Knowledge Compilation-Based Exact Inference for Quantum Simulation

Yipeng Huang
Princeton University
Resource estimation for quantum simulation

Why is simulation important?

• "Developing good classical simulations (or even attempting to and failing) would also help clarify the quantum/classical boundary.” —Aram Harrow

• Development and debugging of quantum algorithm implementations
How do we build a quantum simulator?

Be very smart and write a lot of code:
• Clever circuit minimizations (Cirq optimizations, Qiskit transpilation…)
• Massive parallelism (QuEST, efforts by IBM, Google, Alibaba…)
• Compression (Wu et al., Supercomputing 2019, BDD-based methods)
• Emulation (ProjectQ)
• Stabilizer formalism (CHP by Aaronson)

Borrow from existing classical techniques…
Outline: Borrowing classical probabilistic inference for quantum simulation

• Connection between quantum circuits and Bayesian networks

• Our toolchain for quantum simulation: exact Bayesian network inference based on knowledge compilation

• Evaluation of features offered by this approach: structure extraction & more efficient repeated simulation
Outline: Borrowing classical probabilistic inference for quantum simulation

• **Connection between quantum circuits and Bayesian networks**

• Our toolchain for quantum simulation: exact Bayesian network inference based on knowledge compilation

• Evaluation of features offered by this approach: structure extraction & more efficient repeated simulation
Probabilistic graphical models and an example

**Bayesian networks**
- AKA directed graphical models, belief networks

**Markov networks**
- AKA undirected graphical models, Markov random fields

---

Darwiche, A Differential Approach to Inference in Bayesian Networks
# Theory: connection between quantum computing and probabilistic inference

<table>
<thead>
<tr>
<th>Quantum</th>
<th>Probabilistic</th>
</tr>
</thead>
<tbody>
<tr>
<td>program simulation</td>
<td>inference</td>
</tr>
<tr>
<td>qubits</td>
<td>random variables</td>
</tr>
<tr>
<td>amplitudes</td>
<td>probabilities</td>
</tr>
<tr>
<td>operator unitary matrices</td>
<td>conditional probability tables</td>
</tr>
<tr>
<td>superposition states</td>
<td>probability distributions</td>
</tr>
<tr>
<td>entangled qubits</td>
<td>dependent random variables</td>
</tr>
<tr>
<td>measurement</td>
<td>sampling &amp; conditioning</td>
</tr>
</tbody>
</table>

**Key analogies**

- amplitudes are complex-valued
- squares of amplitudes sum to 1
- interference (canceling of amplitudes) possible

**Key distinctions**

- probabilities between 0 and 1
- probabilities sum to 1
- interference impossible
Theory: connection between quantum computing and probabilistic inference

<table>
<thead>
<tr>
<th>Quantum</th>
<th>Probabilistic</th>
</tr>
</thead>
<tbody>
<tr>
<td>program simulation</td>
<td>inference</td>
</tr>
<tr>
<td>qubits</td>
<td>random variables</td>
</tr>
<tr>
<td>amplitudes</td>
<td>probabilities</td>
</tr>
<tr>
<td>operator unitary matrices</td>
<td>conditional probability tables</td>
</tr>
<tr>
<td>superposition states</td>
<td>probability distributions</td>
</tr>
<tr>
<td>entangled qubits</td>
<td>dependent random variables</td>
</tr>
<tr>
<td>measurement</td>
<td>sampling &amp; conditioning</td>
</tr>
<tr>
<td>Key analogies</td>
<td></td>
</tr>
<tr>
<td>Key distinctions</td>
<td></td>
</tr>
<tr>
<td>amplitudes are complex-valued</td>
<td>probabilities between 0 and 1</td>
</tr>
<tr>
<td>squares of amplitudes sum to 1</td>
<td>probabilities sum to 1</td>
</tr>
<tr>
<td>interference (canceling of amplitudes)</td>
<td>interference impossible</td>
</tr>
</tbody>
</table>

Quantum / probabilistic: separated by Gottesman-Knill theorem, ideas can cross-pollinate
Outline: Borrowing classical probabilistic inference for quantum simulation

• Connection between quantum circuits and Bayesian networks

• Our toolchain for quantum simulation:
  exact Bayesian network inference based on knowledge compilation

• Evaluation of features offered by this approach:
  structure extraction & more efficient repeated simulation
Our toolchain for quantum simulation via knowledge compilation exact inference

- Quantum circuit (QASM) to complex-valued Bayesian network
- Bayesian network to conjunctive normal form (CNF)
- CNF to arithmetic circuit (AC)
- Exact inference on AC to obtain quantum simulation
Our toolchain for quantum simulation via knowledge compilation exact inference

• **Quantum circuit (QASM) to complex-valued Bayesian network**

• Bayesian network to conjunctive normal form (CNF)

• CNF to arithmetic circuit (AC)

• Exact inference on AC to obtain quantum simulation
Quantum circuit (QASM) to complex-valued Bayesian network

Quantum circuit DAG → Bayesian network topology

Quantum gate unitary matrices → conditional probability tables

• Bridge to using classical probabilistic inference
• Similar approach used by Boixo et al. for quantum simulation (they used Markov undirected networks)
Our toolchain for quantum simulation via knowledge compilation exact inference

• Quantum circuit (QASM) to complex-valued Bayesian network

• *Bayesian network to conjunctive normal form (CNF)*

• *CNF to arithmetic circuit (AC)*

• Exact inference on AC to obtain quantum simulation
Bayesian networks to arithmetic circuits

