Logical Abstractions for Noisy Variational Quantum Algorithm Simulation

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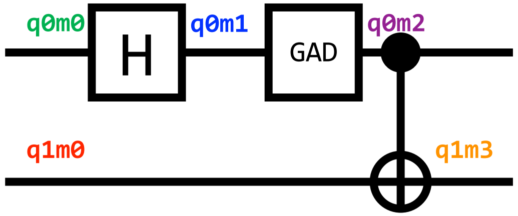
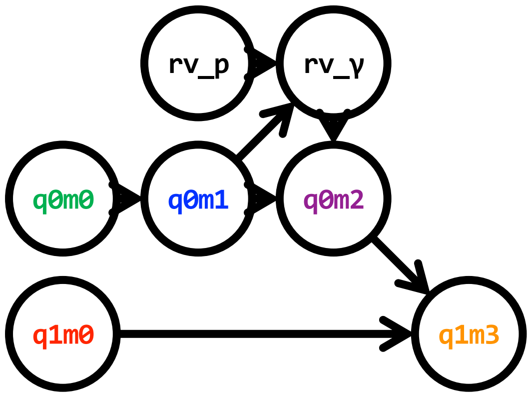
March 10, 2021

What this talk is about:

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

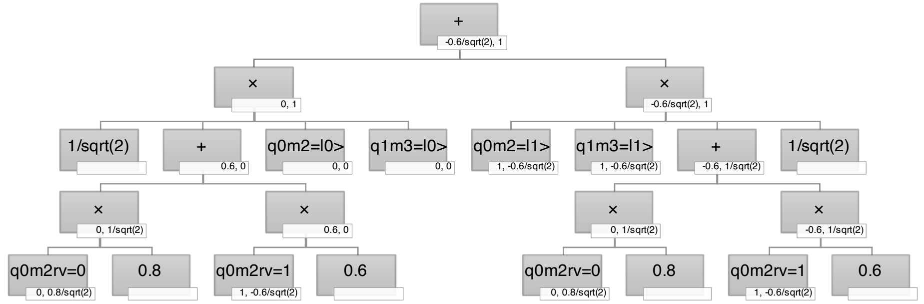
- A new way to represent noisy quantum circuits as probabilistic graphical models.
- A new way to encode quantum circuits as conjunctive normal forms and arithmetic circuits.
- A new way to manipulate quantum circuits using logical equation satisfiability solvers.
- Improved simulation and sampling performance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





The Hadamard gate:

```
q0m0=|0> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|0> AND q0m1=|1> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|1> -> -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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NISQ systems target variational algorithms.

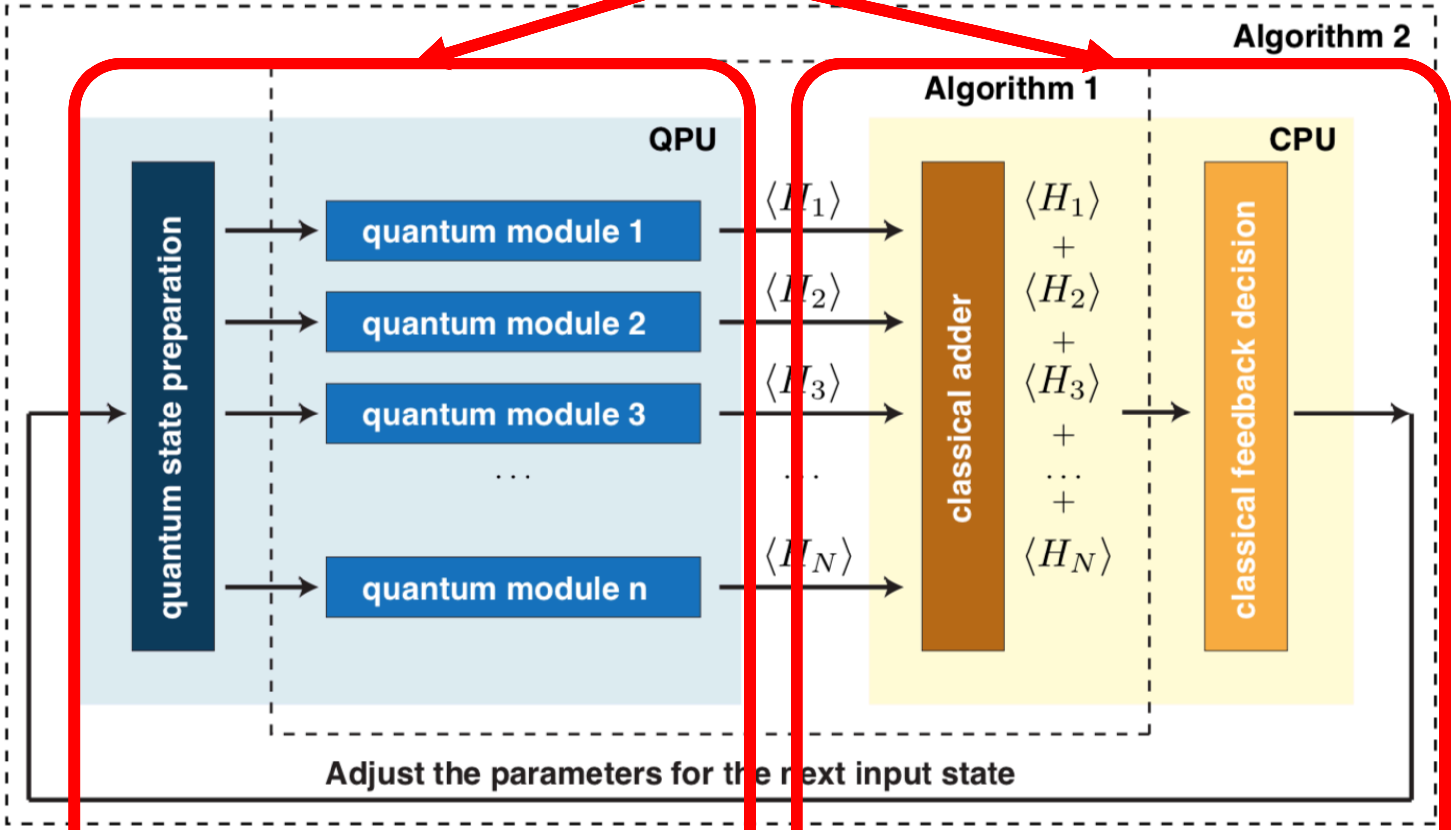
Near-term Intermediate Scale Quantum (NISQ) systems have ~100 qubits with at best 0.1% error rate.

