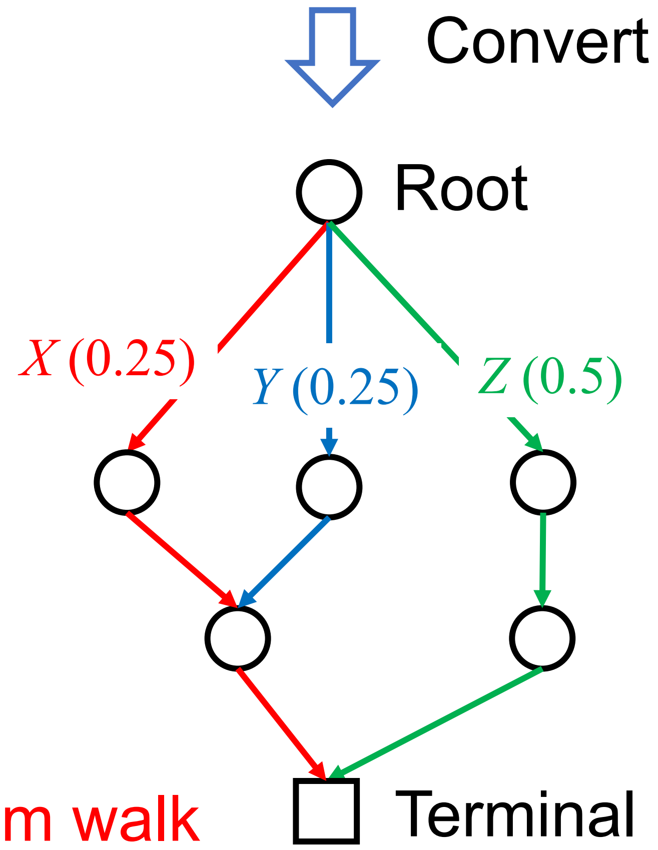
•Single-qubit Pauli-operator
•Weight $w(e) \in (0,1]$ ⇐ Probability of selecting edge

Requirements:

- $v \in V$ has at least one out-going edge
- For out-going edge of v ($e \in \mathrm{out}(v)$), $\sum_{e \in \mathrm{out}(v)} w(e) = 1$

Path: Corresponds measurement basis

$$H = 0.25XXX + 0.25YYX + 0.5ZZZ$$

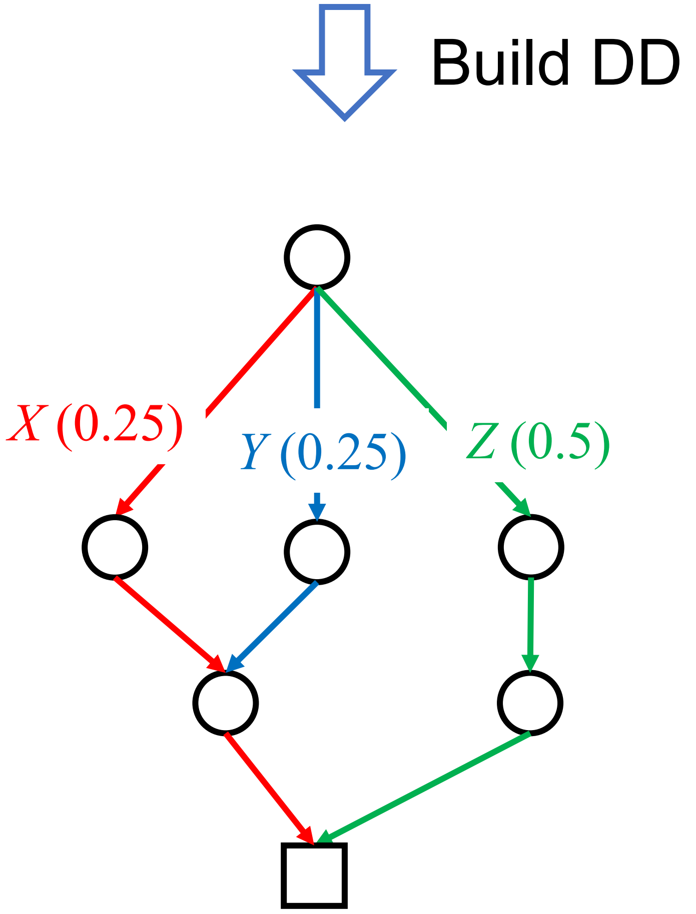


Estimate $\mathrm{Tr}(H\rho)$ using measurement basis obtain by random walk

Factor of variance: Edge weight, Shape of graph

Building method for DD

$$H = 0.25XXX + 0.25YYX + 0.5ZZZ$$



Flow of existing building method for DD

- Reduce Hamiltonian
  Reduce # of Pauli-operators
  Tuning probability distribution

- Initialize DD
  Build DD from reduced Hamiltonian

- Normalize DD
  Normalize edge weights
  Eliminate redundant nodes

Reduce Hamiltonian

$$H = -0.810IIII + 0.045XXXX + 0.045XXYY + 0.045YYXX + 0.045YYYY + 0.172ZIIII - 0.225IZII + 0.172\mathrm{IIZI}$$
$$-0.225IIIZ + 0.120ZZII + 0.168ZIZI + 0.166ZIIZ + 0.166IZZI + 0.174IZIZ + 0.120IIZZ$$

