Noisy Variational Quantum Algorithm Simulation via Knowledge Compilation for Repeated Inference: Extended Abstract

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***Abstract*—We present a quantum circuit simulation toolchain targeted for simulating variational algorithms. We do so by encoding quantum amplitudes and noise probabilities in a probabilistic graphical model, and we use *knowledge compilation* to compile the circuits to logical equations that support efficient repeated simulation of and sampling from quantum circuits for different parameters. Compared to state-of-the-art state vector and density matrix quantum circuit simulators, our simulation approach offers greater performance when sampling from circuits with at least eight to 20 qubits and with around 12 operations on each qubit. And versus quantum circuit simulation techniques based on tensor network contraction, our simulation approach offers a 66 times reduction in sampling cost for simulating ideal shallow quantum circuits with 32 qubits, making the approach ideal for simulating near-term variational quantum algorithms.**

1. Motivation & Key Insights

Due to the limitations of existing quantum prototypes, quantum circuit simulation continues to be a vital tool for validating next generation quantum computers and for studying variational quantum algorithms. Existing quantum circuit simulators do not address the common traits of variational algorithms, namely: 1) their ability to work with noisy qubits and operations, 2) their repeated execution of the same circuits but with different parameters, and 3) the fact that they sample from circuit final wavefunctions to drive an optimization routine [2]. Quantum computing research would benefit from a simulator that supports variational algorithms specifically, which would require a simulator that 1) simulates the probabilistic effects of noise, 2) can handle more qubits, and 3) can reuse computation results between simulation runs with different parameters.

The key insight of our paper is that *knowledge compilation*——a technique for efficient repeated inference originating in artificial intelligence research—can be generalized to work on complex-valued quantum amplitudes, such that the technique serves as the basis for a quantum circuit simulation toolchain geared for variational quantum algorithms. In knowledge compilation, AI models such as Bayesian networks encode probabilistic knowledge about the world in a factorized format. The Bayesian networks compile down to minimized data structures called arithmetic circuits (ACs) that enable repeated inference and sampling queries with different parameters and new pieces of evidence [1]. These features of the knowledge compilation approach—namely, 1) the ability to represent and manipulate probabilistic information, 2) the ability to compile probabilistic model structural information into minimized formats, 3) the ability to efficiently sample from the same model but for varying parameters and evidence—match well with the requirements for variational quantum algorithm simulation.

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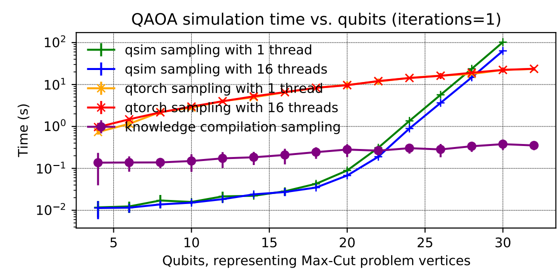
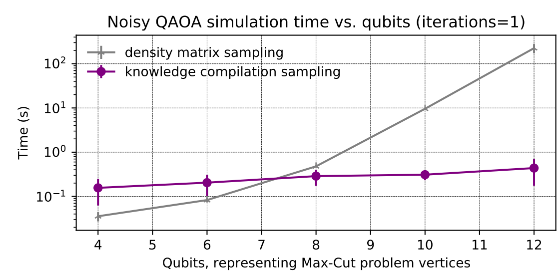


(a) Versus state vector (qsim) and tensor network (qTorch [3]) for ideal circuits



(b) Versus density matrix simulation (Cirq) for noisy circuits

Figure 1: Knowledge compilation sampling performance.

2. Our Knowledge Compilation Approach

We built a knowledge compilation toolchain for quantum algorithm simulation that excels at simulating noisy circuits

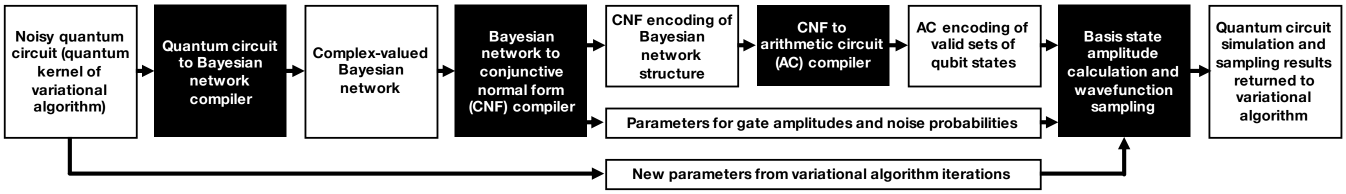


Figure 2: Toolchain stages and intermediate representations for quantum algorithm simulation via knowledge compilation.

TABLE 1: Program transformations converting a noisy quantum circuit to conjunctive normal form (CNF).

