

Graphical models and logical abstractions for quantum systems

Yipeng Huang

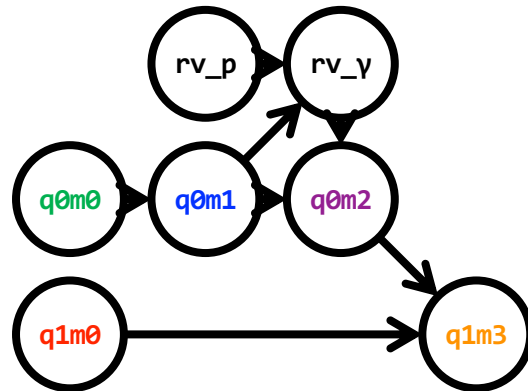
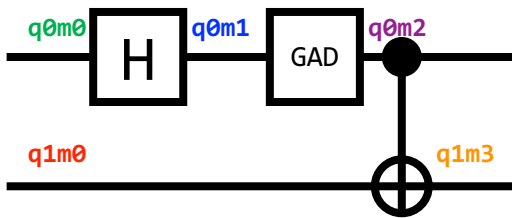
November 15, 2021



What this talk is about:

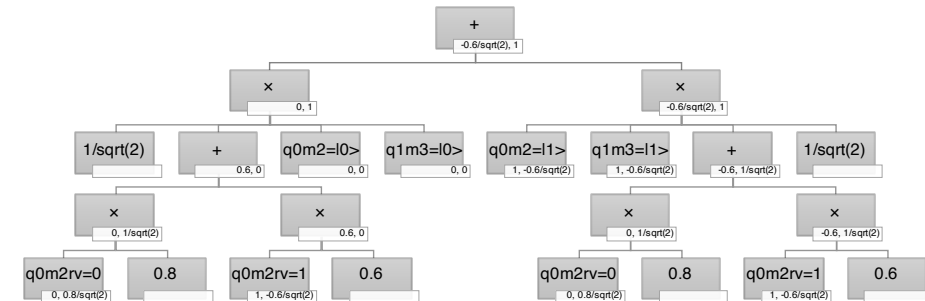
Using classical probabilistic inference techniques as an abstraction for quantum computing.

- A new way to represent noisy quantum circuits as probabilistic graphical models.
- A new way to encode quantum circuits as conjunctive normal forms and arithmetic circuits.
- A new way to manipulate quantum circuits using logical equation satisfiability solvers.
- Improved simulation and sampling performance for important near-term quantum algorithms.



The Hadamard gate:

$q_{0m0}=|0\rangle$ AND $q_{0m1}=|0\rangle \rightarrow +1/\sqrt{2}$
 $q_{0m0}=|0\rangle$ AND $q_{0m1}=|1\rangle \rightarrow +1/\sqrt{2}$
 $q_{0m0}=|1\rangle$ AND $q_{0m1}=|0\rangle \rightarrow +1/\sqrt{2}$
 $q_{0m0}=|1\rangle$ AND $q_{0m1}=|1\rangle \rightarrow -1/\sqrt{2}$



Where we are going:

What are quantum variational algorithms?

- Why are they different and important?

What is quantum circuit simulation?

- Why are the conventional techniques insufficient?

How do we represent quantum circuits as logic formulas?

- Why does it help with variational algorithm simulation, and by how much?

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Limitations of near-term quantum computers

- Limited number of qubits (the fundamental information units and devices in quantum computing).
- Noisy, unreliable operations.
- Limited operations on each qubit.
- Error correction too costly (needs ~million qubits), not available.

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NISQ systems target variational algorithms.

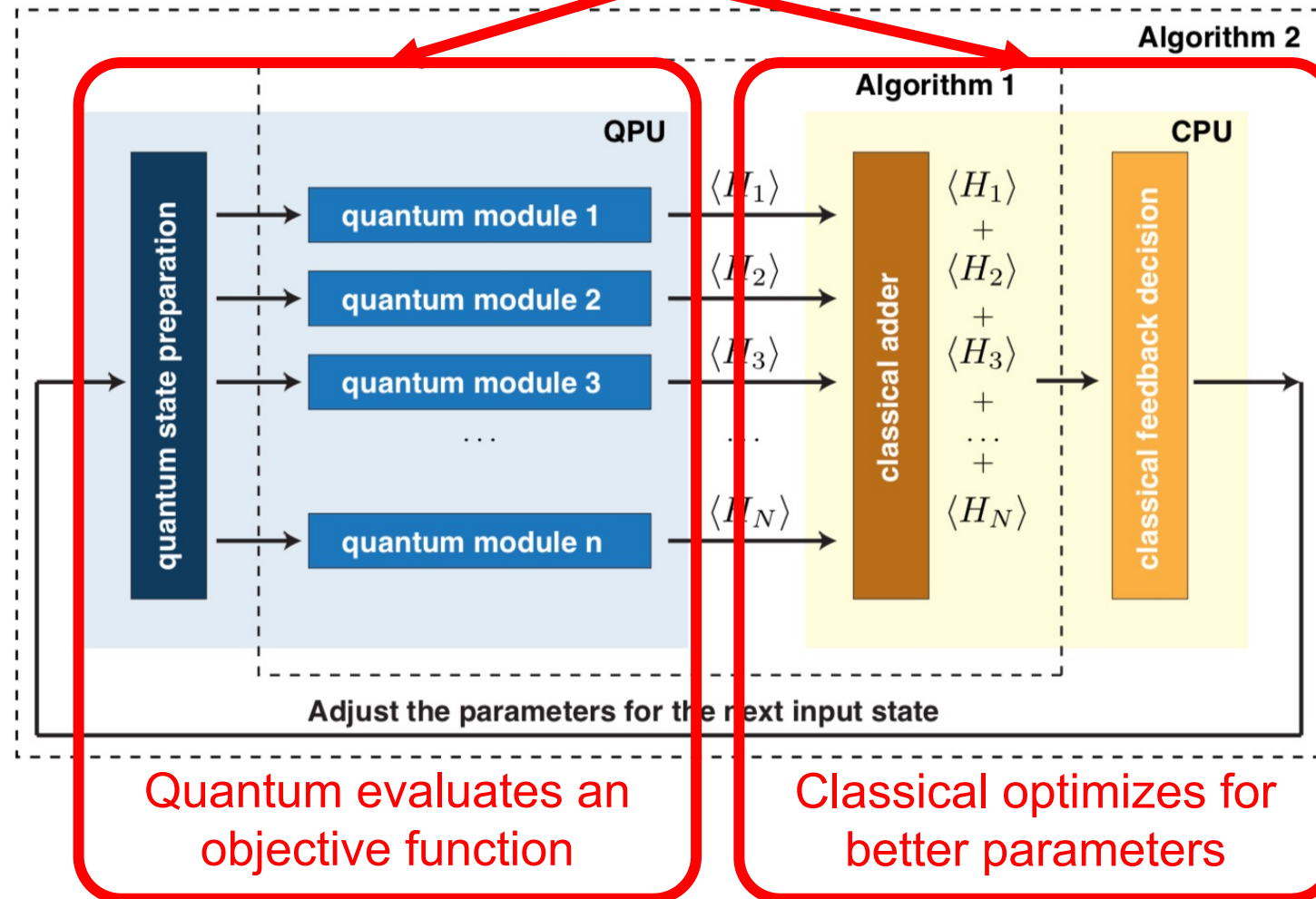
Near-term Intermediate Scale Quantum (NISQ) systems have ~100 qubits with at best 0.1% error rate.

With that capacity and reliability, error correction, along with famous algorithms such as Grover's search and Shor's factoring are infeasible.

The soonest candidates for useful quantum computation involve quantum-classical variational algorithms.

Hybrid quantum-classical variational algos

Use quantum & classical computation



It's like using a classical computer to train a quantum neural network.

Unique traits of variational algorithms

Provides meaningful results with noise even without error correction.

Draws on strengths of quantum and classical:

- Repeatedly prepare and measure quantum states.
- Optimize for a set of optimal parameters based on classical measurements.

Wide but shallow circuits (not many operations on many qubits).

Specific examples of variational algorithms

Variational quantum eigensolver (VQE)

Simulate quantum mechanics.

Quantum approximate optimization algorithm (QAOA)

Approximate solutions to constraint satisfaction problems (CSPs).

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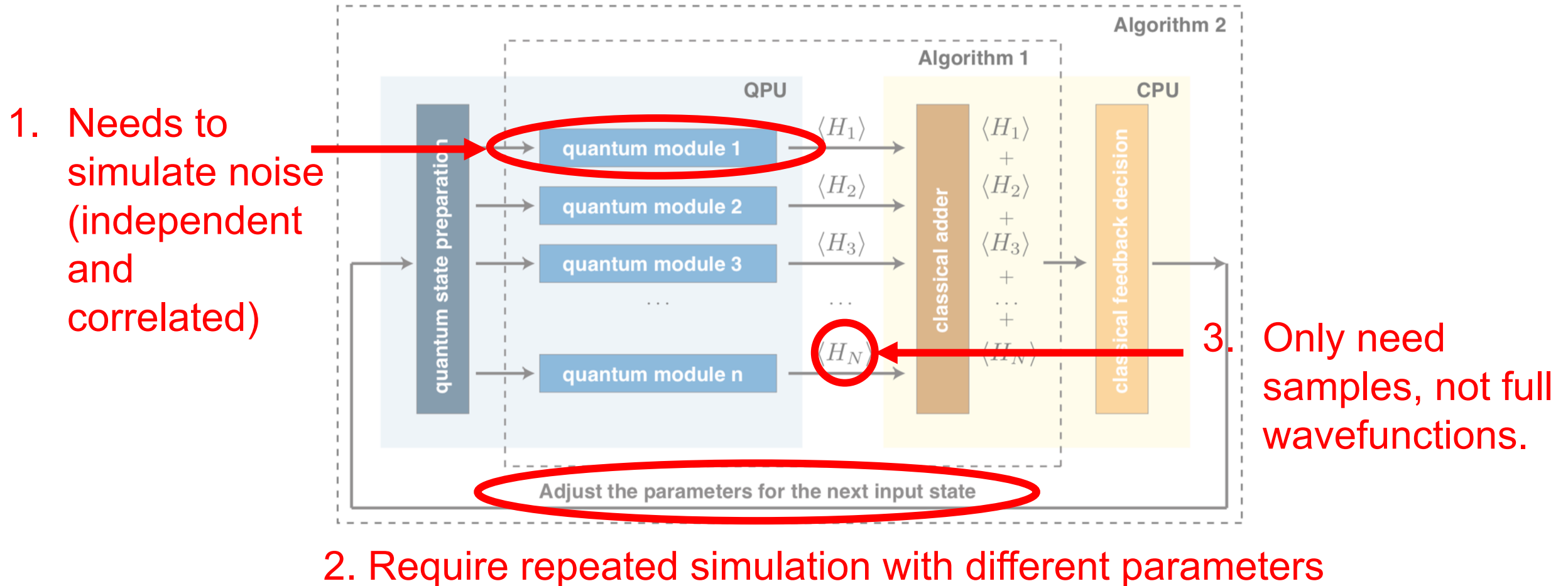
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The unique challenge of simulating noisy variational algorithms