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



Quantum evaluates an objective function

Classical optimizes for better parameters

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

Image source: Peruzzo et al., 2013

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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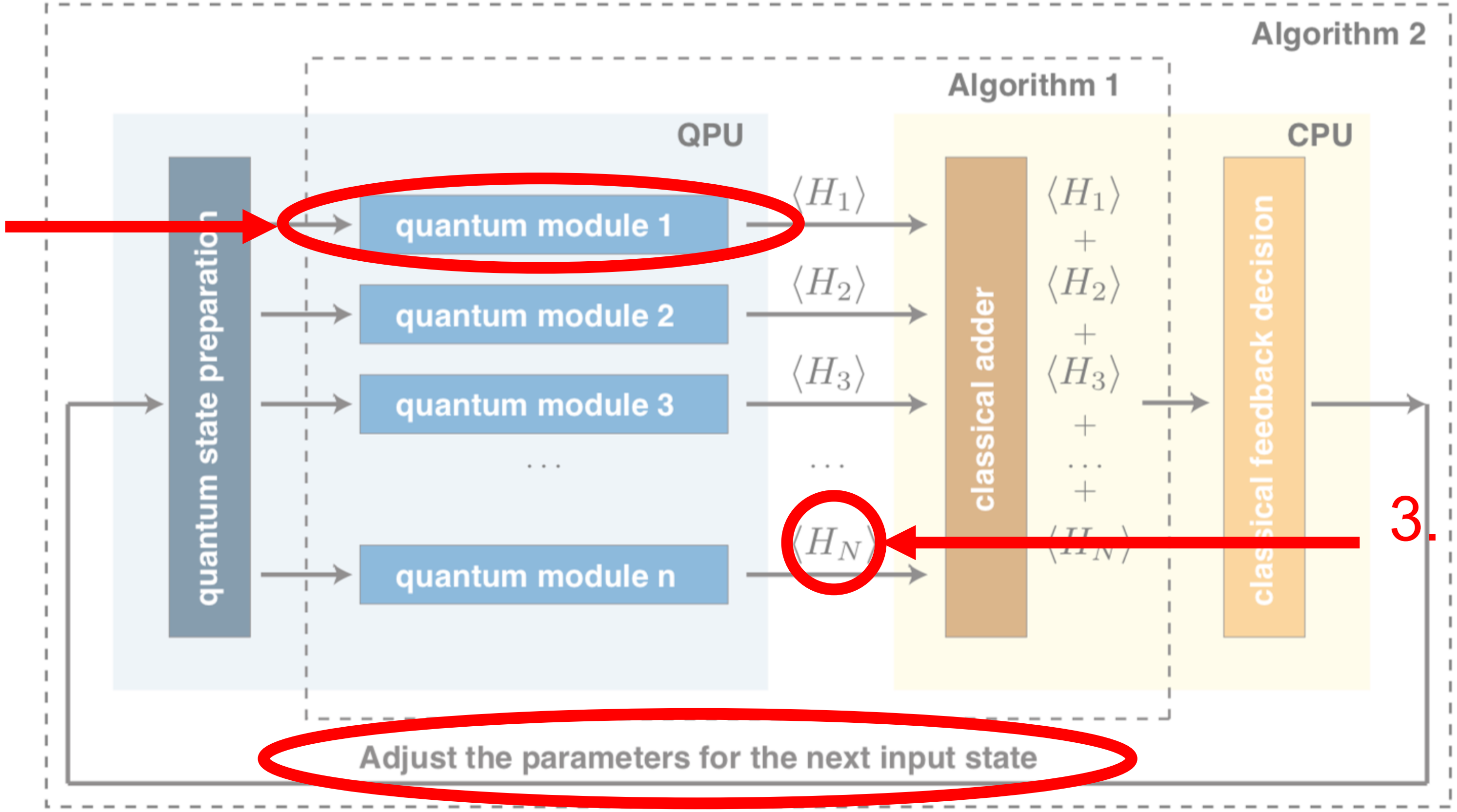
The unique challenge of simulating noisy variational algorithms

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

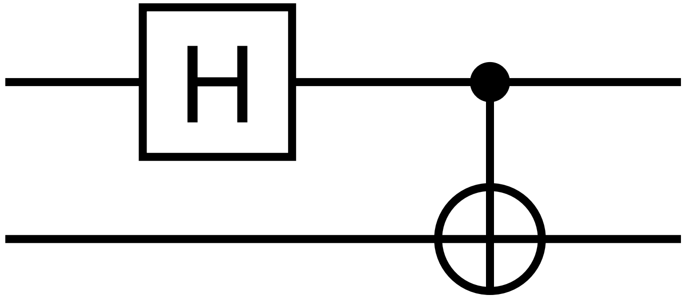
Image source: Peruzzo et al., 2013

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



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

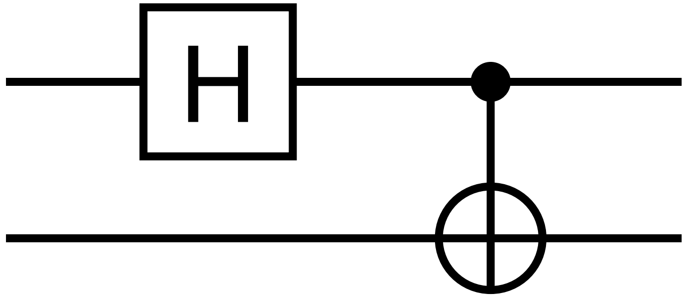
Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

	Schrödinger simulation QuEST, qSim, …; parallel matrix vector multiplication
1. Does it excel at simulating wide but shallow circuits?	✗
2. Does it extract structure for repeated simulation with different parameters?	✗
3. Does it efficiently sample from the final wavefunction?	✓

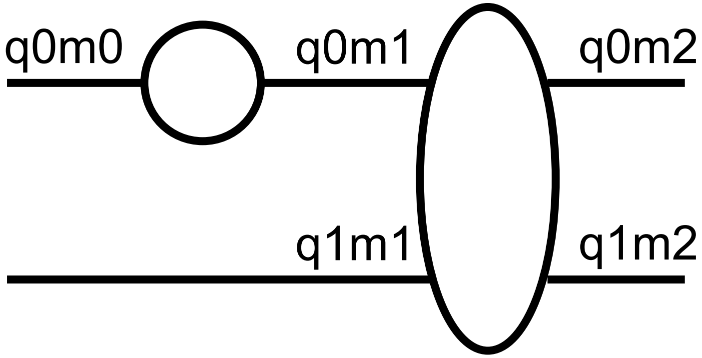
Rock, paper, scissors: Existing simulation techniques are not suited for variational algorithms

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

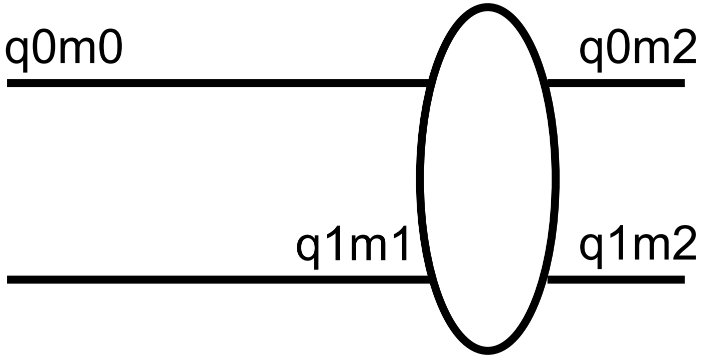
Feynman quantum circuit simulation



	q0m0=$\|0\rangle$	q0m0=$\|1\rangle$
q0m1=$\|0\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
q0m1=$\|1\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{-1}{\sqrt{2}}$



		q0m1=$\|0\rangle$		q0m1=$\|1\rangle$	
		q1m1=$\|0\rangle$	q1m1=$\|1\rangle$	q1m1=$\|0\rangle$	q1m1=$\|1\rangle$
q0m2=$\|0\rangle$	q1m2=$\|0\rangle$	1	0	0	0
	q1m2=$\|1\rangle$	0	1	0	0
q0m2=$\|1\rangle$	q1m2=$\|0\rangle$	0	0	0	1
	q1m2=$\|1\rangle$	0	0	1	0



		q0m0=$\|0\rangle$		q0m0=$\|1\rangle$	
		q1m1=$\|0\rangle$	q1m1=$\|1\rangle$	q1m1=$\|0\rangle$	q1m1=$\|1\rangle$
q0m2=$\|0\rangle$	q1m2=$\|0\rangle$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
	q1m2=$\|1\rangle$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
q0m2=$\|1\rangle$	q1m2=$\|0\rangle$	0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
	q1m2=$\|1\rangle$	$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0

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

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

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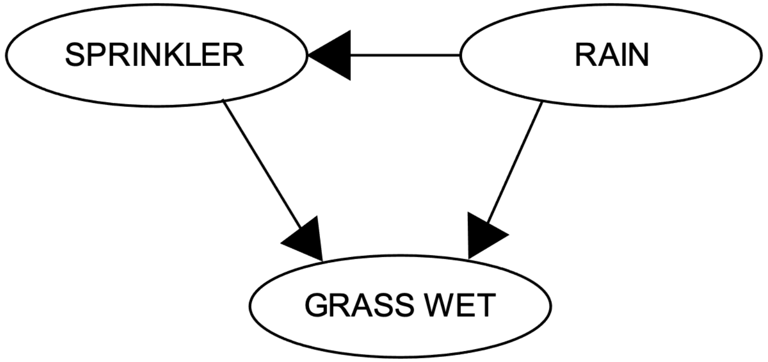
Bayesian networks: AI models that encode probabilistic knowledge in a factorized format

RAIN	SPRINKLER T	SPRINKLER F
F	0.4	0.6
T	0.01	0.99

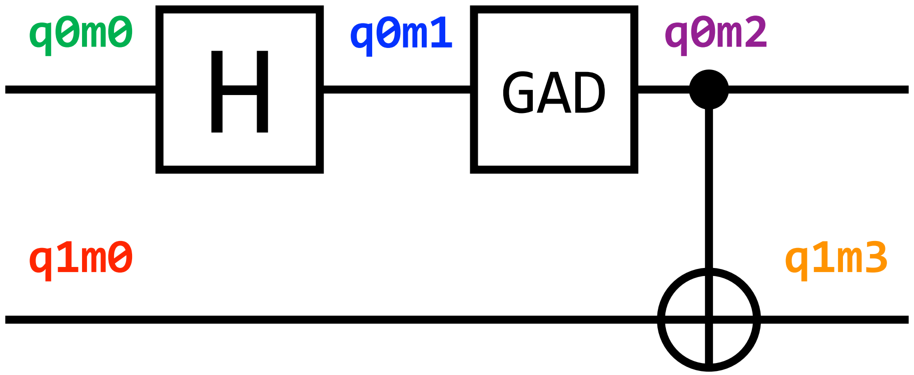


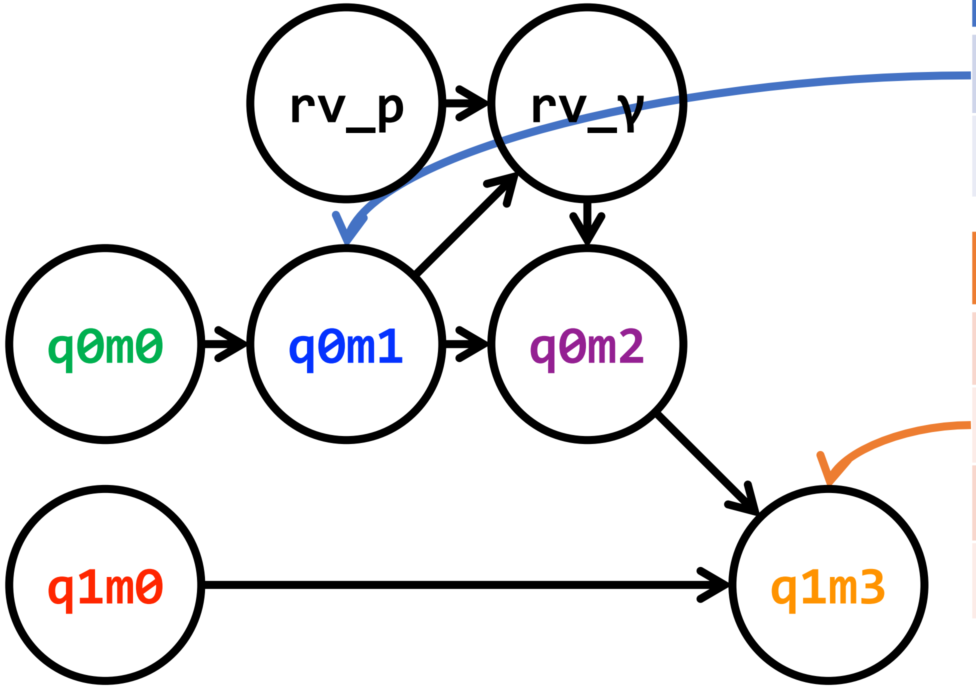
RAIN T	RAIN F
0.2	0.8

SPRINKLER	RAIN	GRASS WET T	GRASS WET F
F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01

Image source: Wikimedia

Noisy quantum circuits to Bayesian network





q0m0	P(q0m1=|0⟩)	P(q0m1=|1⟩)
|0⟩	$+1/\sqrt{2}$	$+1/\sqrt{2}$
|1⟩	$+1/\sqrt{2}$	$-1/\sqrt{2}$

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.