Reduce (Pauli grouping)

- Merge Pauli-operators
- Tuning probability distribution

Reduced Hamiltonian $\mathcal{R}(H)$

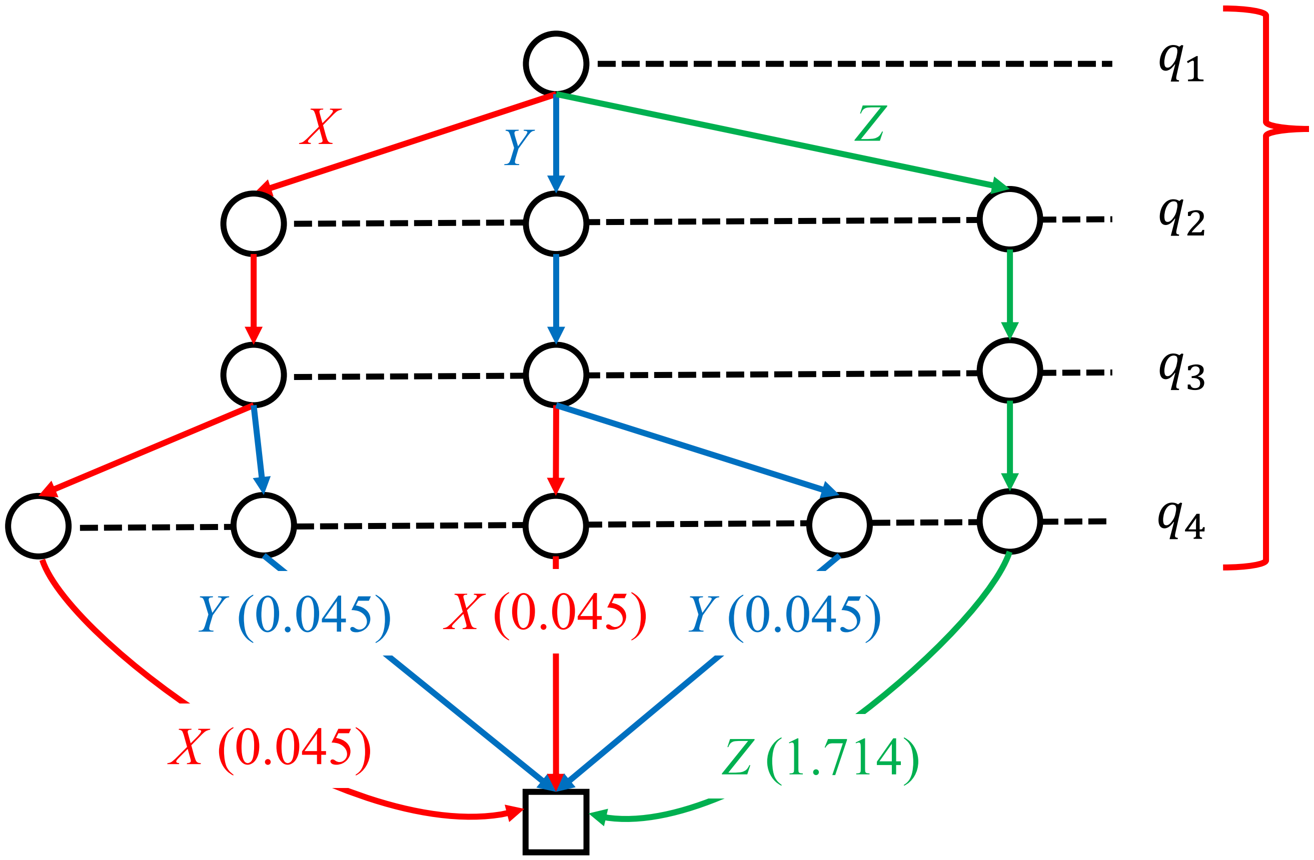
$$= 0.045XXXX + 0.045XXYY + 0.045YYXX + 0.045YYYY + 1.714ZZZZ$$

Coefficients correspond to probability distribution over measurement basis

Algorithm:
Check whether merging is possible for all combinations of terms

Initialize DD

$$\mathcal{R}(H) = 0.045X_1X_2X_3X_4 + 0.045X_1X_2Y_3Y_4 + 0.045Y_1Y_2X_3X_4 + 0.045Y_1Y_2Y_3Y_4 + 1.714Z_1Z_2Z_3Z_4$$