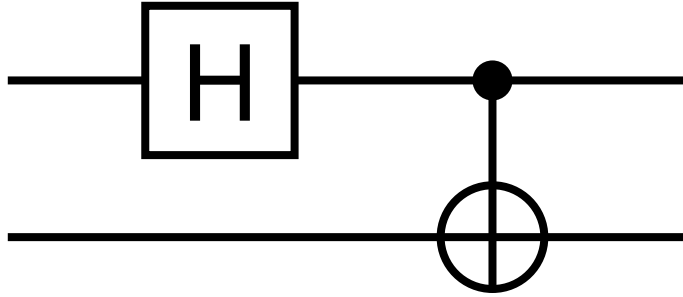


Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

Schrödinger simulation

QuEST, IBM, Google;
parallel matrix vector
multiplication

Schrödinger quantum circuit simulation



$$\text{CNOT}(H \otimes I|00\rangle) = \text{CNOT}(H|0\rangle \otimes I|0\rangle) = \text{CNOT} \begin{bmatrix} \frac{1}{\sqrt{2}} [1] \\ \frac{1}{\sqrt{2}} [0] \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix} = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

Schrödinger simulation

QuEST, qSim, ...;
parallel matrix vector
multiplication

1. Does it excel at
simulating wide but
shallow circuits?

X

2. Does it extract
structure for repeated
simulation with different
parameters?

X

3. Does it efficiently
sample from the final
wavefunction?

✓

Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

Schrödinger simulation

QuEST, qSim, ...;
parallel matrix vector
multiplication

Feynman simulation

qTorch; graphical
model tensor network
contraction

1. Does it excel at
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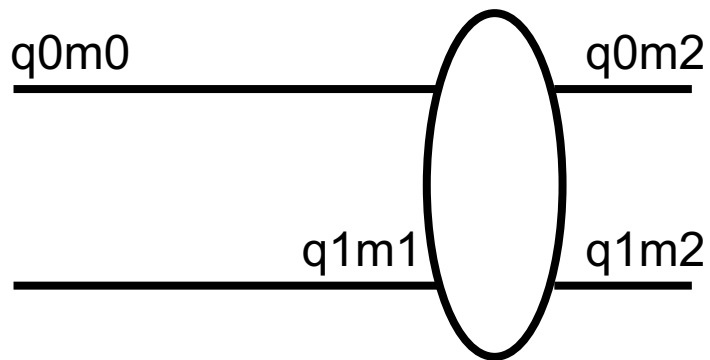
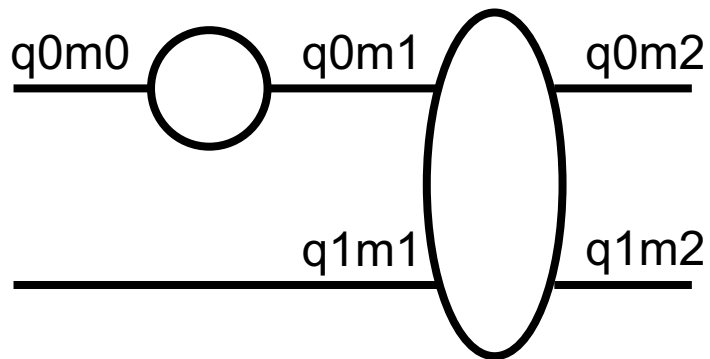
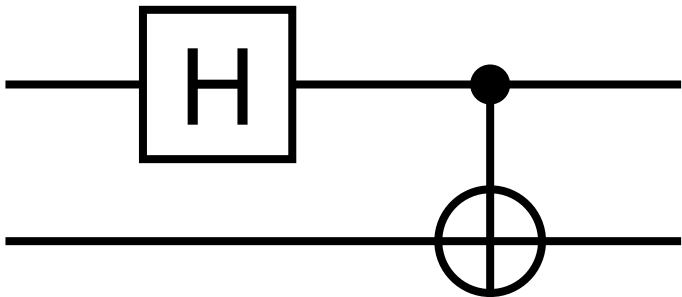
X

2. Does it extract
structure for repeated
simulation with different
parameters?

X

3. Does it efficiently
sample from the final
wavefunction?

✓



q0m
0= $|0\rangle$

q0m
0= $|1\rangle$

q0m 1= $ 0\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
q0m 1= $ 1\rangle$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

q0m2= $|0\rangle$ q1m2= $|0\rangle$
 q1m2= $|1\rangle$

q0m2= $|1\rangle$ q1m2= $|0\rangle$
 q1m2= $|1\rangle$

q0m2= $|0\rangle$ q1m2= $|0\rangle$
 q1m2= $|1\rangle$

q0m2= $|1\rangle$ q1m2= $|0\rangle$
 q1m2= $|1\rangle$

Feynman quantum circuit simulation

q0m1= $ 0\rangle$		q0m1= $ 1\rangle$	
q1m1= $ 0\rangle$	q1m1= $ 1\rangle$	q1m1= $ 0\rangle$	q1m1= $ 1\rangle$
1	0	0	0
0	1	0	0
0	0	0	1
0	0	1	0

q0m0= $ 0\rangle$		q0m0= $ 1\rangle$	
q1m1= $ 0\rangle$	q1m1= $ 1\rangle$	q1m1= $ 0\rangle$	q1m1= $ 1\rangle$
$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0

Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

	<u>Schrödinger simulation</u>	<u>Feynman simulation</u>
	QuEST, IBM, Google; parallel matrix vector multiplication	qTorch; graphical model tensor network contraction
1. Does it excel at simulating wide but shallow circuits?	X	✓
2. Does it extract structure for repeated simulation with different parameters?	X	?
3. Does it efficiently sample from the final wavefunction?	✓	X

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Our toolchain: Bayesian network knowledge compilation for noisy quantum circuit simulation and sampling

1. Noisy quantum circuits to Bayesian network
2. Bayesian networks to conjunctive normal form (CNF)
3. CNF to arithmetic circuit (AC)
4. Exact inference on AC for quantum circuit simulation
5. Gibbs sampling on AC to sample from final wavefunction

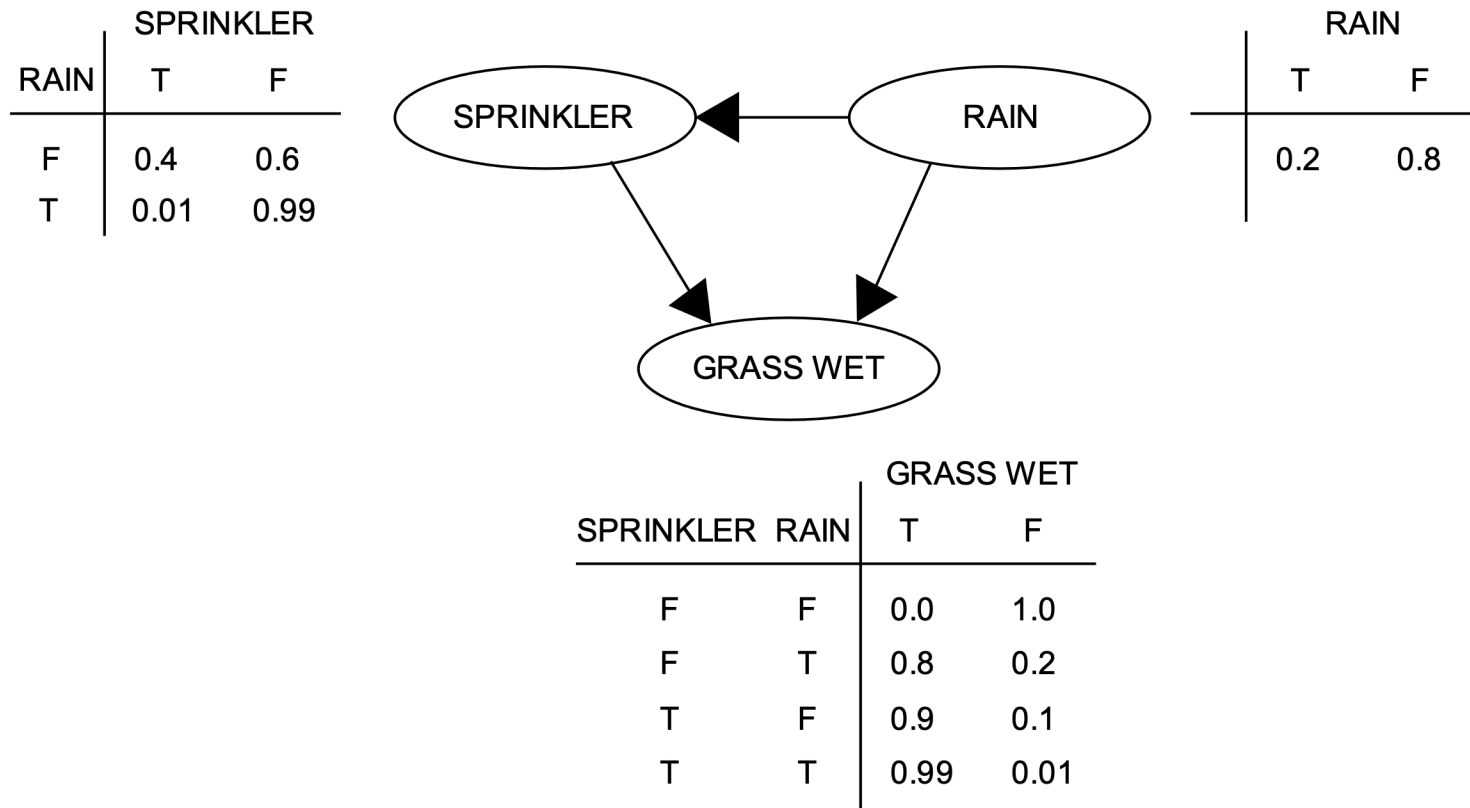
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- 
1. Needs to simulate noise
 2. Repeated simulation with different parameters
 3. Only need samples, not full wavefunctions