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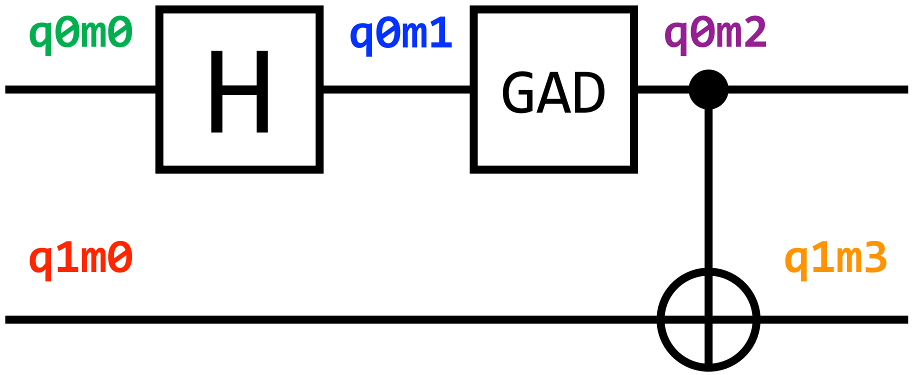
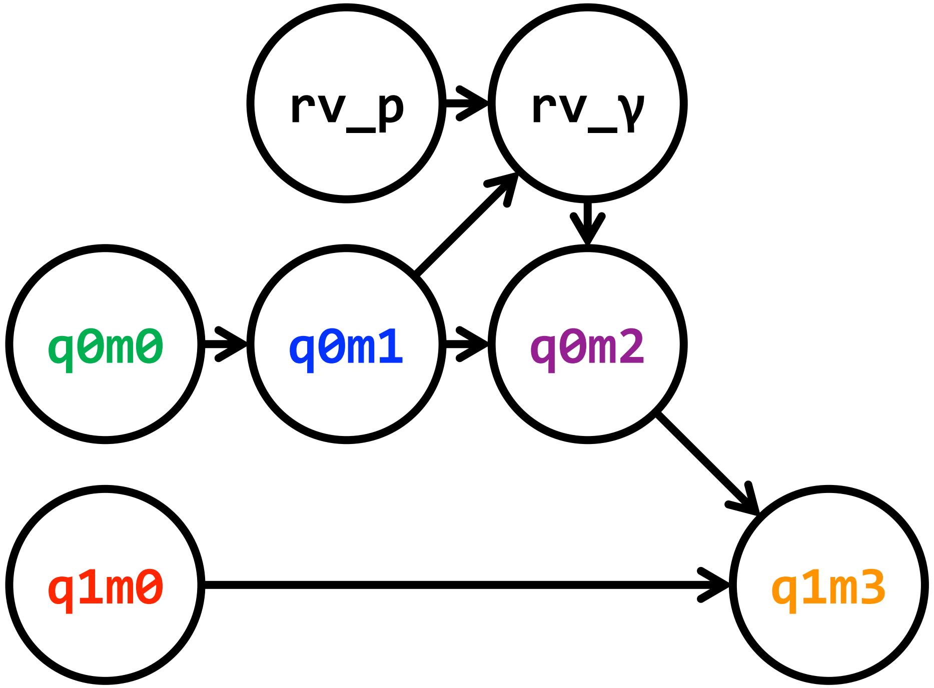
Bayesian networks to conjunctive normal form (CNF)





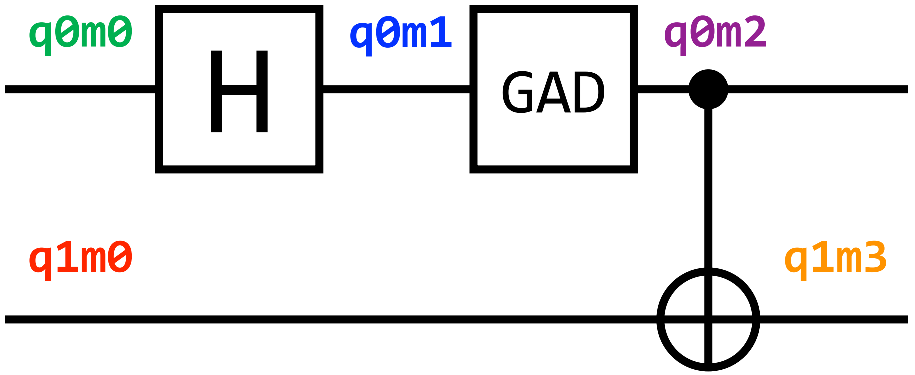
Think about circuit as logic equation

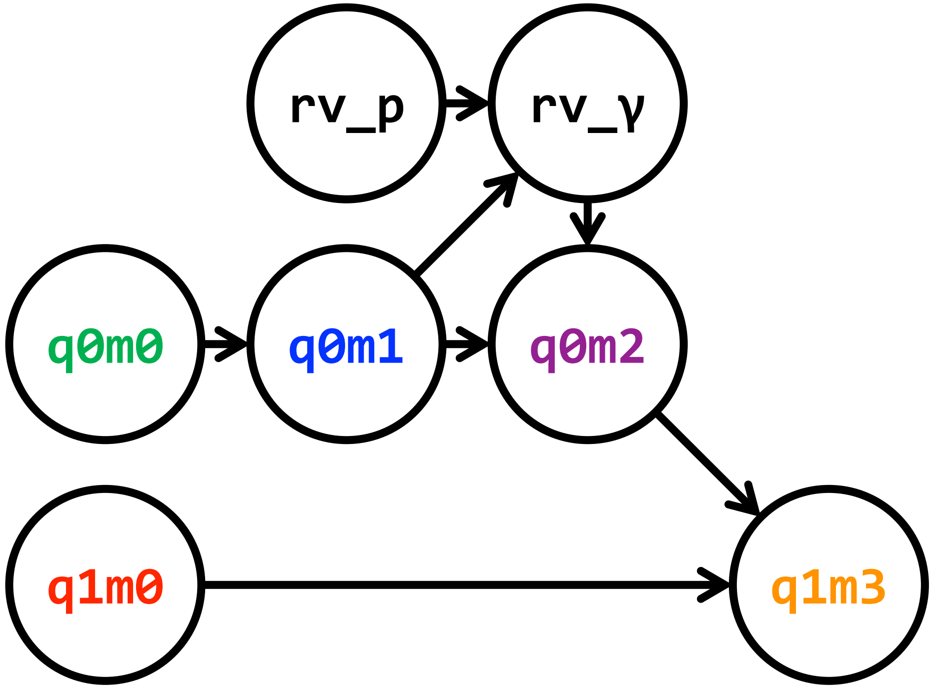
Compile & minimize this logic equation

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)



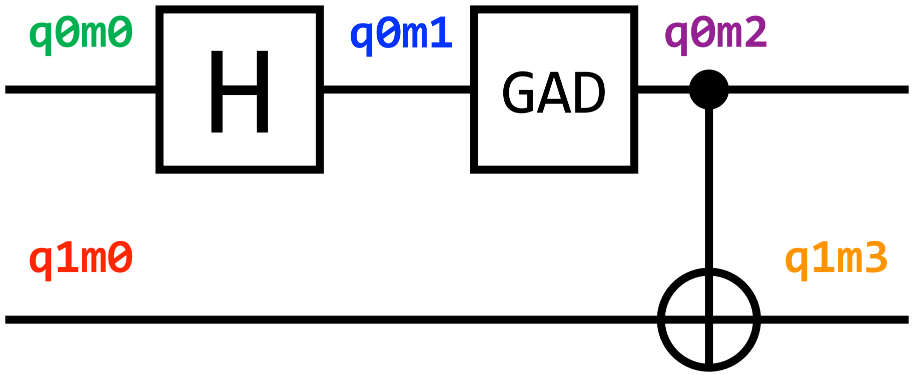


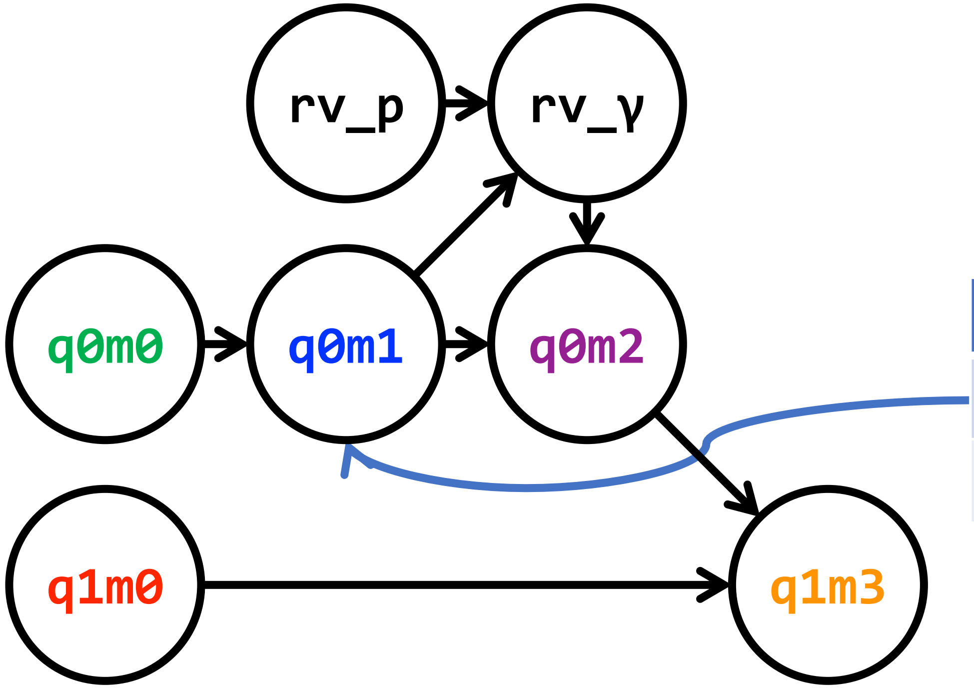
Qubits take on binary values:

q0m0=|0> XOR q0m0=|1>
q0m1=|0> XOR q0m1=|1>
q0m2=|0> XOR q0m2=|1>

q1m0=|0> XOR q1m0=|1>
q1m3=|0> XOR q1m3=|1>

Bayesian networks to conjunctive normal form (CNF)



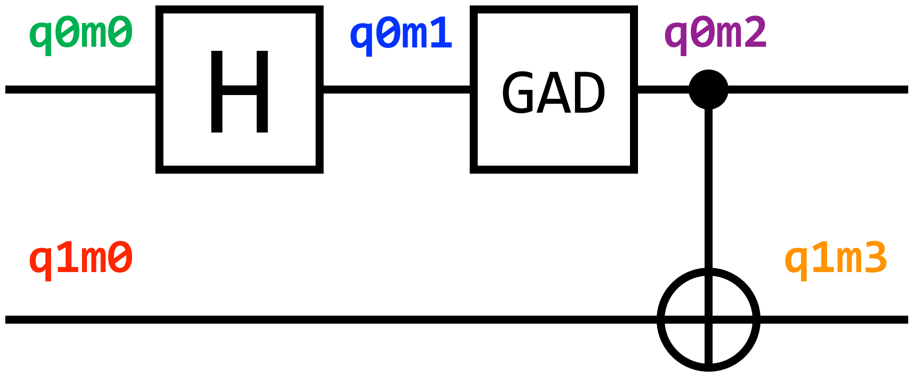


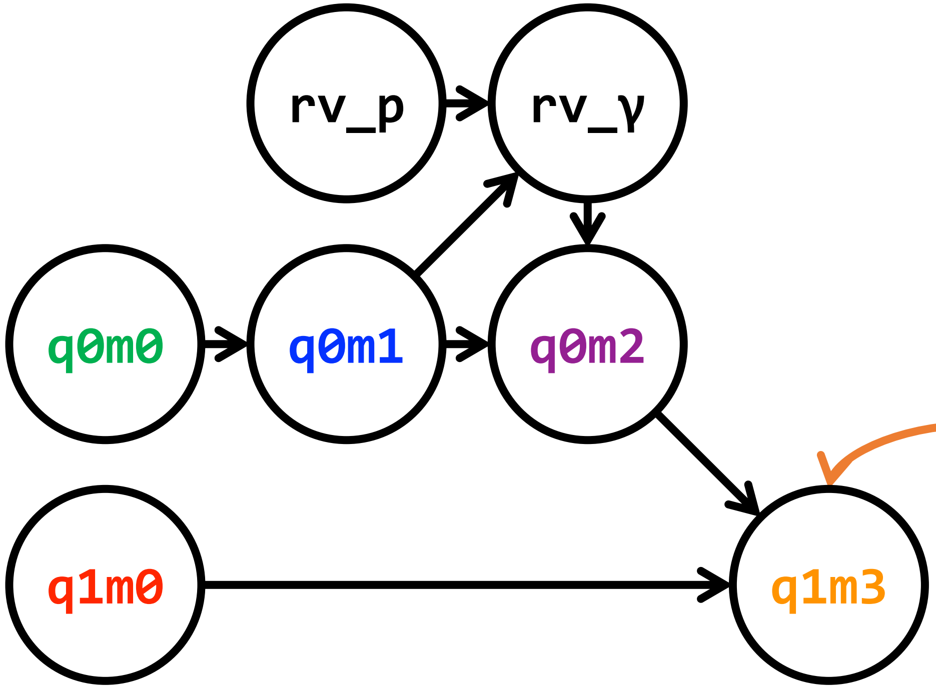
The Hadamard gate:

```
q0m0=|0> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|0> AND q0m1=|1> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|1> -> -1/sqrt(2)
```

q0m0	P(q0m1=$\|0\rangle$)	P(q0m1=$\|1\rangle$)
$\|0\rangle$	$+1/\sqrt{2}$	$+1/\sqrt{2}$
$\|1\rangle$	$+1/\sqrt{2}$	$-1/\sqrt{2}$

Bayesian networks to conjunctive normal form (CNF)





The CNOT gate:

q0m2=|0> AND q1m0=|0> -> q1m3=|0>
q0m2=|0> AND q1m0=|1> -> q1m3=|1>
q0m2=|1> AND q1m0=|0> -> q1m3=|1>
q0m2=|1> AND q1m0=|1> -> q1m3=|0>

Control q0m2	Target q1m0	P(q1m3=|0⟩)	P(q1m3=|1⟩)
|0⟩	|0⟩	1.	0.
|0⟩	|1⟩	0.	1.
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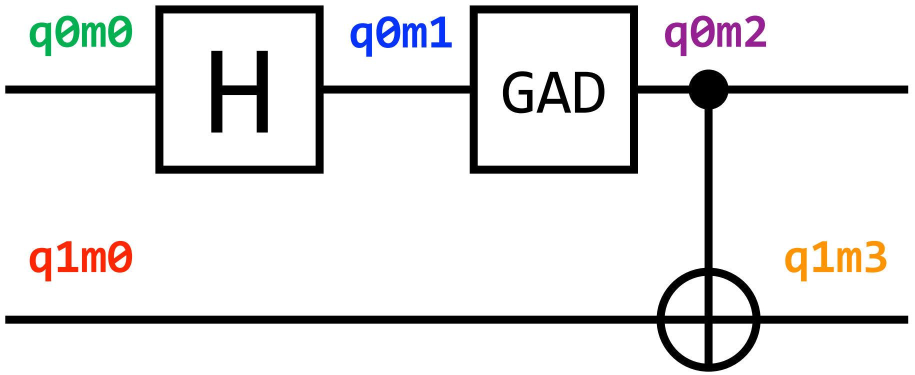
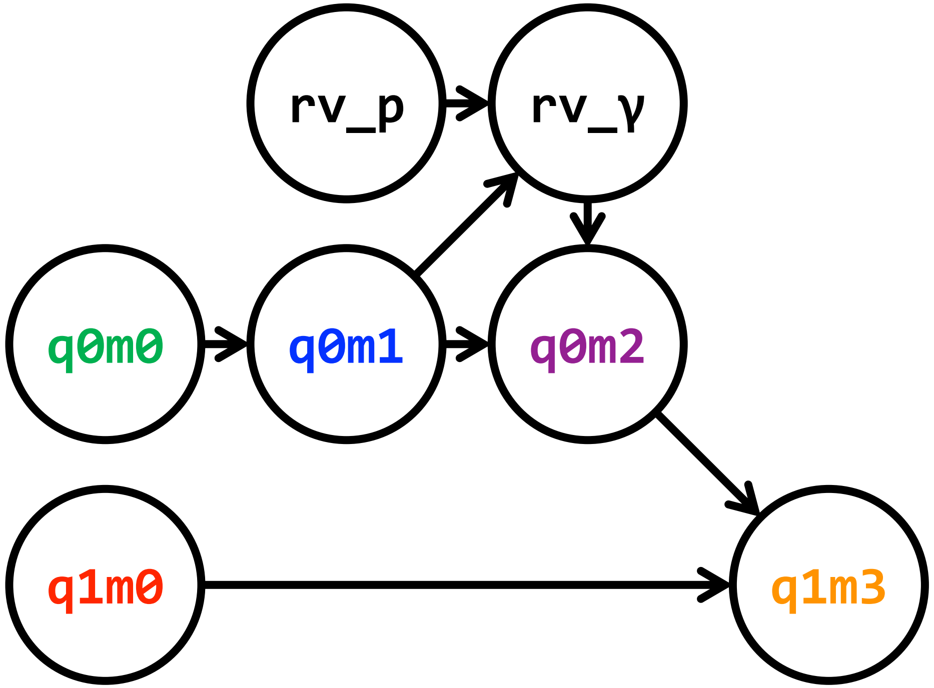
Bayesian networks to conjunctive normal form (CNF)





Put all the sentences together!

