Validation of Quantum Simulations

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Outline

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Introduction

How to validate the results of a *quantum* simulation?

Goals:

- Study state-of-the-art validation techniques;
- Implement/develop a validation protocol in a quantum computer - IBM Q.

Outline

Quantum Simulation

"(...) Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws." - Feynman, 1982

Applications of quantum simulations:

- Condensed matter physics;
- Cosmology;
- Chemistry;
- Schrödinger equation, interferometry, quantum thermodynamics...

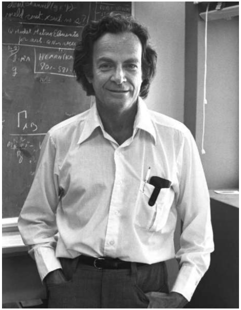


Figure: Richard P. Feynman (1974)
Source: Los Angeles Times

Quantum Simulation

General recipe for quantum simulation:

- Take a quantum system with some degree of controllability;
- Prepare the initial state;
- Evolve the system according a desired Hamiltonian;
- Measure some quantity of interest.

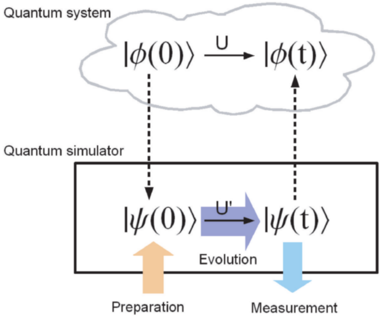


Figure: Schematic representation of a quantum system and a corresponding quantum simulator. I. M. Georgescu et al. (2013). "Quantum Simulation". In: arXiv: 1308.6253

How does one system simulate another?

Analog Quantum Simulator (AQS)

Quantum systems whose Hamiltonians can be engineered to map those of a subset of models put forward to describe a real system. The simulator mimics the continuous evolution of another system.

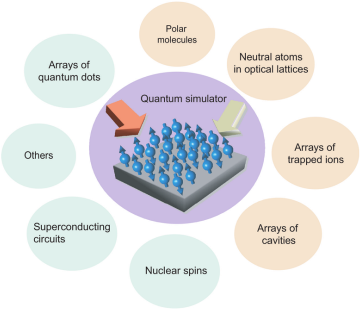


Figure: Different systems that could implement a specialized quantum simulator for the study of problems in condensed-matter physics. I. M. Georgescu et al. (2013). "Quantum Simulation". In: arXiv: 1308.6253

How does one system simulate another?

Digital Quantum Simulator (DQS)

The state of the simulated system is encoded using qubits, and its unitary evolution can be decomposed into a sequence of single and two-qubit gates.

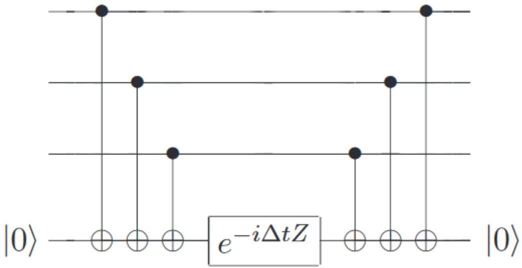


Figure: Quantum Circuit for simulating the Hamiltonian $H = Z_1 \otimes Z_2 \otimes Z_3$ for time Δt
Michael A. Nielsen and Isaac L. Chuang (2010). *Quantum Computation and Quantum Information*. P. 702. arXiv: `arXiv:1011.1669v3`.

Efficiency in DQS

Exponential boost

Consider a system with N two-state (e.g. spin 1/2) variables:

Classical simulator

- Storing the state requires 2^N bits of memory;
- Calculating its time evolution requires the exponentiation of a $2^N \times 2^N$ matrix.

A quantum computer requires only N quantum bits for the same system. However, an *arbitrary* quantum transformation on those N qubits involves the multiplication of a 2^N-dimensional state vector by a $2^N \times 2^N$ matrix.

Efficiency in DQS

Exponential boost

The time evolution of real (observed) quantum systems is NOT arbitrary. These systems evolve according local interactions[1].

A closed Hamiltonian system with local interactions can be written in the form:

$$H = \Sigma_{i=1}^{\ell} H_i$$

As such, a time evolution $U = e^{iHt}$ can be approximated as:

$$e^{iHt} \approx (e^{iH_1 t/n} \dots e^{iH_\ell t/n})^n$$

[1] Seth Lloyd (1996). "Universal Quantum Simulators". In: *Science* 2023.1957, pp. 1073–1078. arXiv: 1606.02734.

Efficiency in DQS

Exponential boost

So the simulation takes place within some degree of accuracy, the time slicing needs to be regulated as[2]:

$$e^{iHt} = (e^{iH_1 t/n} \dots e^{iH_\ell t/n})^n + \sum_{i>j} [H_i, H_j] t^2/2n + \sum_{k=3}^{\infty} E(k)$$

- For higher order error terms *E(k)*: $\|E(k)\|_{sup}\, n \leqslant \|Ht/n\|_{sup}^{k} / k!$
- Error in approximating e^{iHt} is less than $\left\| n(e^{iHt/n} - 1 - iHt/n \right\|_{sup}$

n can be picked sufficiently large to ensure that the simulation always tracks the correct time evolution to within some error $\epsilon > 0$

[2] Malvin H Kalos (2012). *Monte Carlo Methods in Quantum Problems*. Vol. 125. Springer Science & Business Media.

Efficiency in DQS

Exponential boost

Each H_j acts on a Hilbert space of only m_j dimensions, so the number of operations needed to simulate $e^{iH_j t/n}$ approximates to $\approx m_j^2$.