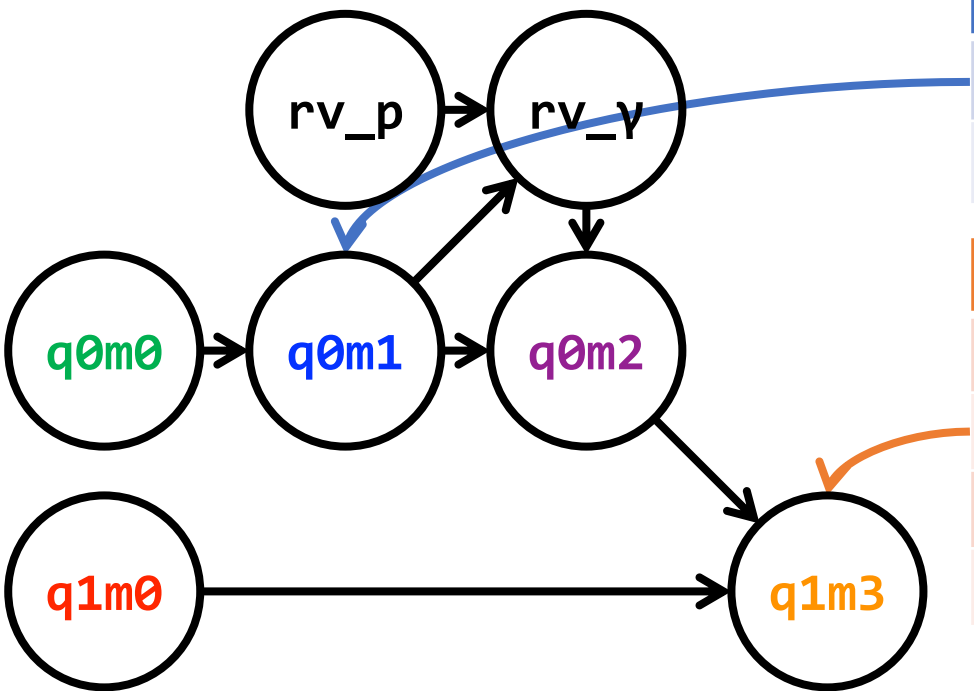
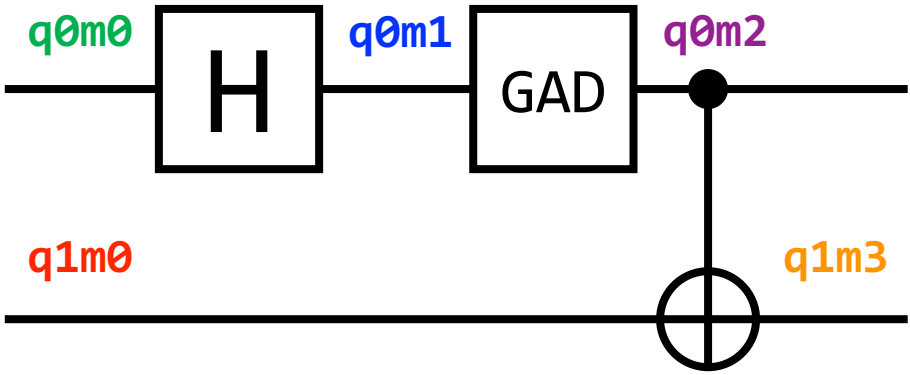
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Bayesian networks: AI models that encode probabilistic knowledge in a factorized format



Noisy quantum circuits to Bayesian network



q0m0	P(q0m1= 0>)	P(q0m1= 1>)
0>	+1/√2	+1/√2
1>	+1/√2	-1/√2

Control q0m2	Target q1m0	P(q1m3= 0>)	P(q1m3= 1>)
0>	0>	1.	0.
0>	1>	0.	1.
1>	0>	0.	1.
1>	1>	1.	0.

Connection between quantum circuits and probabilistic graphical models

	Quantum	Probabilistic
Key analogies	program simulation qubits amplitudes operator unitary matrices superposition states entangled qubits measurement	inference random variables probabilities conditional probability tables probability distributions dependent random variables sampling & conditioning
Key distinctions	amplitudes are complex-valued squares of amplitudes sum to 1 interference (canceling of amplitudes) possible	probabilities between 0 and 1 probabilities sum to 1 interference impossible

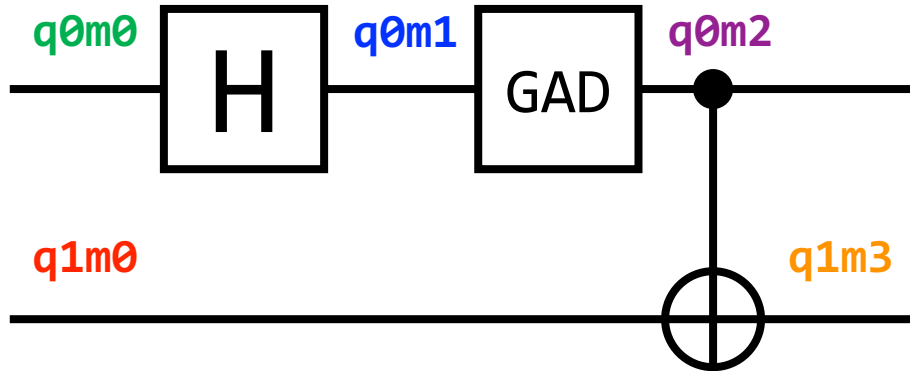
Quantum / probabilistic:

Separated by Gottesman-Knill theorem, ideas can cross-pollinate

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Bayesian networks to conjunctive normal form (CNF)

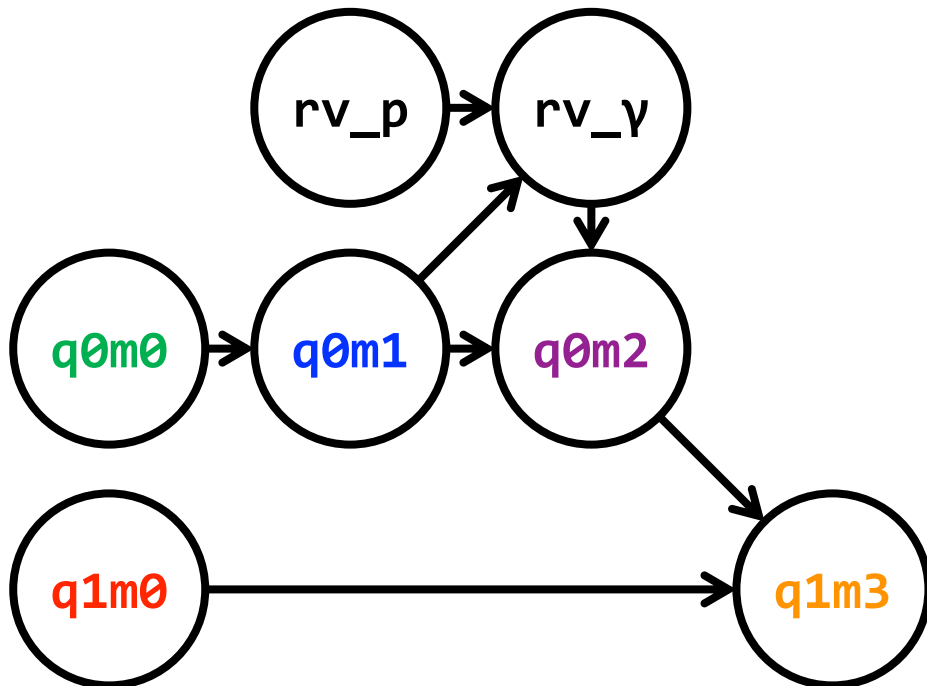


Think about circuit as logic equation

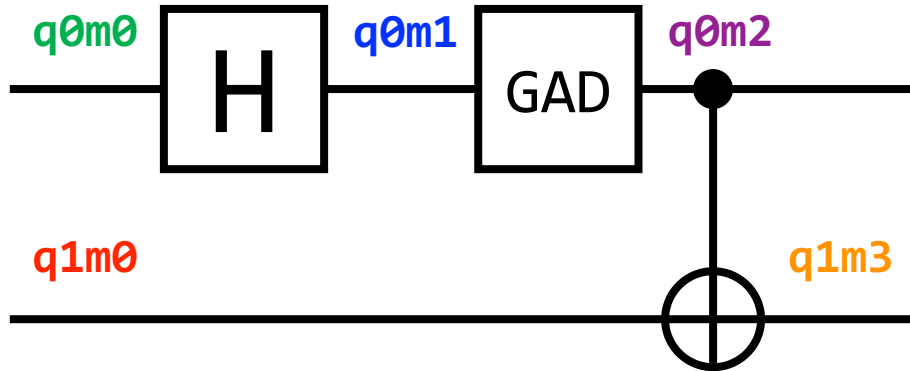
Compile & minimize this logic equation

Variable assignments that satisfy CNF are valid Feynman paths through algorithm

- Model count on variable assignments yields quantum circuit simulation



Bayesian networks to conjunctive normal form (CNF)



Qubits take on binary values:

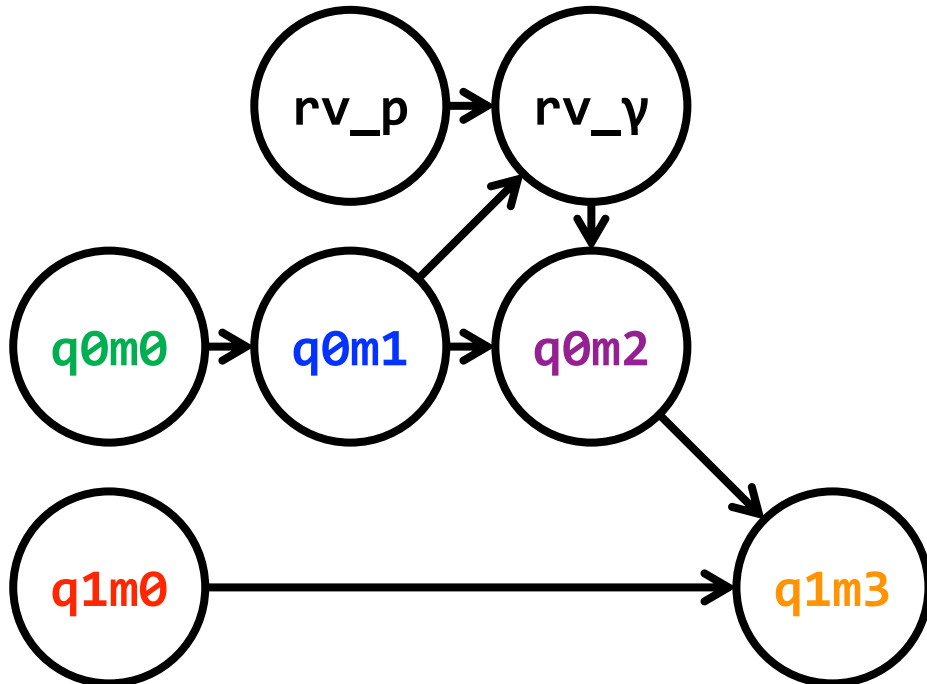
$q_{0m0} = |0\rangle$ XOR $q_{0m0} = |1\rangle$

$q_{0m1} = |0\rangle$ XOR $q_{0m1} = |1\rangle$

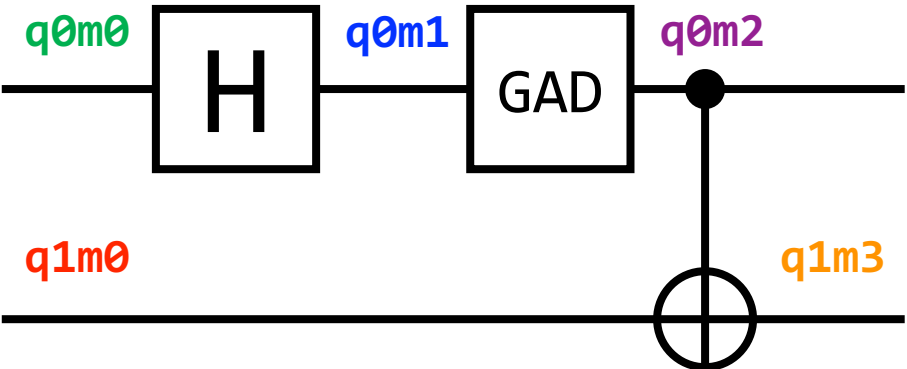
$q_{0m2} = |0\rangle$ XOR $q_{0m2} = |1\rangle$

$q_{1m0} = |0\rangle$ XOR $q_{1m0} = |1\rangle$

$q_{1m3} = |0\rangle$ XOR $q_{1m3} = |1\rangle$

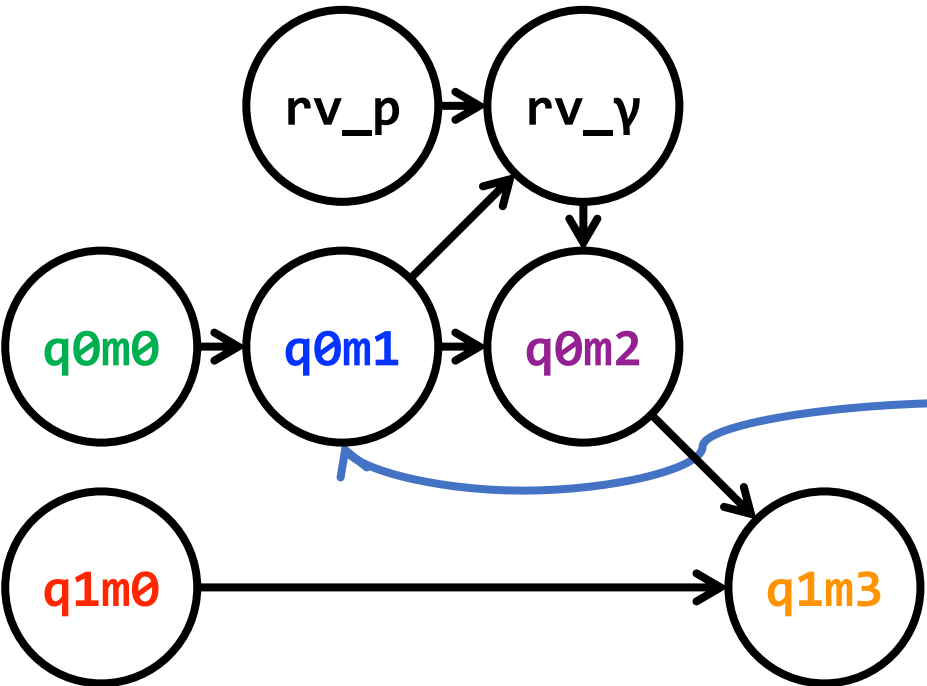


Bayesian networks to conjunctive normal form (CNF)



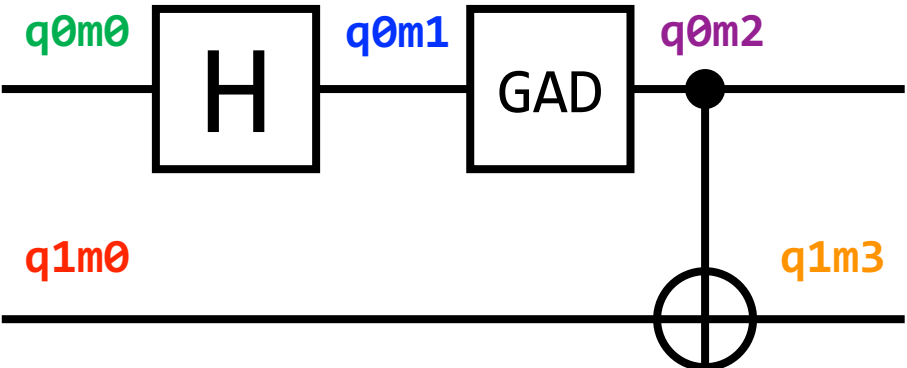
The Hadamard gate:

$$\begin{aligned} q_{0m0} = |0\rangle \text{ AND } q_{0m1} = |0\rangle &\rightarrow +1/\text{sqrt}(2) \\ q_{0m0} = |0\rangle \text{ AND } q_{0m1} = |1\rangle &\rightarrow +1/\text{sqrt}(2) \\ q_{0m0} = |1\rangle \text{ AND } q_{0m1} = |0\rangle &\rightarrow +1/\text{sqrt}(2) \\ q_{0m0} = |1\rangle \text{ AND } q_{0m1} = |1\rangle &\rightarrow -1/\text{sqrt}(2) \end{aligned}$$



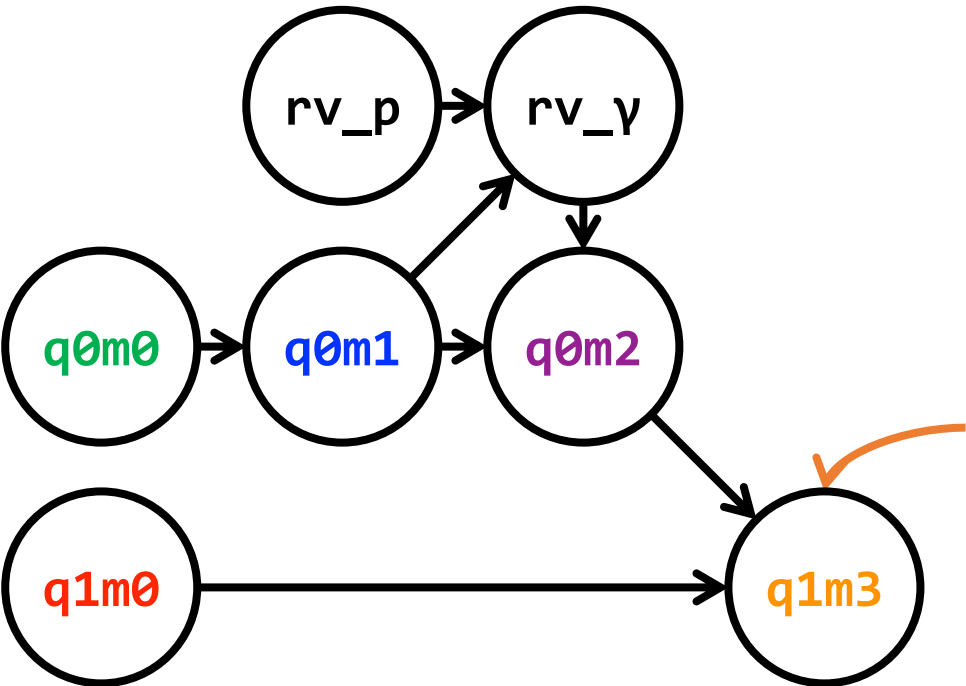
q_{0m0}	$P(q_{0m1}= 0\rangle)$	$P(q_{0m1}= 1\rangle)$
$ 0\rangle$	$+1/\sqrt{2}$	$+1/\sqrt{2}$
$ 1\rangle$	$+1/\sqrt{2}$	$-1/\sqrt{2}$

Bayesian networks to conjunctive normal form (CNF)



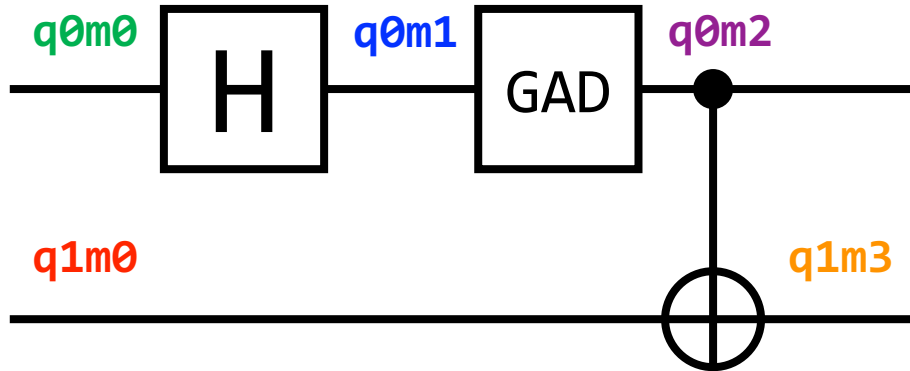
The CNOT gate:

$q_{0m2} = |0\rangle$ AND $q_{1m0} = |0\rangle \rightarrow q_{1m3} = |0\rangle$
 $q_{0m2} = |0\rangle$ AND $q_{1m0} = |1\rangle \rightarrow q_{1m3} = |1\rangle$
 $q_{0m2} = |1\rangle$ AND $q_{1m0} = |0\rangle \rightarrow q_{1m3} = |1\rangle$
 $q_{0m2} = |1\rangle$ AND $q_{1m0} = |1\rangle \rightarrow q_{1m3} = |0\rangle$



Control q_{0m2}	Target q_{1m0}	$P(q_{1m3}= 0\rangle)$	$P(q_{1m3}= 1\rangle)$
$ 0\rangle$	$ 0\rangle$	1.	0.
$ 0\rangle$	$ 1\rangle$	0.	1.
$ 1\rangle$	$ 0\rangle$	0.	1.
$ 1\rangle$	$ 1\rangle$	1.	0.