Convert logical implications "→" to logical disjunctions

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

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

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3. ***CNF to arithmetic circuit (AC)***
4. Exact inference on AC for quantum circuit simulation
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CNF to arithmetic circuit (AC)

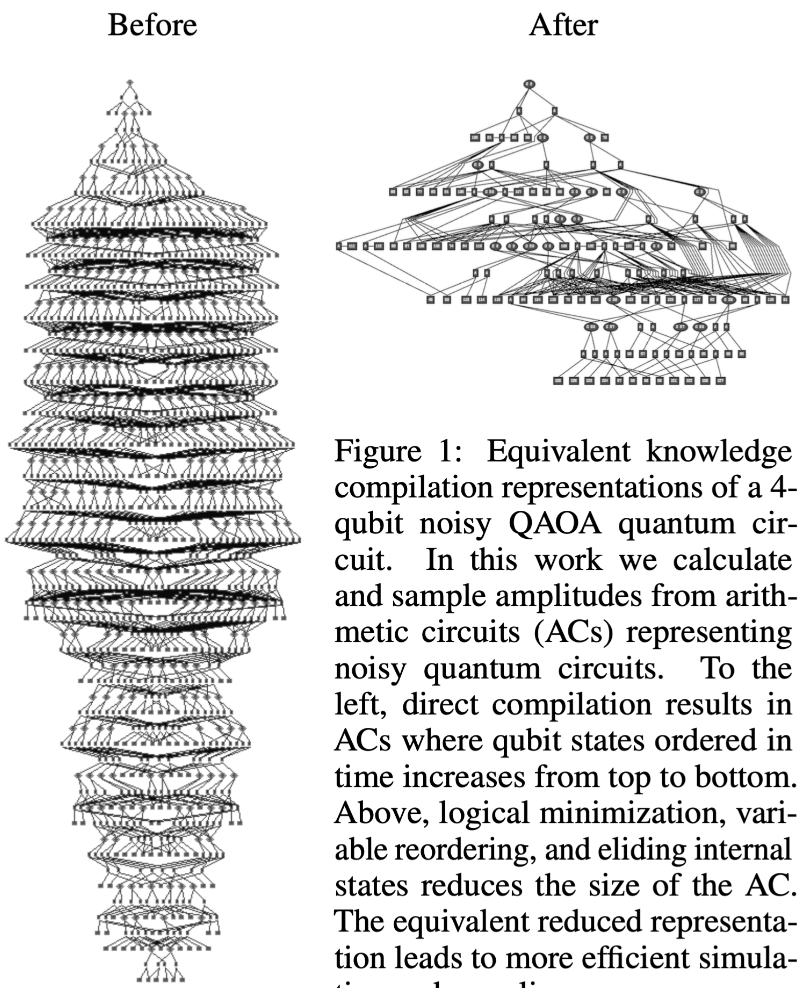

Figure 1: Equivalent knowledge compilation representations of a 4-qubit noisy QAOA quantum circuit. In this work we calculate and sample amplitudes from arithmetic circuits (ACs) representing noisy quantum circuits. To the left, direct compilation results in ACs where qubit states ordered in time increases 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.

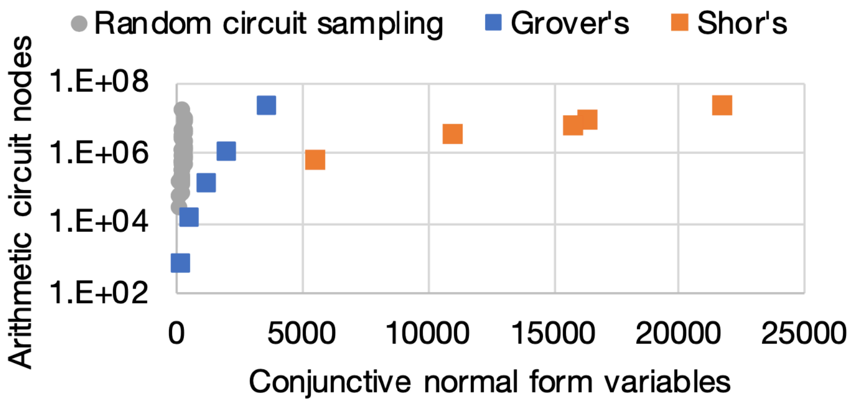

Figure 6: Simulation resource requirements vs. quantum circuit size for three quantum algorithms

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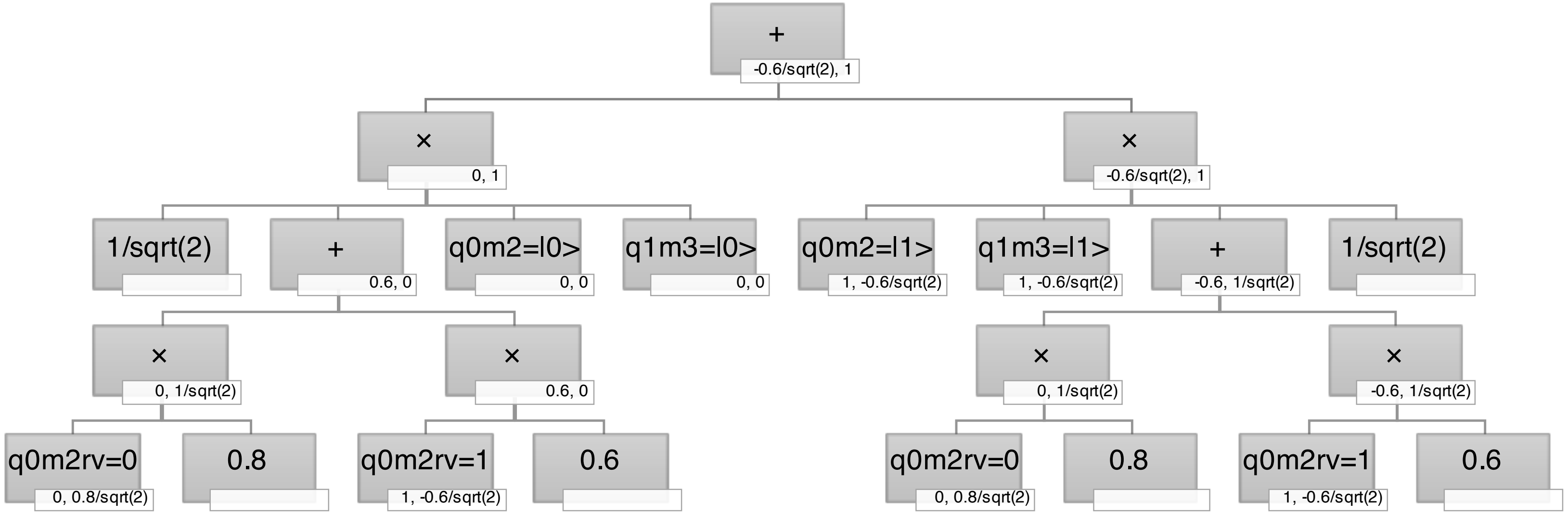
Exact inference on AC for quantum circuit simulation



- Quantum simulation becomes tree traversal on AC

Exact inference on AC for quantum circuit simulation

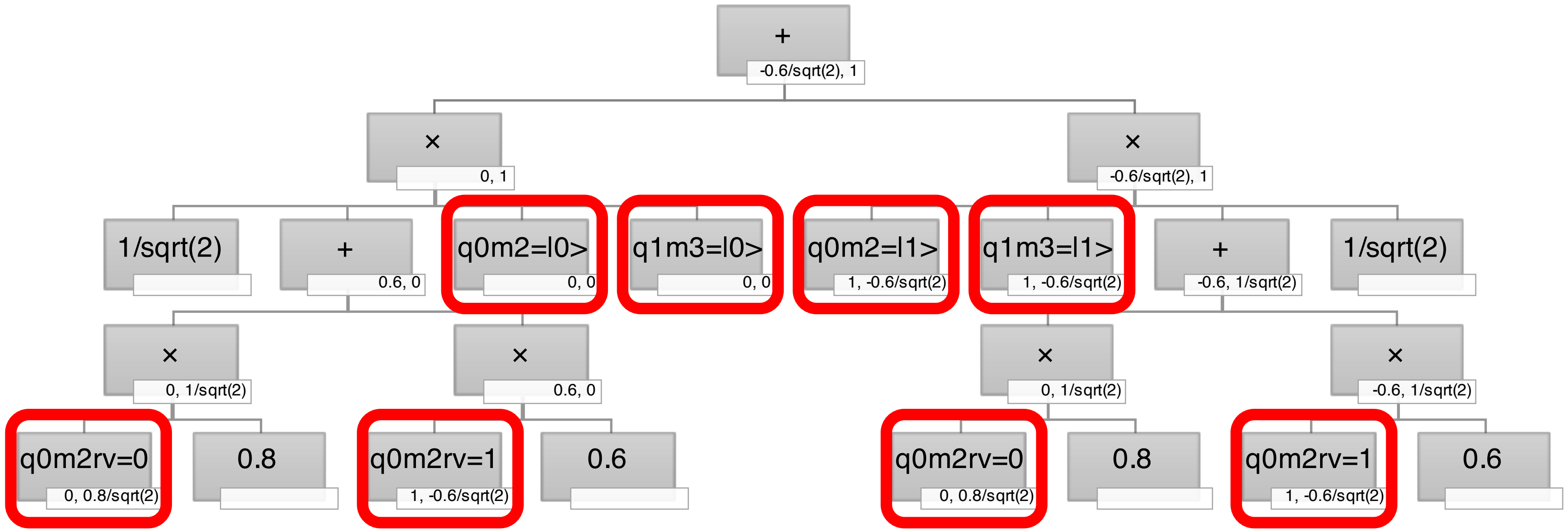
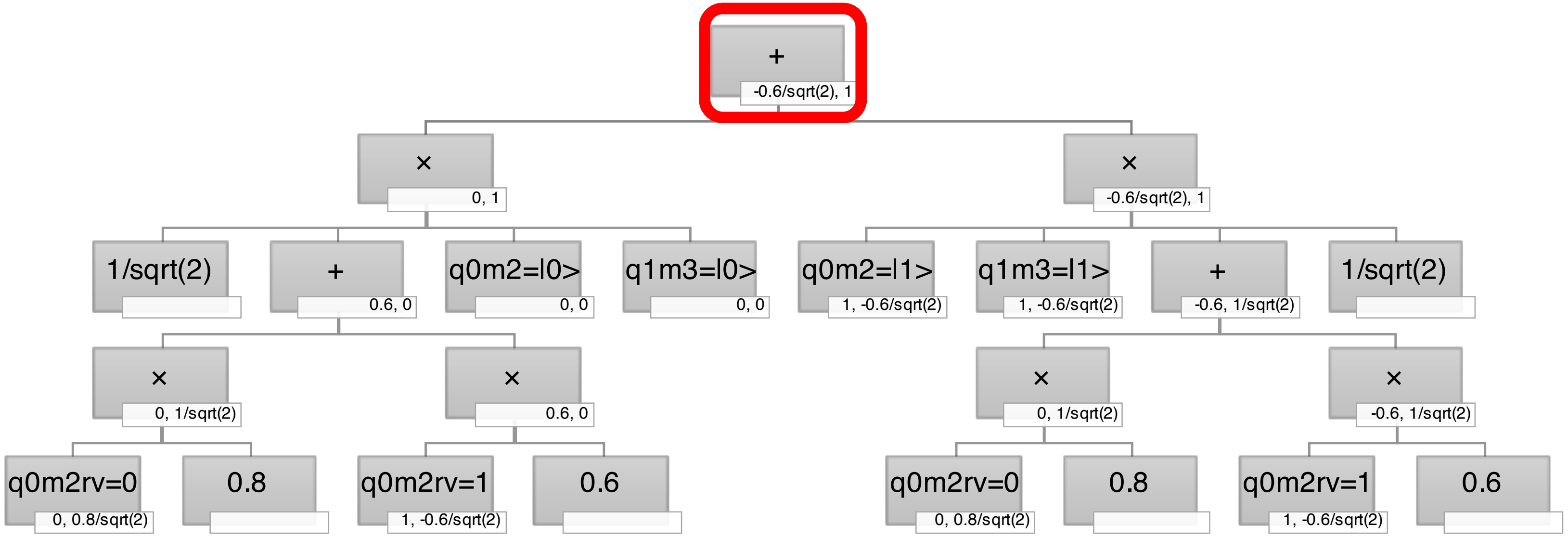


Table 9: Upward pass for finding amplitudes