Qubit order:
Order in which bits are referenced

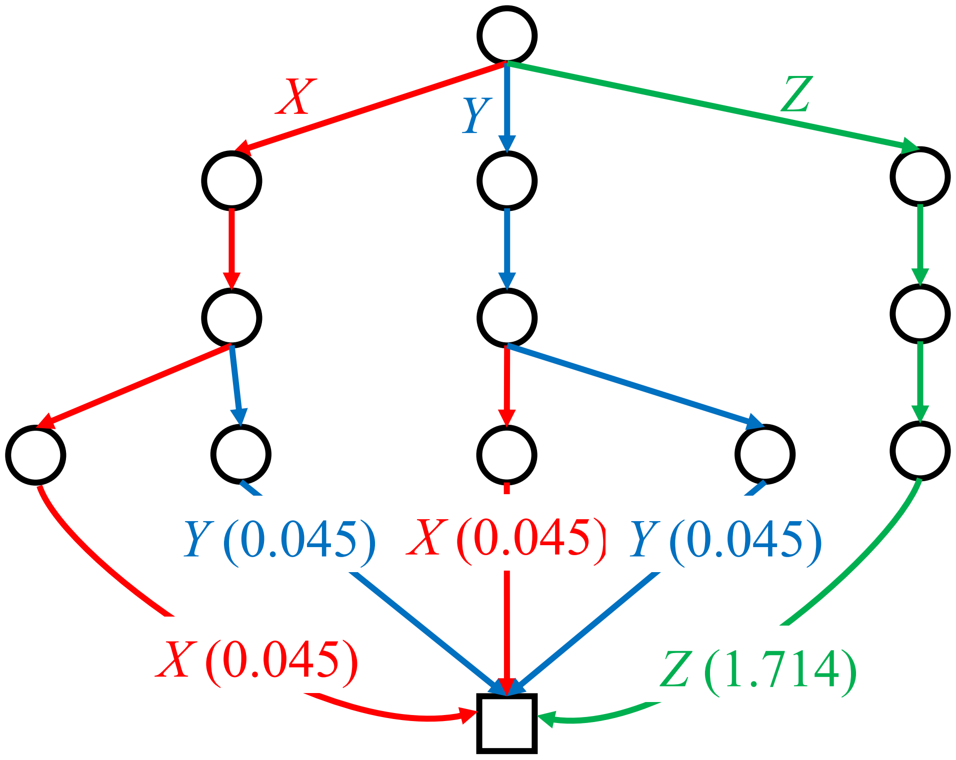
- Create path for each pauli-operator
- Give weight to bottom edge
(Weight corresponds to coefficient)

Next, normalize this DD
- Normalize edge weights
- Merge some nodes

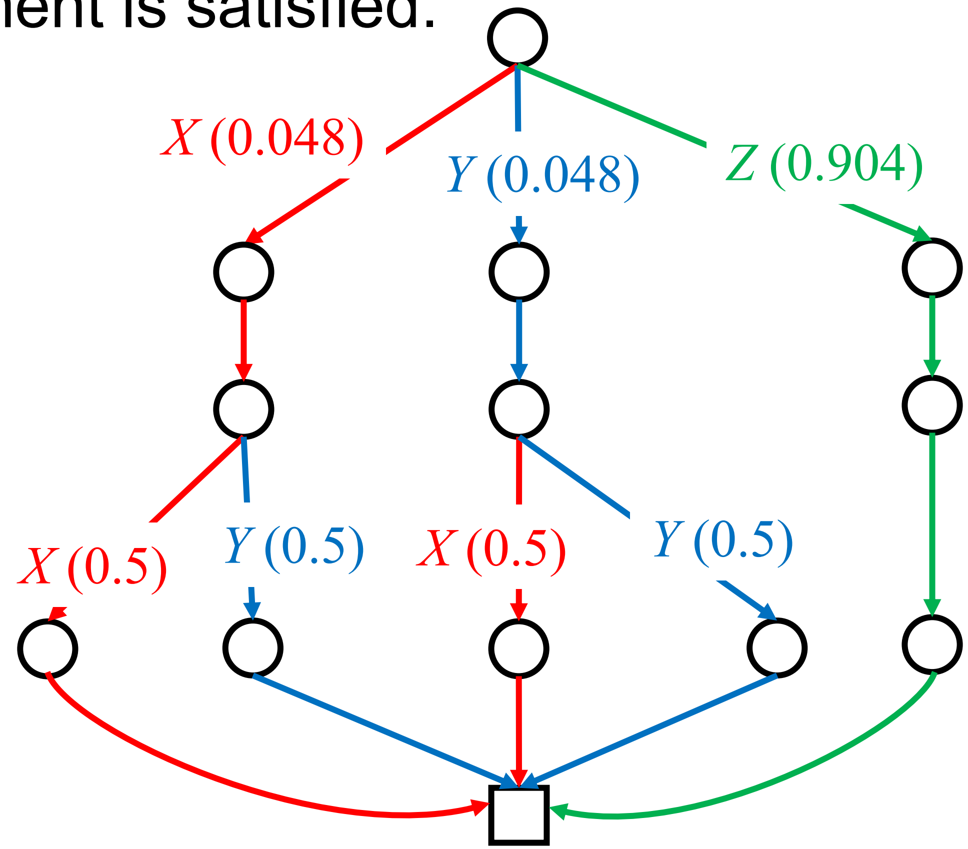
Normalize edge weight

Requirement for edge weight:
For out-going edge of v ($e \in \mathrm{out}(v)$), $\sum_{e \in \mathrm{out}(v)} w(e) = 1$

While propagating weight to root node,
normalize edge weight so that above requirement is satisfied.