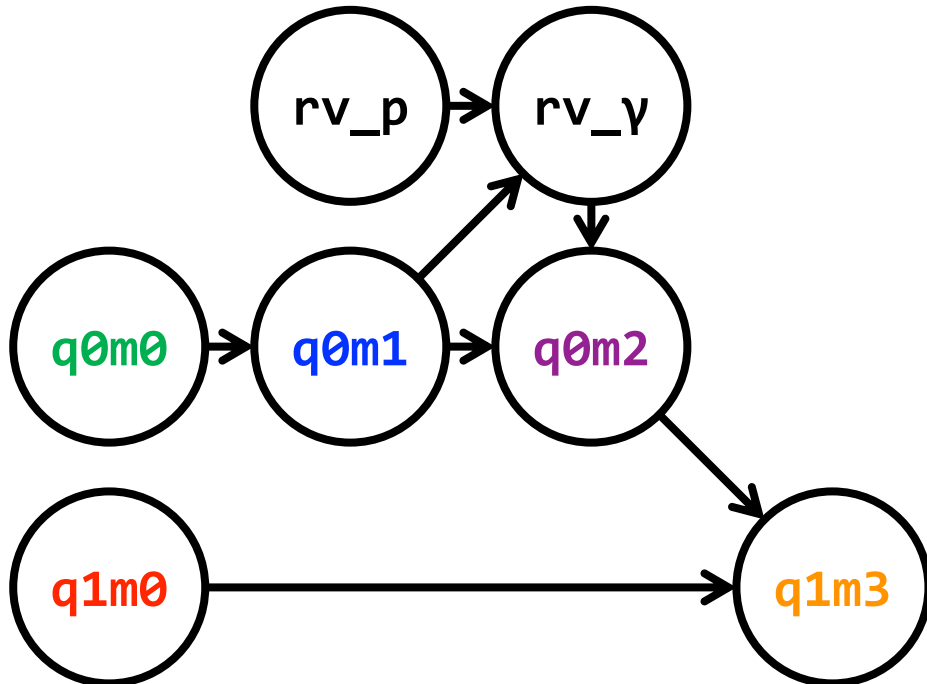
Bayesian networks to conjunctive normal form (CNF)



Put all the sentences together!

Convert logical implications " \rightarrow " to logical disjunctions

Conjoin all the disjunctive clauses together to form CNF (i.e., AND all the ORs together)



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CNF to arithmetic circuit (AC)

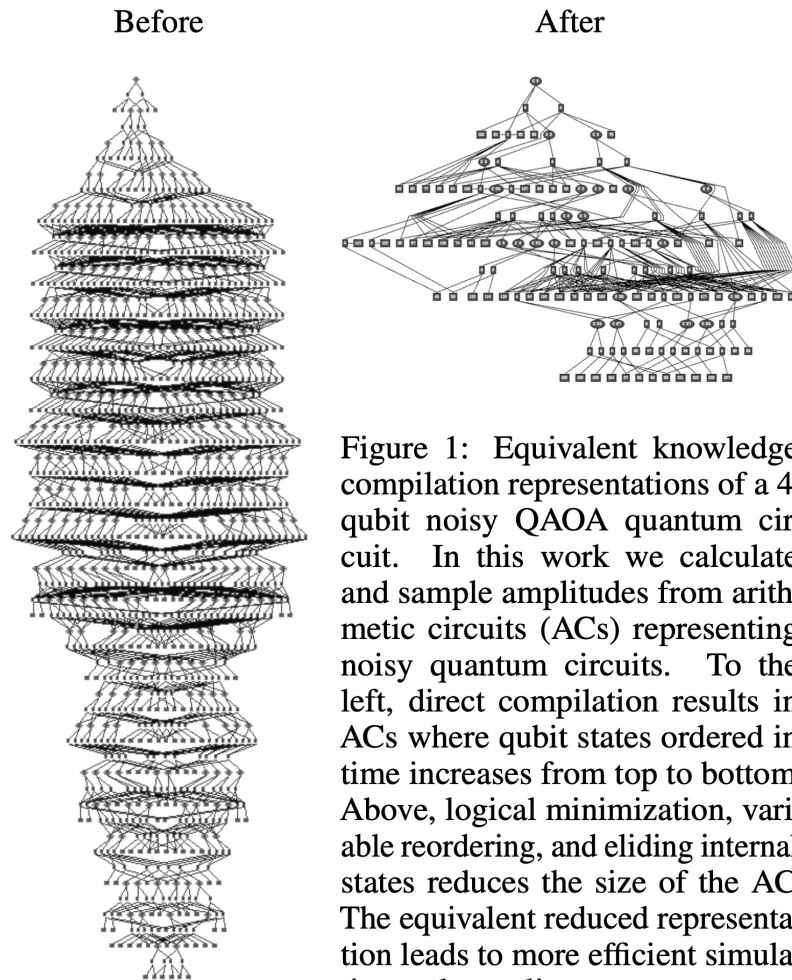


Figure 1: Equivalent knowledge compilation representations of a 4-qubit noisy QAOA quantum circuit. In this work we calculate and sample amplitudes from arithmetic circuits (ACs) representing noisy quantum circuits. To the left, direct compilation results in ACs where qubit states ordered in time increases from top to bottom. Above, logical minimization, variable reordering, and eliding internal states reduces the size of the AC. The equivalent reduced representation leads to more efficient simulation and sampling.

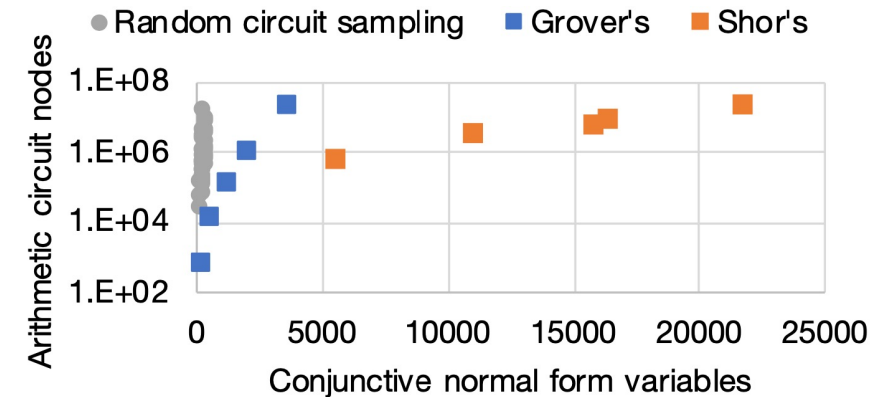
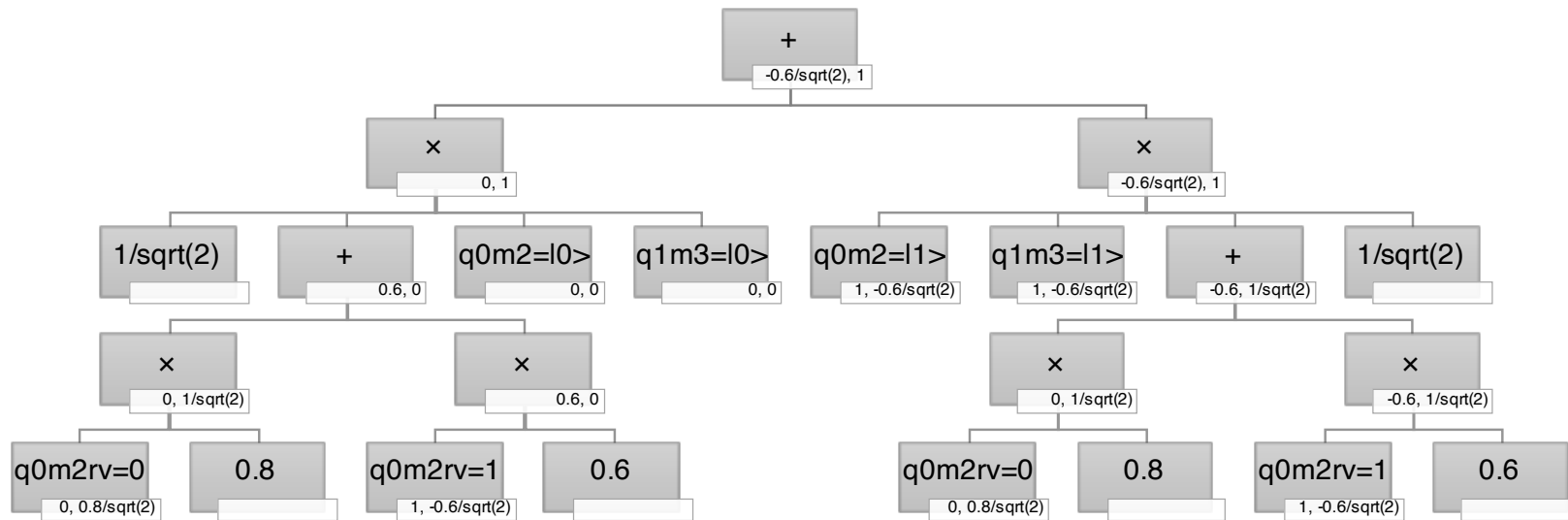


Figure 6: Simulation resource requirements vs. quantum circuit size for three quantum algorithms

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Exact inference on AC for quantum circuit simulation