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

- 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

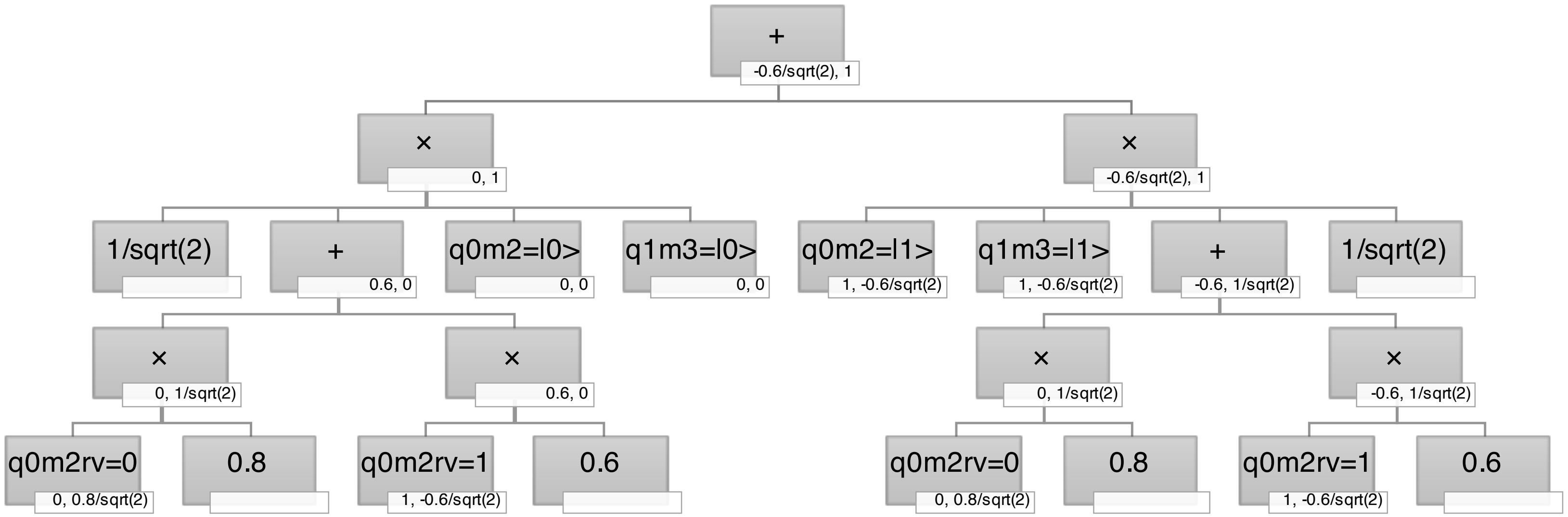
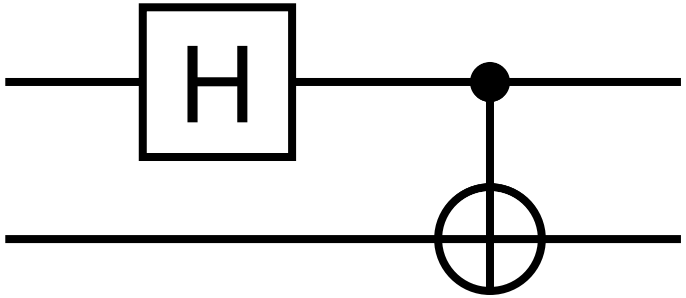


Table 10: Downward pass for finding derivatives for Gibbs sampling MCMC

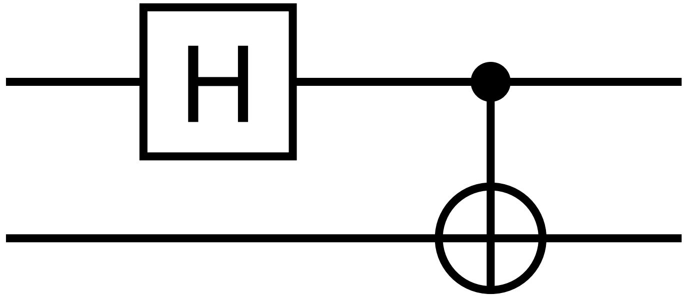
	q0m2rv	q0m2	q1m3	amplitude
Present sample	1	$\lvert 1\rangle$	$\lvert 1\rangle$	$0.6\frac{-1}{\sqrt{2}}$
Gibbs sample noise	0	$\lvert 1\rangle$	$\lvert 1\rangle$	$0.8\frac{1}{\sqrt{2}}$
Gibbs sample qubits	1	$\lvert 0\rangle$	$\lvert 1\rangle$	0
Gibbs sample qubits	1	$\lvert 1\rangle$	$\lvert 0\rangle$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

Schrödinger quantum circuit simulation

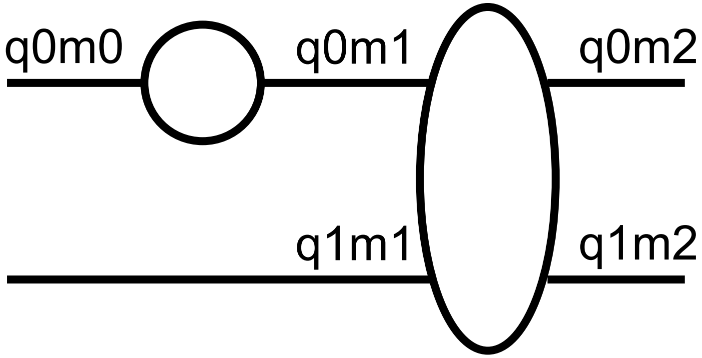


$$\mathrm{CNOT}(\mathrm{H} \otimes \mathrm{I}|00\rangle) = \mathrm{CNOT}(\mathrm{H}|0\rangle \otimes \mathrm{I}|0\rangle) = \mathrm{CNOT}\begin{bmatrix} \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} \\ \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 & & & \\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

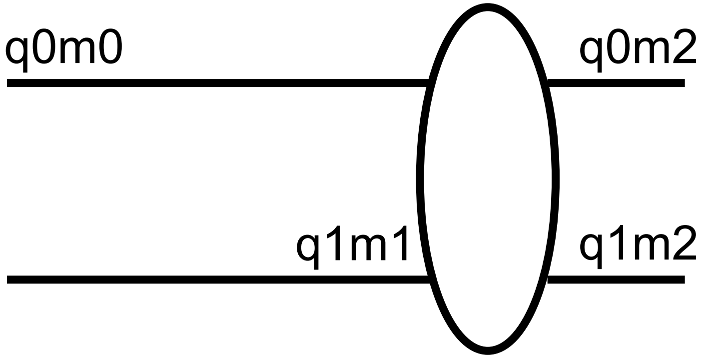
Feynman quantum circuit simulation



	q0m0=$|\mathbf{0}\rangle$	q0m0=$|\mathbf{1}\rangle$
q0m1=$|\mathbf{0}\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