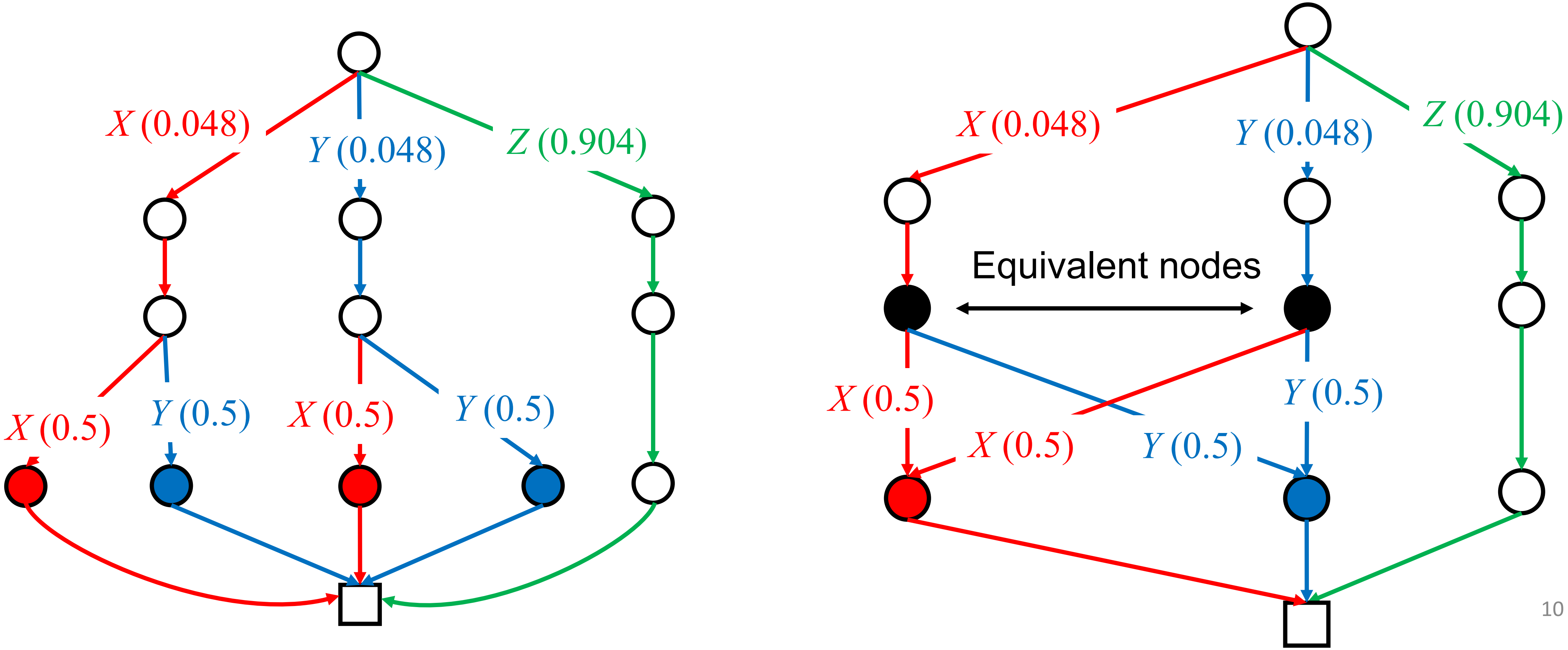
Initial DD



Normalized weight

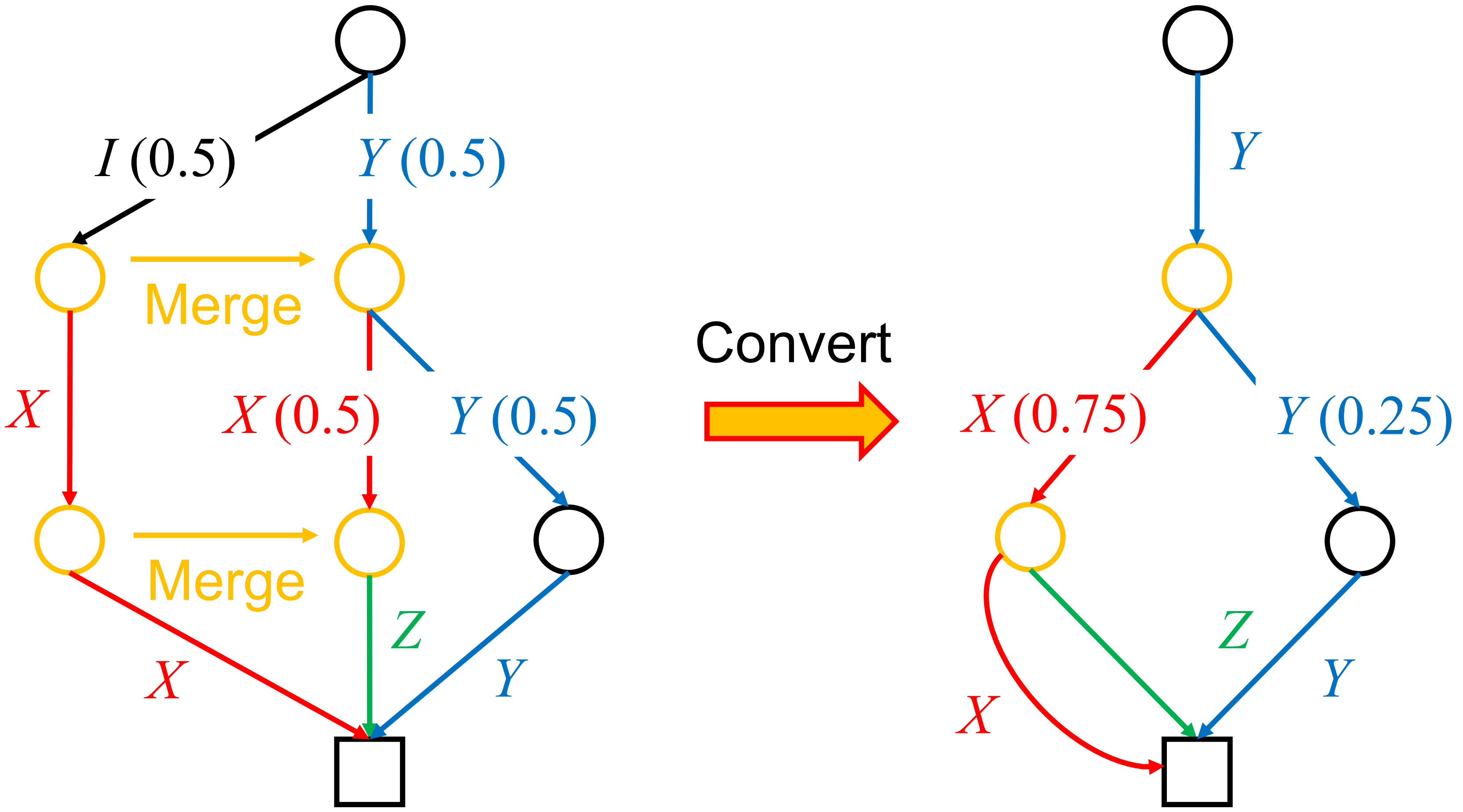
Merge equivalent node

Merge node v, u, when the two nodes satisfy following conditions.
(1) V_c (child-nodes of node v) = V_c' (child-nodes of node u)
(2) For any node $a \in V_c$,
Pauli-operation and weight of edge (v, a) and edge (u, a) are equivalent.



Node reduction by merging I-edges

When graph satisfies some conditions, following operation can be applied



# of nodes = 7

# of nodes = 5

Our contribution

Issue of DD:

Size of Hamiltonian: Large $\Longrightarrow$ Size of DD: Large

⇨ Can not be applied to large-size Hamitonian

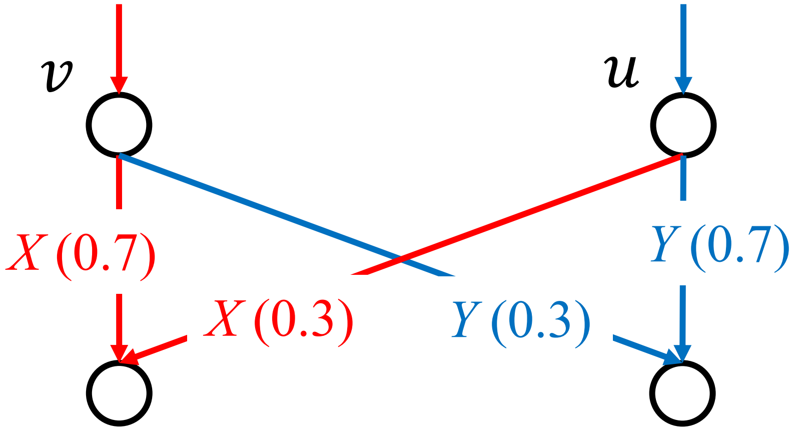
Our contribution:

- Propose a method for reducing size of DD
- Our method does not compromise accuracy of estimator

Relaxing condition of equivalent nodes

Merge nodes v, u, when the two nodes satisfy the following conditions
(1) V_c (child-nodes of node v) = V_c' (child-nodes of node u)
(2) For any node $a \in V_c$, Pauli operations of edge (v, a) and edge (u, a) are equivalent

Difference from existing method: Ignore edge weight



Existing method: v, u are not equivalent

Proposed method: v, u are equivalent

# of nodes merged is increased

⇨ Reduce # of nodes in DD

Edge weighting scheme

$$\mathrm{Var}(\nu) = \frac{1}{S}\left(\left(\sum_{P,Q} \alpha_P \alpha_Q g(P,Q,\beta)\mathrm{Tr}(PQ\rho)\right) - \left(\mathrm{Tr}(H\rho)\right)^2\right)$$