Quantum circuit semantics encoded	**The logical sentences comprising the CNF for a noisy Bell state quantum circuit example**		**Compilation / simplification rules**
Qubits take on binary values; supply initial qubit values	$\texttt{q0m0} = \|0\rangle \oplus \texttt{q0m0} = \|1\rangle$ $\texttt{q0m0} = \|0\rangle$ $\texttt{q0m1} = \|0\rangle \oplus \texttt{q0m1} = \|1\rangle$	$\texttt{q1m0} = \|0\rangle \oplus \texttt{q1m0} = \|1\rangle$ $\texttt{q1m0} = \|0\rangle$ $\texttt{q1m3} = \|0\rangle \oplus \texttt{q1m3} = \|1\rangle$	Combine initial value sentences into binary constraint sentences using logical unit resolution.
Hadamard gate	$\texttt{q0m0} = \|0\rangle \wedge \texttt{q0m1} = \|0\rangle \implies +\frac{1}{\sqrt{2}}$ $\texttt{q0m0} = \|1\rangle \wedge \texttt{q0m1} = \|0\rangle \implies +\frac{1}{\sqrt{2}}$	$\texttt{q0m0} = \|0\rangle \wedge \texttt{q0m1} = \|1\rangle \implies +\frac{1}{\sqrt{2}}$ $\texttt{q0m0} = \|1\rangle \wedge \texttt{q0m1} = \|1\rangle \implies -\frac{1}{\sqrt{2}}$	Weight variables stand in for parameters for amplitudes or probabilities; compiler stores equal-value parameters as a single variable.
Phase damping noise channel	$\texttt{q0m2rv} = 0 \oplus \texttt{q0m2rv} = 1$ $\texttt{q0m1} = \|0\rangle \implies \texttt{q0m2rv} = 0$	$\texttt{q0m1} = \|1\rangle \wedge \texttt{q0m2rv} = 0 \implies +0.8$ $\texttt{q0m1} = \|1\rangle \wedge \texttt{q0m2rv} = 1 \implies -0.6$	The simulator resolves variables with values that change for repeated simulations.
CNOT gate	$\texttt{q0m1} = \|0\rangle \wedge \texttt{q1m0} = \|0\rangle \implies \texttt{q1m3} = \|0\rangle$ $\texttt{q0m1} = \|0\rangle \wedge \texttt{q1m0} = \|1\rangle \implies \texttt{q1m3} = \|1\rangle$	$\texttt{q0m1} = \|1\rangle \wedge \texttt{q1m0} = \|0\rangle \implies \texttt{q1m3} = \|1\rangle$ $\texttt{q0m1} = \|1\rangle \wedge \texttt{q1m0} = \|1\rangle \implies \texttt{q1m3} = \|0\rangle$	Deterministic parameters (*i.e.*, 0 or 1) are factored to logic without weight variables.

for variational algorithms (Fig. 2). It comprises:

1) A front-end for converting noisy quantum circuits (specified in Google's Cirq framework[1]) to complex-valued Bayesian networks [4], which we extend to correctly encode quantum noise mixtures and channels. Compared to conventional quantum circuits where complex-valued quantum amplitudes and real-valued noise probabilities are treated separately, the Bayesian network encoding unifies quantum states and noise events in a single representation.
2) A compiler that converts Bayesian networks representing noisy quantum circuits into conjunctive normal form (CNF) logic equations. The CNFs encode the quantum circuits' topological information. The sets of logic variable assignments that satisfy the CNF correspond to all sets of qubit state assignments that are consistent with a quantum circuit's semantics (Tab. 1). The structural information can be reused across simulations independently of quantum amplitude and noise probability parameters, which vary across simulations. More importantly, CNF logical equation encodings for quantum circuits permits using logical equation compilers based on SAT solvers to minimize the representation.
3) A compiler that converts CNFs to ACs. An AC enumerates and assigns a weight value to each set of variable assignments that satisfy a logical equation [1]. Summing the weights across all qubit state assignments results in the output amplitudes that we seek to find in the quantum circuit simulation task. The ACs enable the quantum circuit simulator to find the probability amplitude for an outcome, without incurring the cost of finding the amplitudes of intermediate qubit states. The ACs further memoize the calculated results from prior queries such that subsequent queries update values only as necessary. The ACs also enable a Markov chain Monte Carlo procedure for sampling sets of qubit outcomes according to their measurement probability.

3. Key Results and Contributions

Our key results are that 1) a quantum circuit simulation approach based on knowledge compilation of probabilistic program representations is correct for a benchmark suite of quantum algorithms, and 2) such an approach offers advantages in simulating near-term variational quantum algorithms, relative to other simulation approaches based on state vectors[2], density matrices, and tensor networks [3] (Fig. 1). The advantages are due to the more compact representation, the circuit minimization and memoization capabilities of our approach, and due to the storage costs for conventional simulators based on matrix representations. The improved simulation performance facilitates studying variational algorithms and validating prototype quantum computer results in the NISQ era of quantum computing.

References

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1. https://github.com/quantumlib/Cirq

2. https://github.com/quantumlib/qsim