q0m1=$|\mathbf{1}\rangle$	$\frac{1}{\sqrt{2}}$	$\frac{-1}{\sqrt{2}}$



		q0m1=$|\mathbf{0}\rangle$		q0m1=$|\mathbf{1}\rangle$	
		q1m1=$|\mathbf{0}\rangle$	q1m1=$|\mathbf{1}\rangle$	q1m1=$|\mathbf{0}\rangle$	q1m1=$|\mathbf{1}\rangle$
q0m2=$|\mathbf{0}\rangle$	q1m2=$|\mathbf{0}\rangle$	1	0	0	0
	q1m2=$|\mathbf{1}\rangle$	0	1	0	0
q0m2=$|\mathbf{1}\rangle$	q1m2=$|\mathbf{0}\rangle$	0	0	0	1
	q1m2=$|\mathbf{1}\rangle$	0	0	1	0



		q0m0=$|\mathbf{0}\rangle$		q0m0=$|\mathbf{1}\rangle$	
		q1m1=$|\mathbf{0}\rangle$	q1m1=$|\mathbf{1}\rangle$	q1m1=$|\mathbf{0}\rangle$	q1m1=$|\mathbf{1}\rangle$
q0m2=$|\mathbf{0}\rangle$	q1m2=$|\mathbf{0}\rangle$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
	q1m2=$|\mathbf{1}\rangle$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
q0m2=$|\mathbf{1}\rangle$	q1m2=$|\mathbf{0}\rangle$	0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
	q1m2=$|\mathbf{1}\rangle$	$1/\sqrt{2}$	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?

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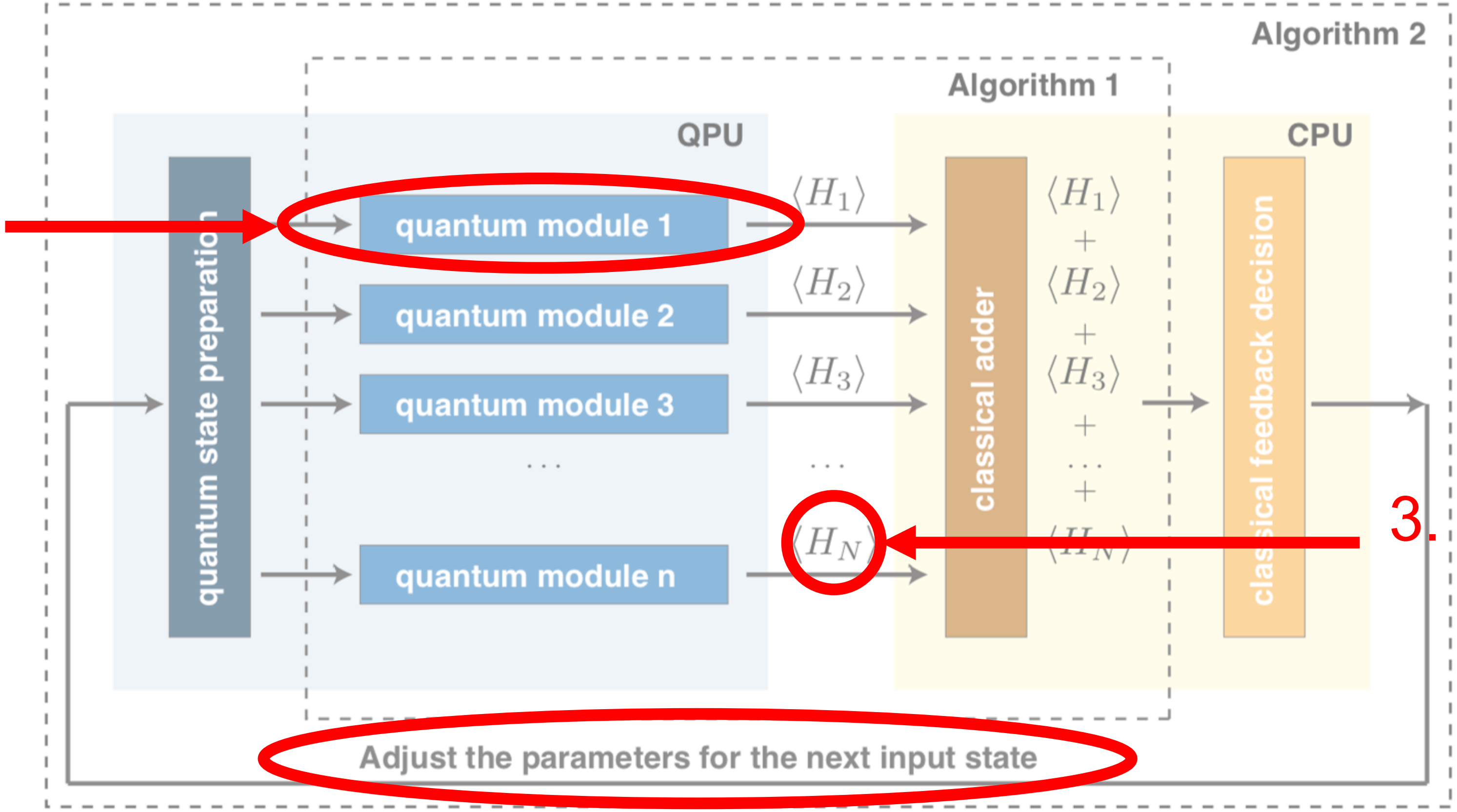
The unique challenge of simulating noisy variational algorithms

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

Image source: Peruzzo et al., 2013

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

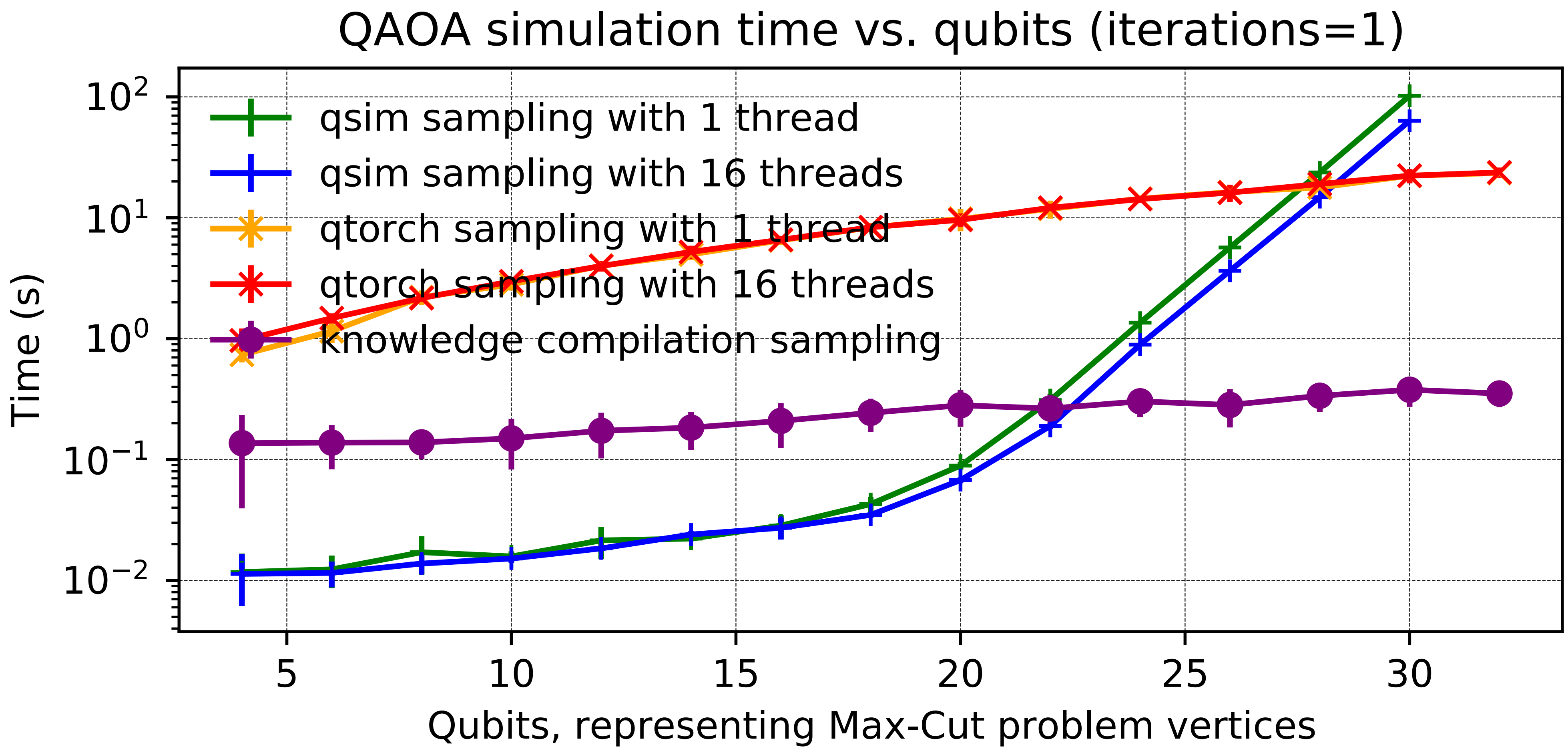
Result 1: It works!