**Bayesian network → CNF**
- Allows weighted model counting
- Equivalent to Feynman path sum

**CNF → arithmetic circuits**
- Reduces the circuit size
- ACs are related to BDDs

Many specific techniques, pick one that doesn’t assume probabilities sum to 1
- We use UCLA’s ACE tool by Chavira & Darwiche

Driven by an underlying solver that needs no special input other than the QASM code
- We use UCLA’s C2D tool by Darwiche
Our toolchain for quantum simulation via knowledge compilation exact inference

• Quantum circuit (QASM) to complex-valued Bayesian network

• Bayesian network to conjunctive normal form (CNF)

• CNF to arithmetic circuit (AC)

• *Exact inference on AC to obtain quantum simulation*
Exact inference on AC to obtain quantum simulation

- Quantum simulation becomes tree traversal on AC

Darwiche, A Differential Approach to Inference in Bayesian Networks
Exact inference on AC to obtain quantum simulation

- Quantum simulation becomes tree traversal on AC

- Quantum measurement outcomes are probabilistic evidence

Darwiche, A Differential Approach to Inference in Bayesian Networks
Exact inference on AC to obtain quantum simulation

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

- **Amplitude for given outcome comes from root node**

Darwiche, A Differential Approach to Inference in Bayesian Networks
Outline: Borrowing classical probabilistic inference for quantum simulation

• Connection between quantum circuits and Bayesian networks

• Our toolchain for quantum simulation: exact Bayesian network inference based on knowledge compilation

• Evaluation of features offered by this approach: structure extraction & more efficient repeated simulation
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, BV, Grover’s, Shor’s, random circuit sampling

In general, works with exact inference methods

• E.g., variable elimination, weighted model counting

In general, fails with approximate inference methods

• E.g., Sampling, Markov chain Monte Carlo
Result 2: Ability to extract quantum circuit structure

**Y-axis:** proportional to resource intensiveness
- Compilation/inference time, memory, storage

**X-axis:** proportional to the number of qubit states
- Quantum circuit width $\times$ depth

<table>
<thead>
<tr>
<th></th>
<th># qubits</th>
<th># gates</th>
<th>AC file size</th>
</tr>
</thead>
<tbody>
<tr>
<td>RCS</td>
<td>42</td>
<td>840</td>
<td>82 MB</td>
</tr>
<tr>
<td>Grover’s</td>
<td>17</td>
<td>2460</td>
<td>530 MB</td>
</tr>
<tr>
<td>Shor’s</td>
<td>13</td>
<td>12247</td>
<td>586 MB</td>
</tr>
</tbody>
</table>

(b) Problem size metrics for largest problem instances.

Workloads taken from Scaffold
Result 3: More efficient repeated simulation with different measurement outcomes

Random circuit sampling

• Samples multiple measurement outcome assignments

Subject of intense competition

• Boixo et al. hinted reusing results between simulations may be useful
Result 3: More efficient repeated simulation with different measurement outcomes

First work where partial simulation results reused for RCS

- Change of sampled measurement outcome only needs tree re-traversal

Up to about depth 29, \(~20\times\) speedup

- Against Boixo et al., on a workstation

Beyond depth 29, no structure to extract
Result 4: More efficient repeated simulation with different operator matrix parameters

Peruzzo et al., 2013

Table 1: Time cost per toolchain stage for each of 88 iterations.

<table>
<thead>
<tr>
<th>Toolchain stage</th>
<th>Computation time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantum circuit to Bayesian network</td>
<td>0.372 ± 0.005</td>
</tr>
<tr>
<td>Bayesian network to CNF</td>
<td>1.219 ± 0.042</td>
</tr>
<tr>
<td>CNF to arithmetic circuit</td>
<td>12.077 (once)</td>
</tr>
<tr>
<td>Inference on AC</td>
<td>1.459 ± 0.350</td>
</tr>
</tbody>
</table>

VQE Benchmark by Teague Tomsesh, Princeton
Outline: Borrowing classical probabilistic inference for quantum simulation

• Connection between quantum circuits and Bayesian networks

• Our toolchain for quantum simulation: exact Bayesian network inference based on knowledge compilation

• Evaluation of features offered by this approach: structure extraction & more efficient repeated simulation
Theory: connection between quantum computing and probabilistic inference

<table>
<thead>
<tr>
<th>Quantum</th>
<th>Probabilistic</th>
</tr>
</thead>
<tbody>
<tr>
<td>program simulation</td>
<td>inference</td>
</tr>
<tr>
<td>qubits</td>
<td>random variables</td>
</tr>
<tr>
<td>amplitudes</td>
<td>probabilities</td>
</tr>
<tr>
<td>operator unitary matrices</td>
<td>conditional probability tables</td>
</tr>
<tr>
<td>superposition states</td>
<td>probability distributions</td>
</tr>
<tr>
<td>entangled qubits</td>
<td>dependent random variables</td>
</tr>
<tr>
<td>measurement</td>
<td>sampling &amp; conditioning</td>
</tr>
</tbody>
</table>

**Key analogies**
- amplitudes are complex-valued
- squares of amplitudes sum to 1
- interference (canceling of amplitudes) possible

**Key distinctions**
- probabilities between 0 and 1
- probabilities sum to 1
- interference impossible

*Quantum / probabilistic: separated by Gottesman-Knill theorem, ideas can cross-pollinate*
Resource estimation for quantum simulation

Why is simulation important?

• "Developing good classical simulations (or even attempting to and failing) would also help clarify the quantum/classical boundary.” —Aram Harrow

• Development and debugging of quantum algorithm implementations
Thank you to my collaborators

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

Teague Tomesh, Margaret Martonosi; Princeton

Members of the EPiQC team

• This work is funded in part by EPiQC, an NSF Expedition in Computing, under grant 1730082.