Small

# of measurement basis covering P, Q : Large

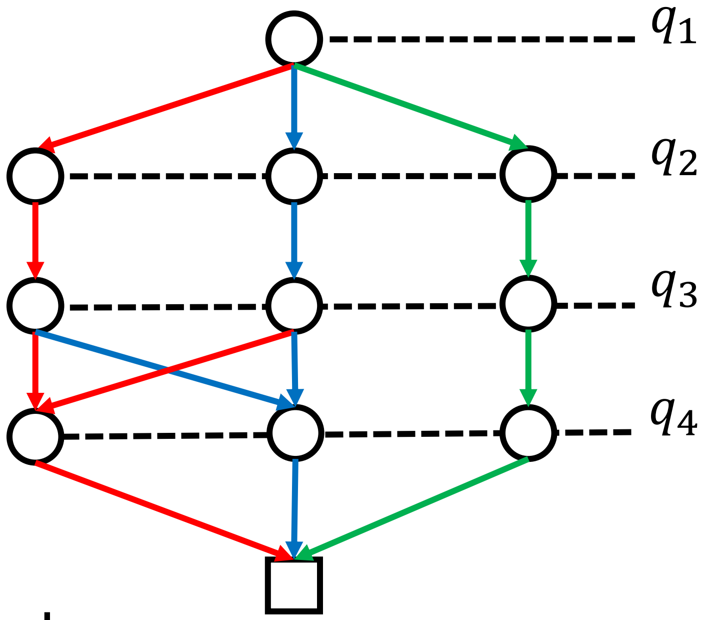
Small

Influence of Pauli operator with large coefficient: Large

# of measurement basis covering P, Q with large coefficient: Large

Edge weighting scheme:
Give a large weight to edges in path corresponding to such measurement basis

Qubit ordering



Reduce # of nodes by qubit ordering

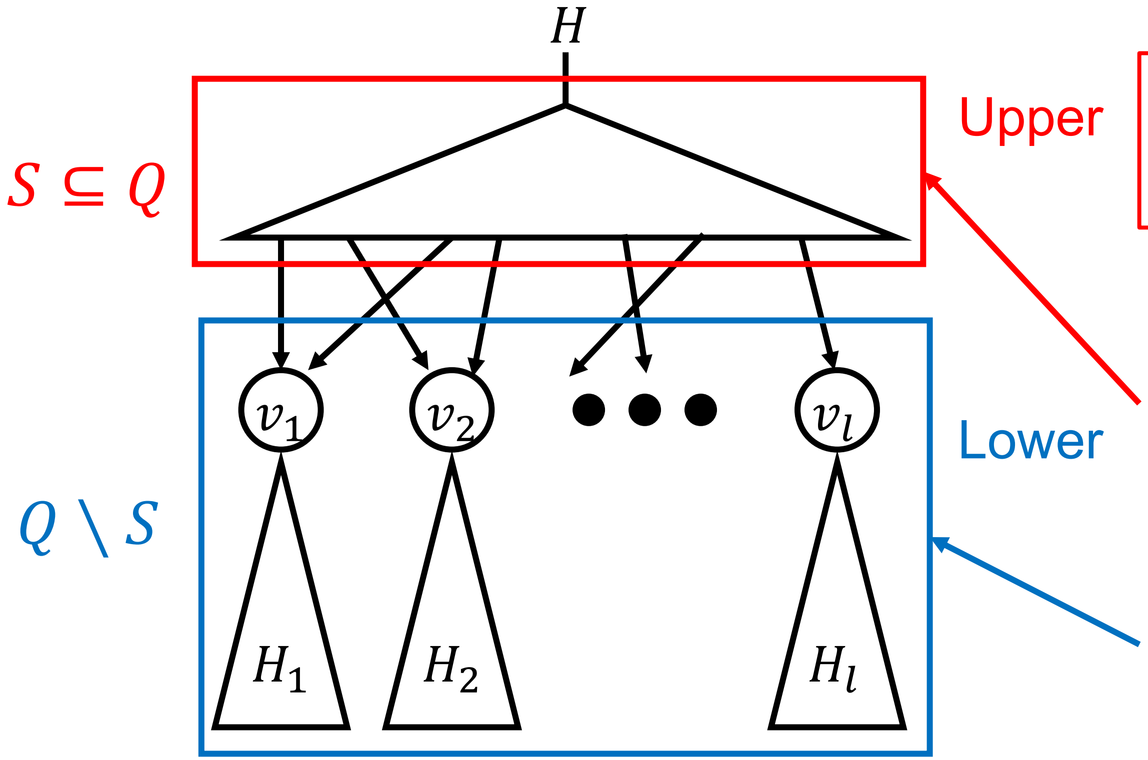
DD for quantum measurements
•# of nodes: Depends on qubit order
BDD (representative DD)
•# of nodes:
Depends on variable order (corresponds to qubit order)

Naïve algorithm for finding qubit order that minimizes # of nodes:
•Examine all qubit orders
•Time complexity: $O(n!)$

Proposed method:
•Fast algorithm based on dynamic programming
(technique utilized in BDD variable ordering)
•Obtain the optimal ordering when ignoring the reduction by merging I-edges