- Quantum simulation becomes tree traversal on AC

Exact inference on AC for quantum circuit simulation

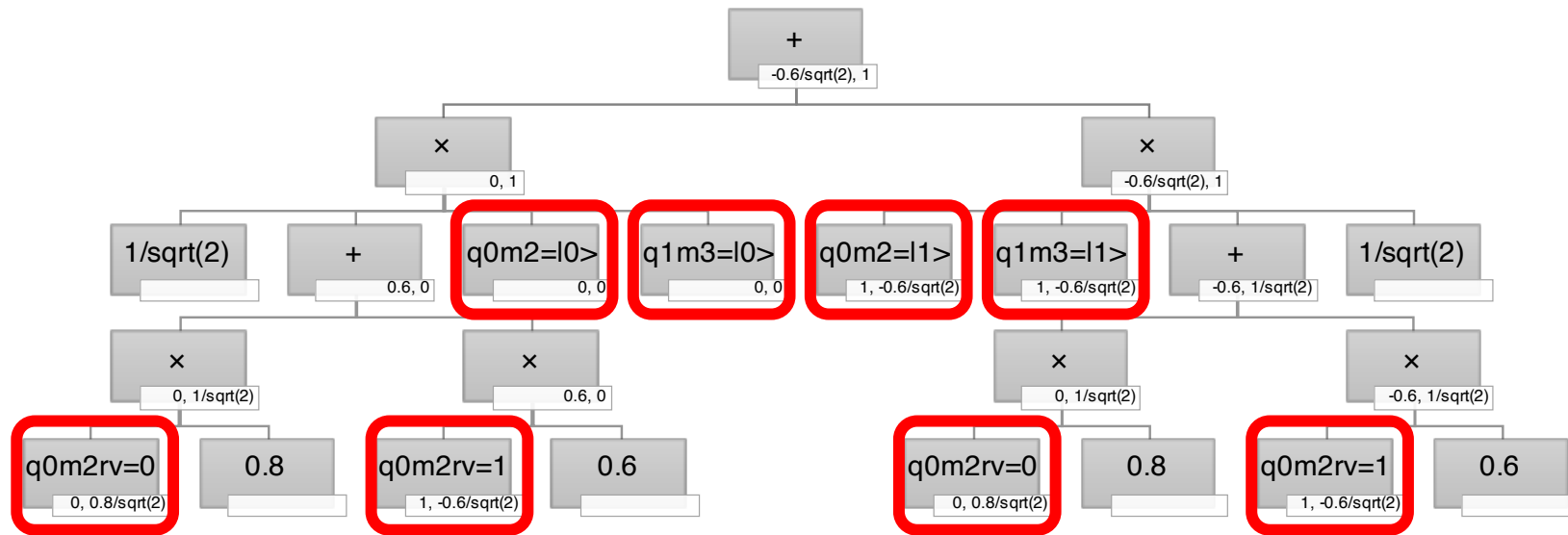


Table 9: Upward pass for finding amplitudes

q0m2rv	q0m2	q1m3	amplitude	density matrix component
0	$ 0\rangle$	$ 0\rangle$	$0.8 \frac{1}{\sqrt{2}}$	0.64 $\begin{bmatrix} +1/2 & 0 & 0 & +1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1/2 & 0 & 0 & +1/2 \end{bmatrix}$
0	$ 0\rangle$	$ 1\rangle$	0	
0	$ 1\rangle$	$ 0\rangle$	0	
0	$ 1\rangle$	$ 1\rangle$	$0.8 \frac{1}{\sqrt{2}}$	
1	$ 0\rangle$	$ 0\rangle$	$0.6 \frac{1}{\sqrt{2}}$	0.36 $\begin{bmatrix} +1/2 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1/2 & 0 & 0 & +1/2 \end{bmatrix}$
1	$ 0\rangle$	$ 1\rangle$	0	
1	$ 1\rangle$	$ 0\rangle$	0	
1	$ 1\rangle$	$ 1\rangle$	$0.6 \frac{-1}{\sqrt{2}}$	

- Quantum simulation becomes tree traversal on AC
- Quantum measurement outcomes are probabilistic evidence

Exact inference on AC for quantum circuit simulation

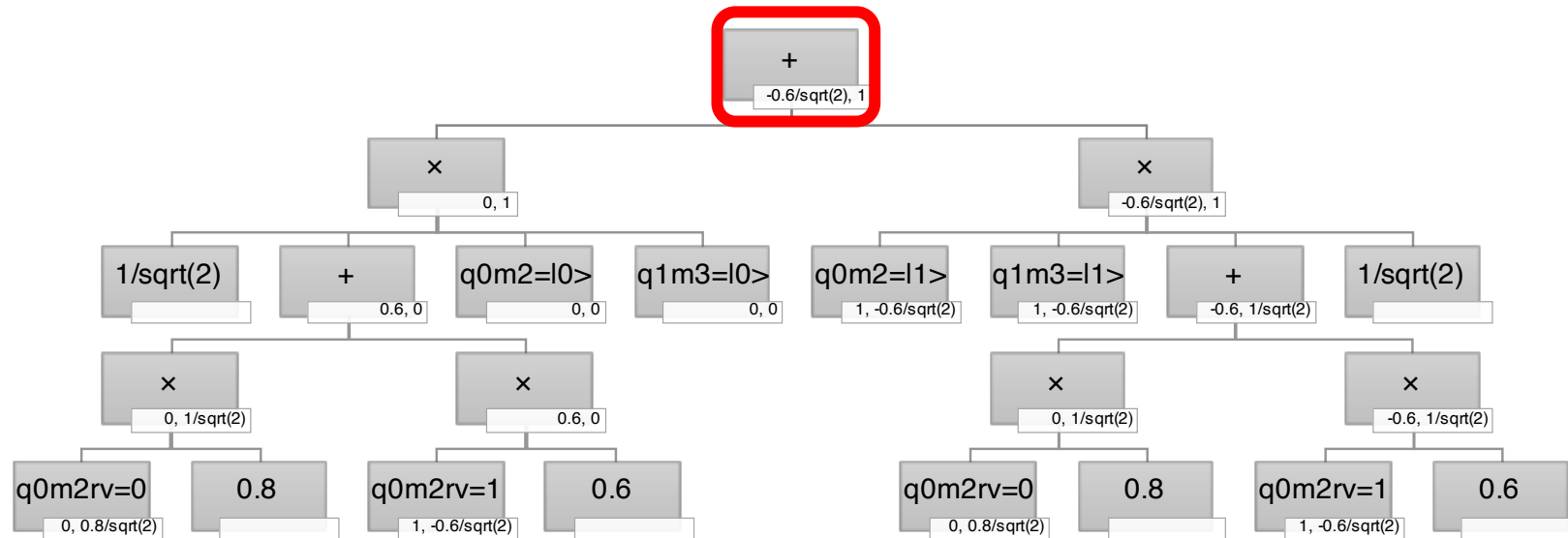


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0	$ 0\rangle$	$ 1\rangle$	0	
0	$ 1\rangle$	$ 0\rangle$	0	
0	$ 1\rangle$	$ 1\rangle$	$0.8 \frac{1}{\sqrt{2}}$	
1	$ 0\rangle$	$ 0\rangle$	$0.6 \frac{1}{\sqrt{2}}$	0.36 $\begin{bmatrix} +1/2 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1/2 & 0 & 0 & +1/2 \end{bmatrix}$
1	$ 0\rangle$	$ 1\rangle$	0	
1	$ 1\rangle$	$ 0\rangle$	0	
1	$ 1\rangle$	$ 1\rangle$	$0.6 \frac{-1}{\sqrt{2}}$	

- Quantum simulation becomes tree traversal on AC
- Quantum measurement outcomes are probabilistic evidence
- **Amplitude for given outcome comes from root node**

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Gibbs sampling on AC to sample from final wavefunction

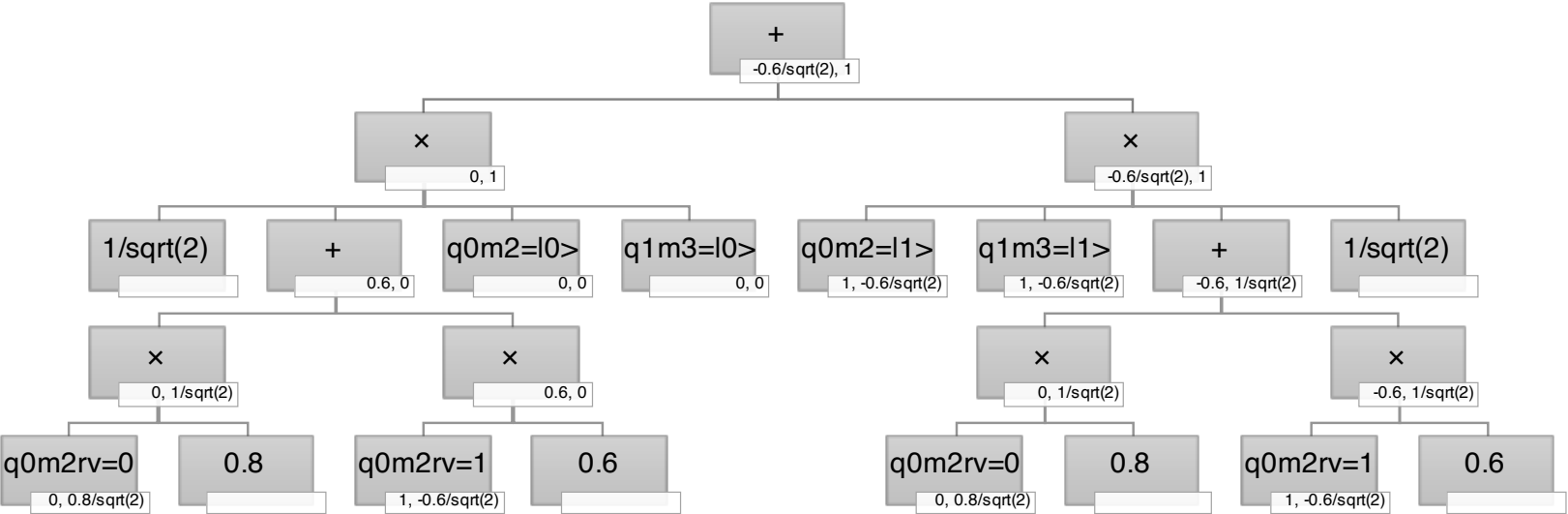
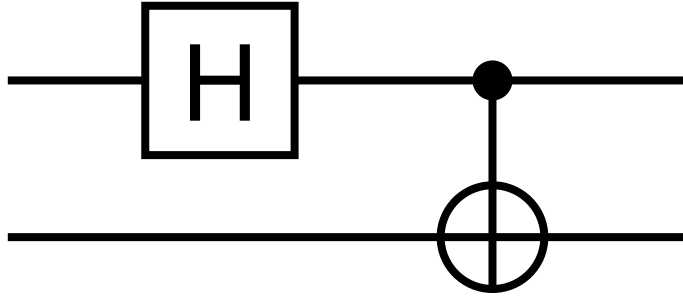