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

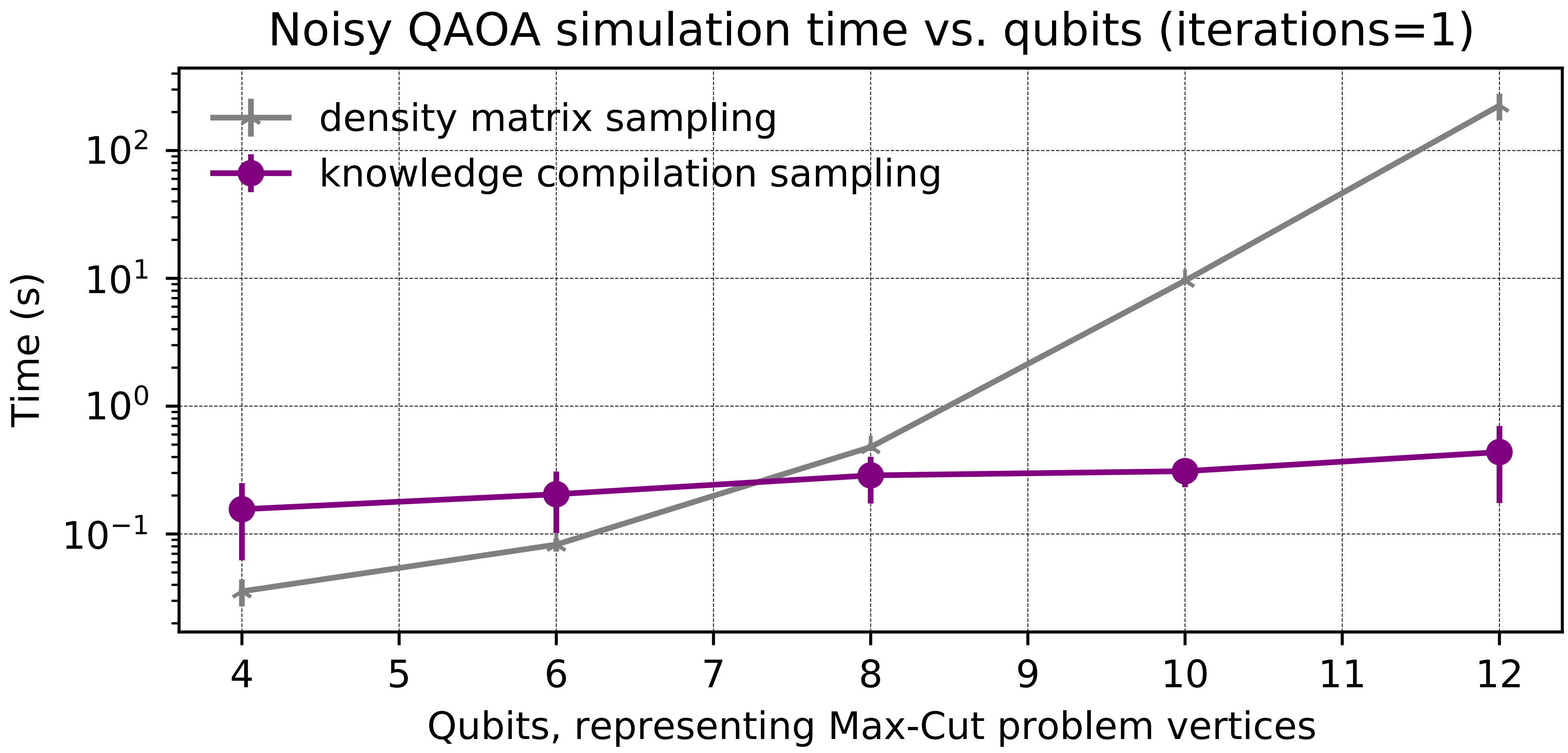
- Can accurately simulate Pauli gates, CNOT, CZ, phase kickback, Toffoli, CHSH protocol, Deutsch-Jozsa, Bernstein-Vazirani, hidden shift, quantum Fourier transform, Shor's, Grover's…

- Passes Google Cirq's suite of test harness for quantum simulators

Result 2: Ideal circuit simulation



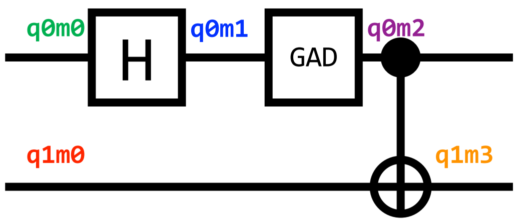
Result 2: Noisy circuit simulation

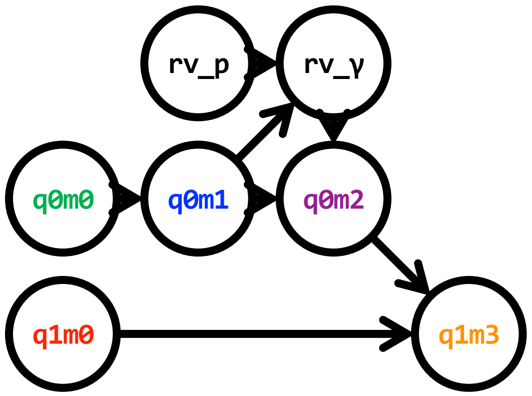


What this talk was about:

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

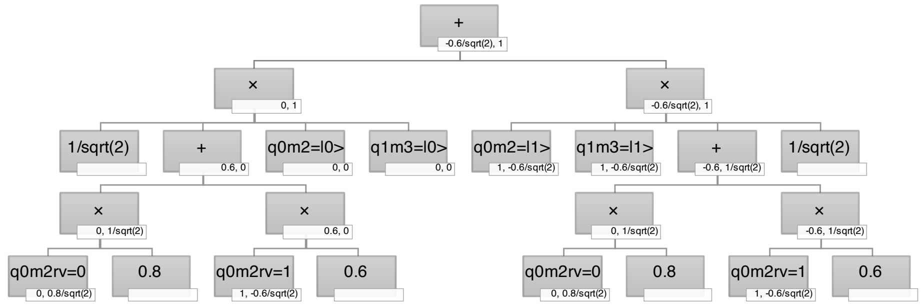
- A new way to represent noisy quantum circuits as probabilistic graphical models.
- A new way to encode quantum circuits as conjunctive normal forms and arithmetic circuits.
- A new way to manipulate quantum circuits using logical equation satisfiability solvers.
- Improved simulation and sampling performance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





The Hadamard gate:

```
q0m0=|0> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|0> AND q0m1=|1> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|0> -> +1/sqrt(2)
q0m0=|1> AND q0m1=|1> -> -1/sqrt(2)
```



Where we have gone:

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- Why are they different and important?

What is quantum circuit simulation?

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How do we represent quantum circuits as logic formulas?

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

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?)

Ongoing work: accelerating quantum research via graphical model inference techniques

1	Improving the correctness of quantum algorithms.	• Genetic algorithms on graphical model topologies for improving variational ansatzes. • Graphical model training to understand variational algorithm progress.
2	Benchmarking the performance of quantum programs on unreliable quantum prototypes.	• Bayesian network sensitivity analysis for debugging misbehaving program implementations. • Bayesian network knowledge compilation to enable more efficient repeated simulation.
3	Probing the limits of classical computing to better understand the potential of quantum computing.	• Classical hardware accelerators for graphical models in support of quantum simulation.

Thank you to my collaborators

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Steven Holtzen, Todd Millstein, Guy Van den Broeck; UCLA

Members of the EPiQC team

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