Divide DD

$Q = \{q_1, q_2, \ldots, q_n\}$ (q_i: Qubits in a DD)



Assumption:
Ignore the reduction by merging I-edges

\# of nodes in upper part:
Independent from lower part qubit order

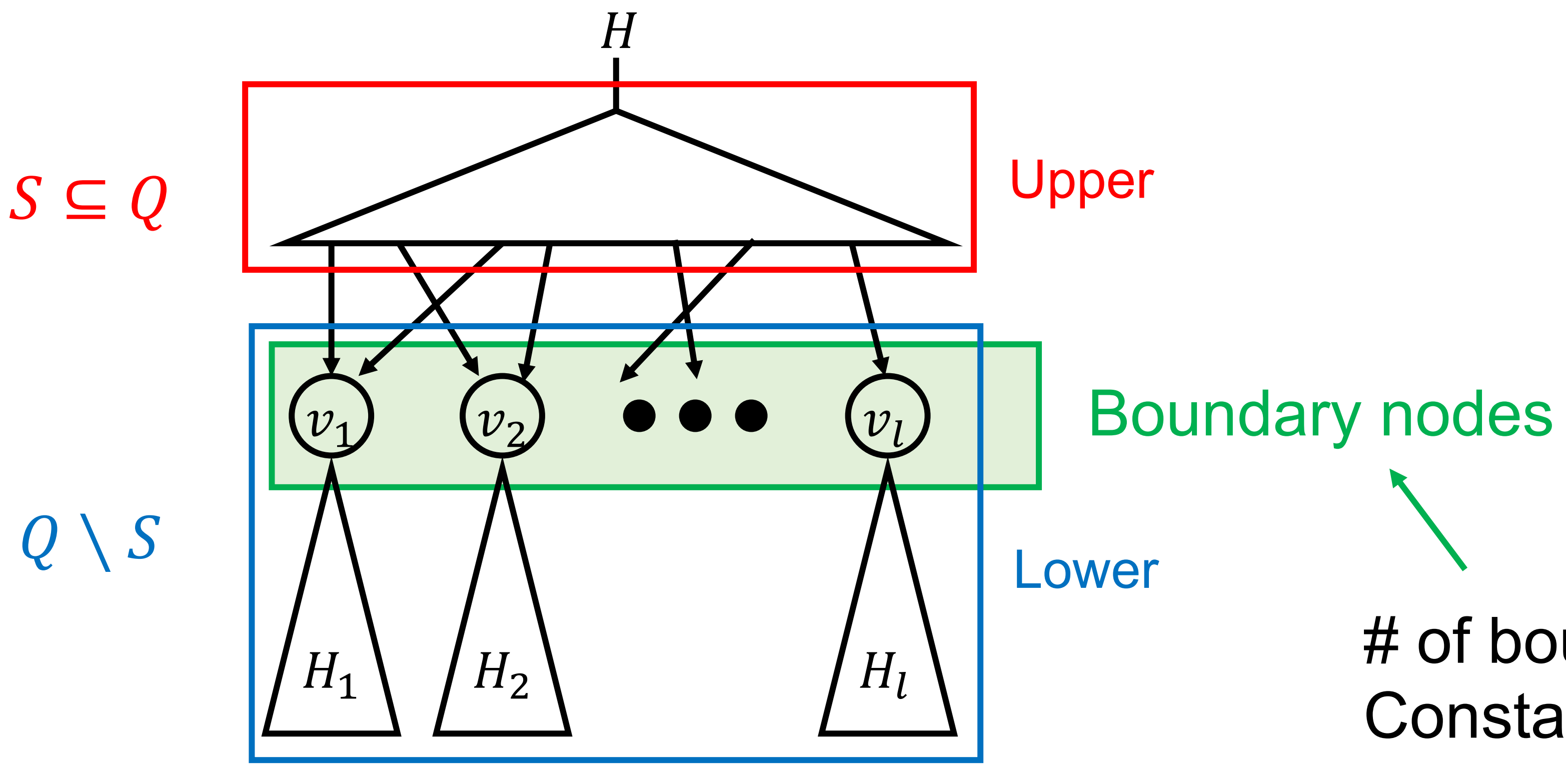
\# of nodes in lower part:
Independent from upper part qubit order

Problem of finding optimal qubit order:
We can separate upper part and lower part