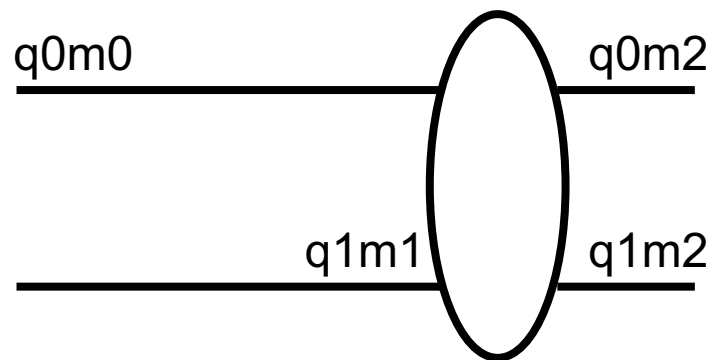
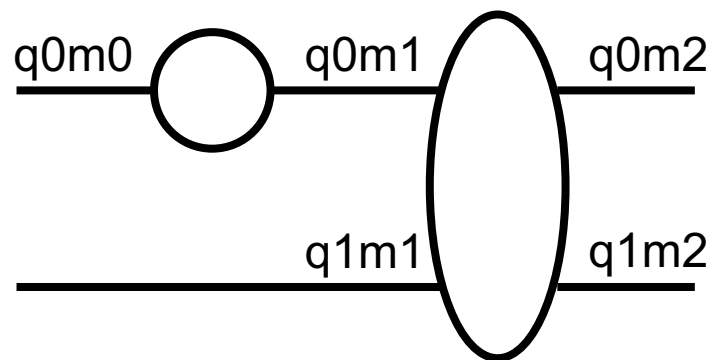
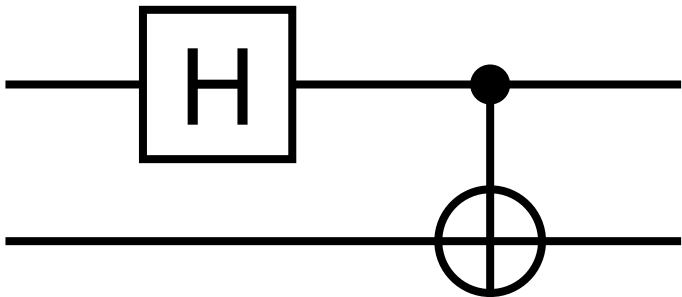
Table 10: Downward pass for finding derivatives for Gibbs sampling MCMC

	q0m2rv	q0m2	q1m3	amplitude
Present sample	1	1⟩	1⟩	$0.6 \frac{-1}{\sqrt{2}}$
Gibbs sample noise	0	1⟩	1⟩	$0.8 \frac{1}{\sqrt{2}}$
Gibbs sample qubits	1	0⟩	1⟩	0
Gibbs sample qubits	1	1⟩	0⟩	0

Schrödinger quantum circuit simulation



$$\text{CNOT}(H \otimes I|00\rangle) = \text{CNOT}(H|0\rangle \otimes I|0\rangle) = \text{CNOT} \begin{bmatrix} \frac{1}{\sqrt{2}} [1] \\ \frac{1}{\sqrt{2}} [0] \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix} = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$



q0m
0= $|0\rangle$ q0m
0= $|1\rangle$

q0m 1= $ 0\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
q0m 1= $ 1\rangle$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

q0m2= $|0\rangle$ q1m2= $|0\rangle$
q1m2= $|1\rangle$
q0m2= $|1\rangle$ q1m2= $|0\rangle$
q1m2= $|1\rangle$

q0m2= $|0\rangle$ q1m2= $|0\rangle$
q1m2= $|1\rangle$
q0m2= $|1\rangle$ q1m2= $|0\rangle$
q1m2= $|1\rangle$

Feynman quantum circuit simulation

q0m1= $ 0\rangle$		q0m1= $ 1\rangle$	
q1m1= $ 0\rangle$	q1m1= $ 1\rangle$	q1m1= $ 0\rangle$	q1m1= $ 1\rangle$
1	0	0	0
0	1	0	0
0	0	0	1
0	0	1	0

q0m0= $ 0\rangle$		q0m0= $ 1\rangle$	
q1m1= $ 0\rangle$	q1m1= $ 1\rangle$	q1m1= $ 0\rangle$	q1m1= $ 1\rangle$
$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0

Where we are going.

What are quantum variational algorithms?

- Why are they different and important?

What is quantum circuit simulation?

- Why are the conventional techniques insufficient?

How do we represent quantum circuits as logic formulas?

- Why does it help with variational algorithm simulation, and by how much?

Where we are going.

What are quantum variational algorithms?

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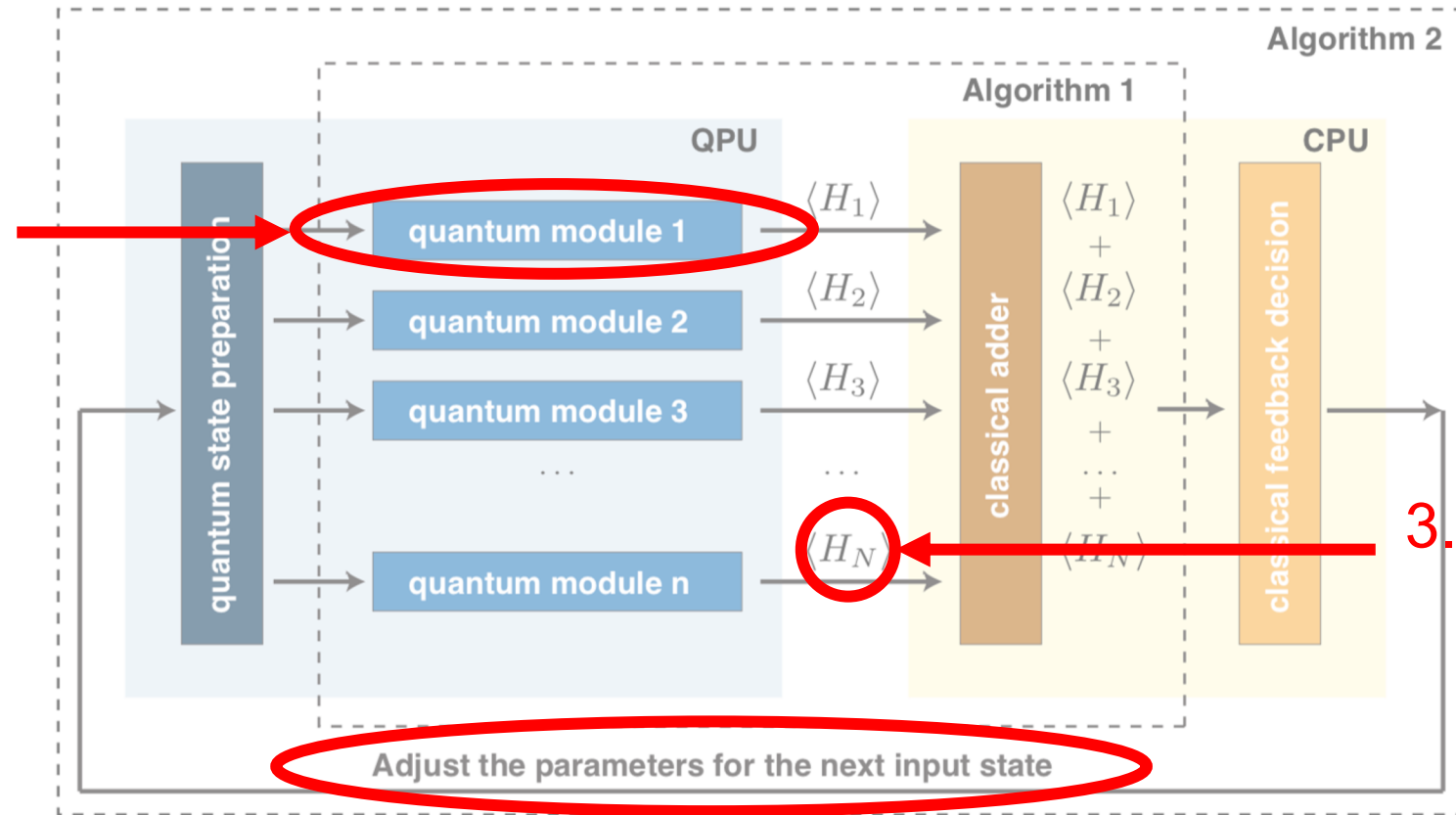
- Why are the conventional techniques insufficient?

How do we represent quantum circuits as logic formulas?