Optimal qubit order: Examine all combinations of S

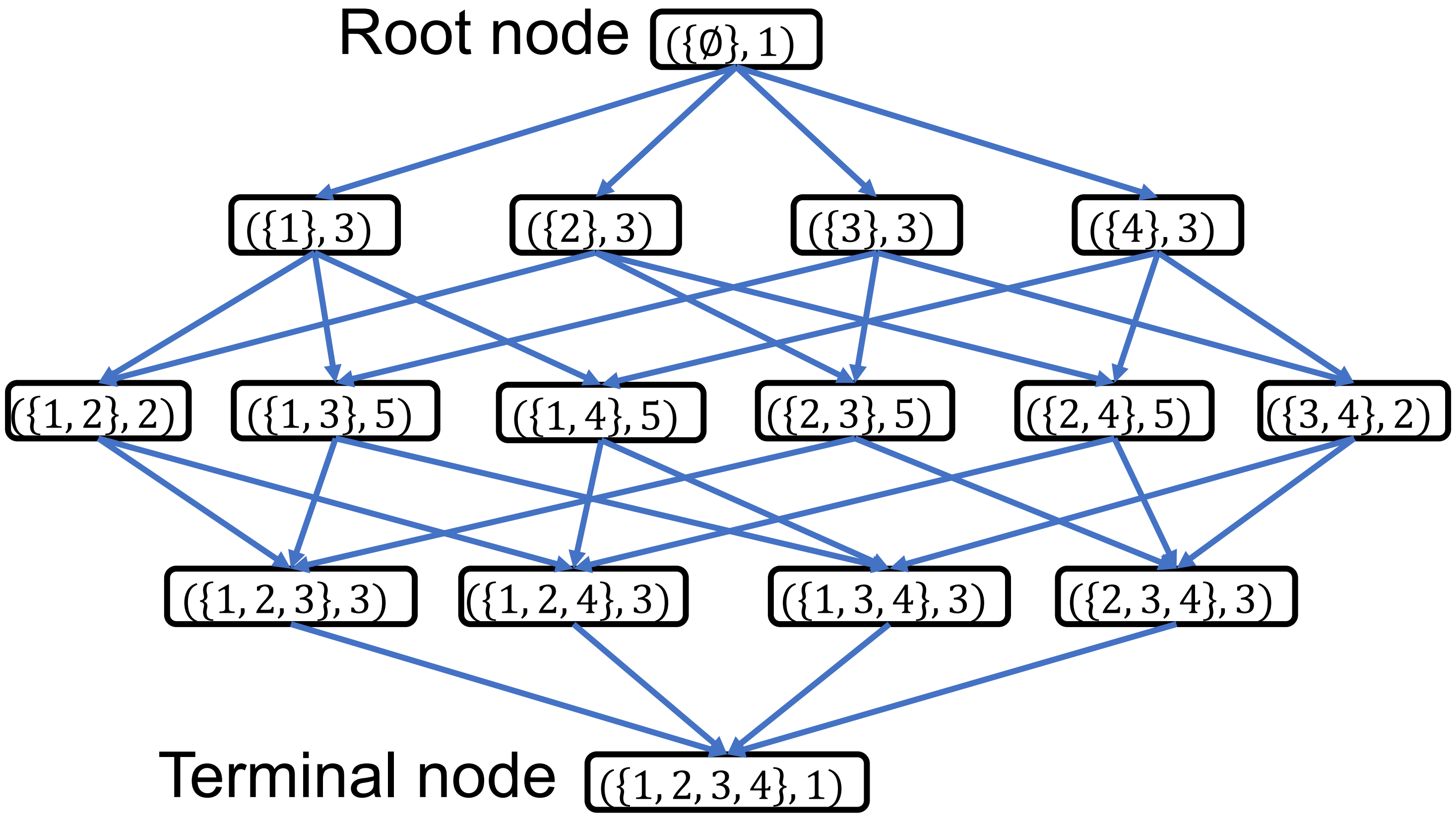
of boundary nodes

Information for finding optimal qubit order:
•Set of qubits S
•# of boundary nodes



# of boundary nodes:
Constant regardless of S

Master Profile Chart(MPC)



Data of nodes: • Set of qubits S
• # of boundary nodes

Edge: Transition of S

Path: Corresponds to qubit order

Path weight: # of nodes in DD

(Node weight: # of boundary nodes)

Finding qubit order that minimize # nodes = Finding minimum weighted path

Breadth fast search can solve this problem

Time complexity: Exponential to # of qubits

Experimental results

Comparison of existing method with proposed method

Molecule	Encode	Terms	CS [4]	Existing DD-based [21]			Proposed		
			Vari.	Node	Edge	Vari.	Node	Edge	Vari.
LiH (12-qubit)	JW	751	266	166	271	11.3	74	137	8.28
	Parity	778	760	215	429	31.2	172	316	36.7
	BK	765	163	290	521	29.6	167	300	44.1
BeH_2 (14-qubit)	JW	796	1792	319	484	123	177	297	314
	Parity	831	3524	375	702	635	266	468	697
	BK	833	2273	336	545	561	226	390	3597
H_2O (14-qubit)	JW	1302	4789	389	682	1444	220	397	1474
	Parity	1332	11209	540	1065	3552	229	492	5660
	BK	1333	26004	476	864	5325	265	487	9481

Proposed methods: Reduce DD size without compromising accuracy

[4] S. Aaronson, "Shadow tomography of quantum states," 2020.
[21] S. Hillmich, et. al, "Decision diagrams for quantum measurements with shallow circuits," 2021.

Conclusion

DD based quantum measurement:
•High accuracy
•Scalability issue regarding DD size

Proposed methods:
•Relax condition of equivalent nodes
•Edge weighting scheme
•Qubit ordering optimization

Experimental results:
•Demonstrate proposed methods can reduce DD size without compromising accuracy