- *Why does it help with variational algorithm simulation, and by how much?*

The unique challenge of simulating noisy variational algorithms


1. Needs to simulate noise, and quantum circuits are wide but shallow



3. Only need samples, not full wavefunctions.

2. Require repeated simulation with different parameters

Our toolchain: Bayesian network knowledge compilation for noisy quantum circuit simulation and sampling

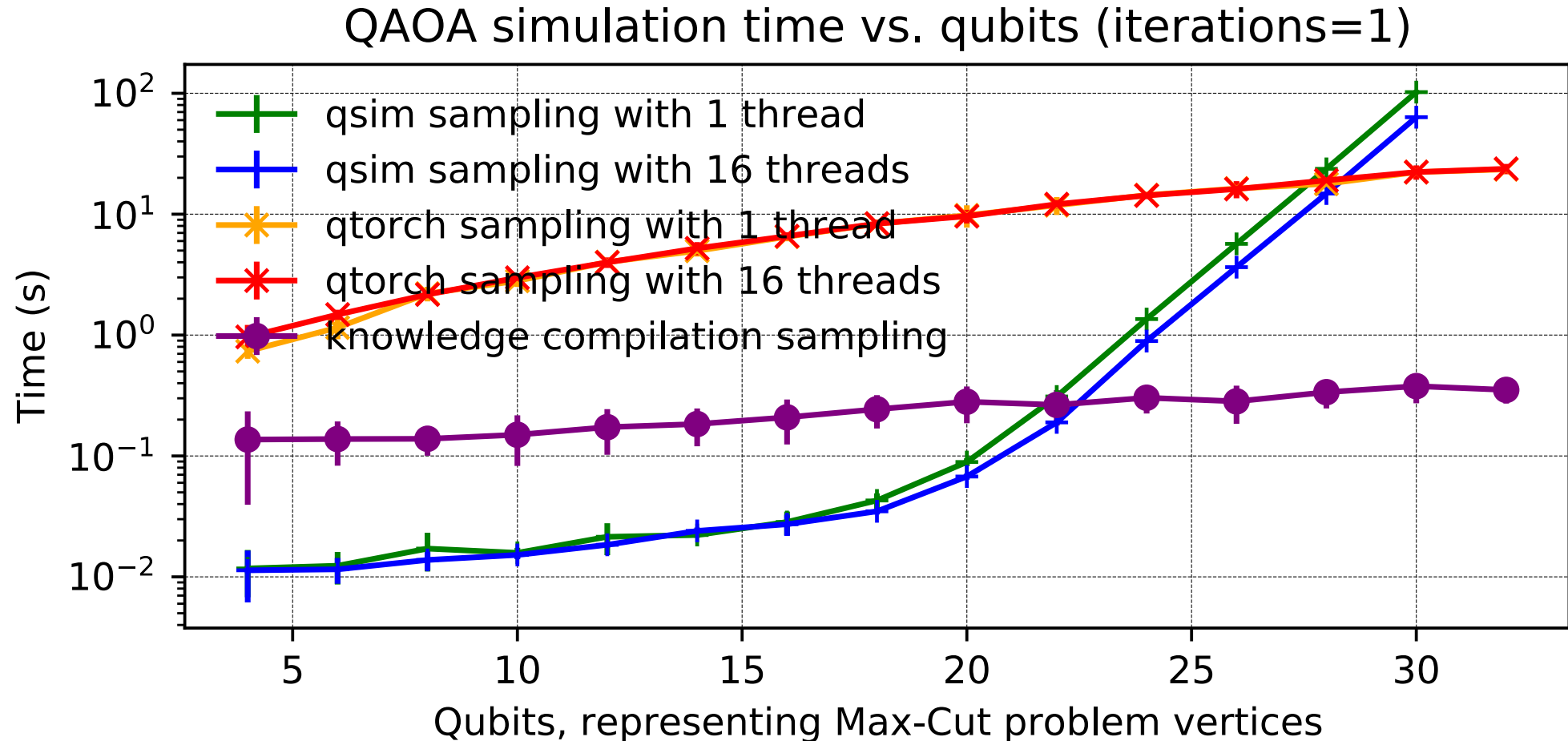
1. Noisy quantum circuits to Bayesian network
 2. Bayesian networks to conjunctive normal form (CNF)
 3. CNF to arithmetic circuit (AC)
 4. Exact inference on AC for quantum circuit simulation
 5. Gibbs sampling on AC to sample from final wavefunction
- 
1. Needs to simulate noise
 2. Repeated simulation with different parameters
 3. Only need samples, not full wavefunctions

Result 1: It works!

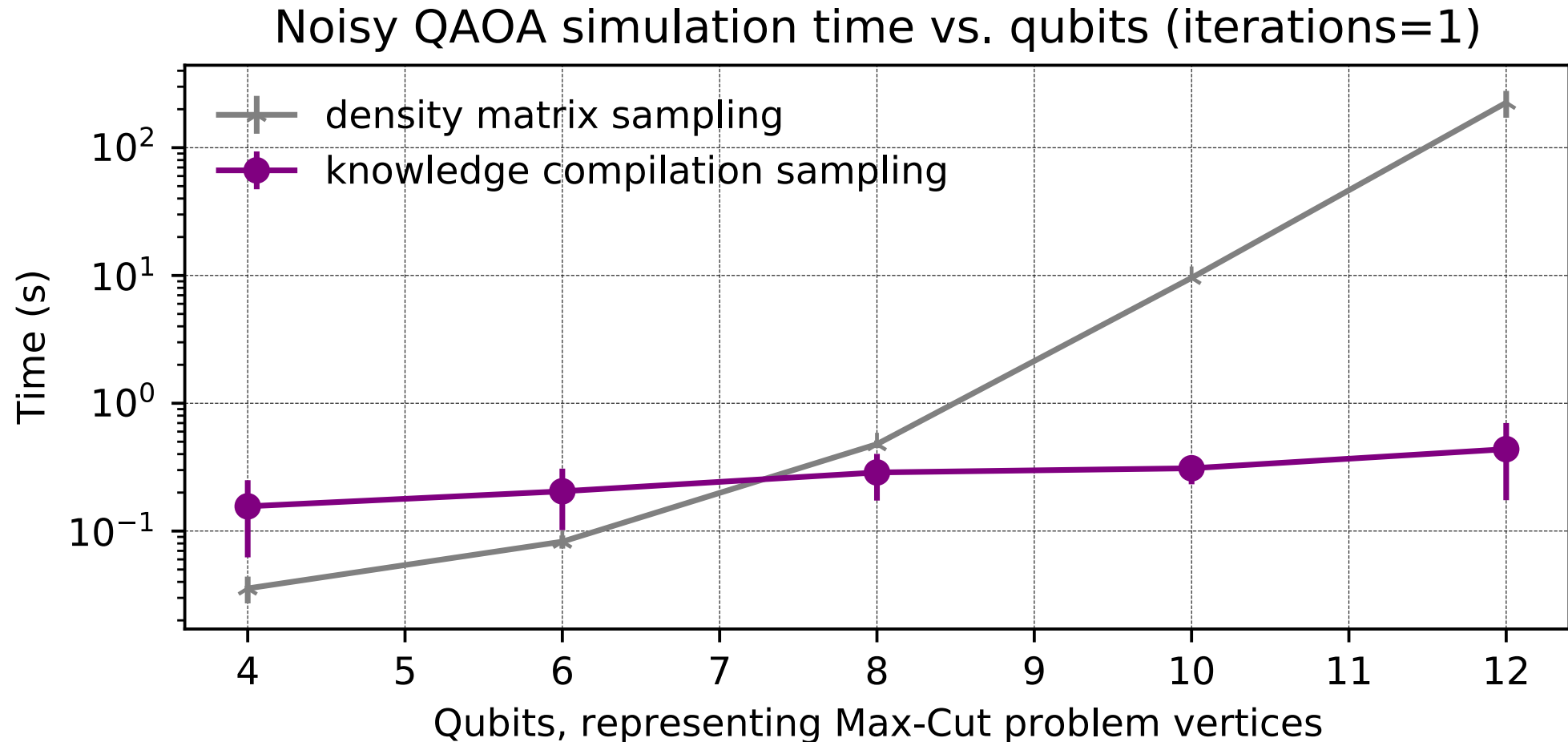
With minimal modification, knowledge compilation exact inference can be repurposed for quantum simulation

- Can accurately simulate Pauli gates, CNOT, CZ, phase kickback, Toffoli, CHSH protocol, Deutsch-Jozsa, Bernstein-Vazirani, hidden shift, quantum Fourier transform, Shor's, Grover's...
- Passes Google Cirq's suite of test harness for quantum simulators

Result 2: Ideal circuit simulation



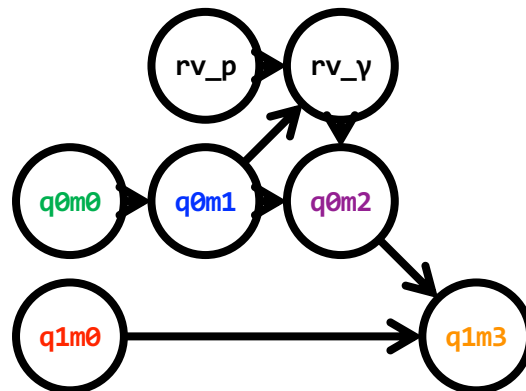
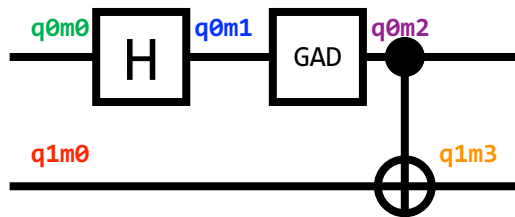
Result 2: Noisy circuit simulation



What this talk was about:

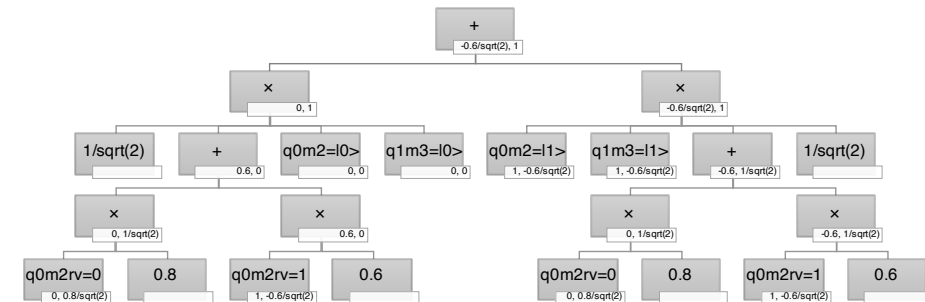
Using classical probabilistic inference techniques as an abstraction for quantum computing.

- A new way to represent noisy quantum circuits as probabilistic graphical models.
- A new way to encode quantum circuits as conjunctive normal forms and arithmetic circuits.
- A new way to manipulate quantum circuits using logical equation satisfiability solvers.
- Improved simulation and sampling performance for important near-term quantum algorithms.



The Hadamard gate:

$q0m0=|0\rangle$ AND $q0m1=|0\rangle \rightarrow +1/\sqrt{2}$
 $q0m0=|0\rangle$ AND $q0m1=|1\rangle \rightarrow +1/\sqrt{2}$
 $q0m0=|1\rangle$ AND $q0m1=|0\rangle \rightarrow +1/\sqrt{2}$
 $q0m0=|1\rangle$ AND $q0m1=|1\rangle \rightarrow -1/\sqrt{2}$



Where we have gone:

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Broader research agenda:
new representations for quantum computing

Schrödinger: state vectors and density matrices

Heisenberg: stabilizer formalism

Feynman: tensor-network path sums

Binary decision diagrams (new?)

Logical satisfiability equations (this work; new?)

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potential
synergies