Since each operator is simulated n times, the total number of operations needed to simulate the time evolution e^{iHt} is:

$$\approx n(\Sigma_{i=1}^{\ell} m_i^2) \leqslant n\ell m^2, \text{ where } m = \max\{m_i\}$$

For typical local interactions such as nearest neighbor or next-nearest neighbor, ℓ is proportional to N.

A **digital quantum simulator** takes resources of time and memory space directly proportional to those of the system being simulated; the number of basic operations needed is proportional to the number of its variables.

Outline

Quantum tomography

Quantum state tomography

Set of techniques for reconstruction of the quantum state from a source quantum system;

- The source must be able to consistently prepare the same state;
- The measurements must be tomographically complete.

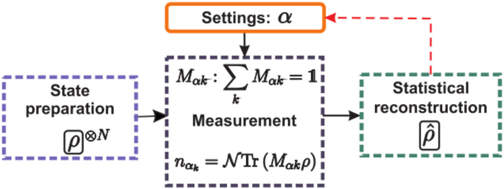


Figure: Diagram for a method of quantum state tomography. Stanislav Straupe (2016). "Adaptive quantum tomography". In: pp. 1–12. arXiv: 1610.02840

Quantum tomography

Quantum process tomography

Set of techniques for reconstruction of the parameters of an unknown transformation of a known quantum state.

Drawbacks of tomography approaches:

- Full tomography of quantum states is extremely computationally intensive, i.e. proportional to the dimension of the system's Hilbert space.
- It hasn't been experimentally demonstrated for states with over 14 qubits[3].

[3] Stanislav Straupe (2016). "Adaptive quantum tomography". In: pp. 1–12. arXiv: 1610.02840.

Quantum interactive proofs

Aharonov and Vazirani[4] argue that the scientific paradigm of "predict and verify" cannot be applied to testing quantum mechanics in the limit of high complexity".

- How can a classical, computationally restricted experimentalist test the high complexity aspects of quantum mechanics?

Quantum interactive proof (QIP)

A QIP is a model of computation where a classically limited verifier can interact with a powerful, untrusted quantum system capable of performing quantum computations.

Although an expermentalist may not be able to check if the outcome of a single experiment is correct, he may devise a specific sequence of experiment and test the consistency of the outcomes.

[4] A. Dorit and V. Umesh (2012). "Is Quantum Mechanics Falsifiable? A computational perspective on the foundations of Quantum Mechanics". In: *arXiv preprint arXiv:1206.3686*, pp. 1–12. arXiv: `arXiv:1206.3686v1`.

Quantum interactive proofs

Existing protocols[5] require the verifier to be able store 3 qubits, and manipulate and exchange them with the prover - Arthur, the experimentalist, needs to have at least some computational power.

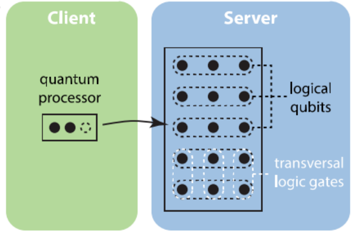


Figure: Setting considered by Aharonov, Ben-Or and Eban. Source: Joseph F. Fitzsimons (2016). "Private quantum computation: An introduction to blind quantum computing and related protocols". In: *npj Quantum Information* December 2016, pp. 1–10. arXiv: 1611.10107

[5] Dorit Aharonov et al. (2017). "Interactive Proofs for Quantum Computations". In: arXiv: 1704.04487.

Blind quantum computation

Blind quantum computation (BQC)

Broad set of techniques seeking to ensure the privacy of a delegated, remote quantum computation. Many of these also allow for verification of the computation being performed.

Similarly to QPIP, progress has come by relaxing restrictions to an ideal BQC protocol[6]:

- By making the client have access to some computational power;
- By delegating the computation to multiple, non-communicating quantum servers sharing entangled qubits.

[6] Joseph F. Fitzsimons and Elham Kashefi (2017). "Unconditionally verifiable blind quantum computation". In: *Physical Review A* 96.1, pp. 1–27. arXiv: 1203.5217.

Outline

IBM Q Network

IBM Q Network is a cloud-based platform where it's possible to program and remotely interact with a quantum computer.

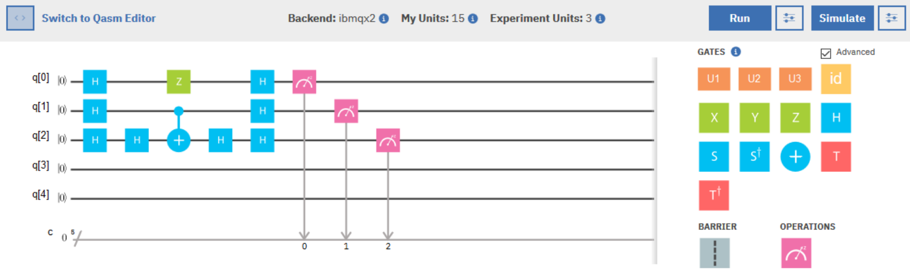


Figure: Online interface for the IBM circuit Composer, here shown implementing Deutsch-Josza's algorithm for an input of 3-bit strings.

Experimental part

Applying a maximum-likelihood quantum state tomography protocol Smolin et al. 2011 with QISKit for a 2-qubit Bell state $\frac{1}{2}(|00\rangle + |11\rangle)$:

Define the classical and quantum registers, and construct the state:

```
qr = Q_program.create_quantum_register('qr', 2)
cr = Q_program.create_classical_register('qr', 2)
bell = Q_program.create_circuit('bell', [qr], [cr])
bell.h(qr[0]
bell.cx(qr[0], qr[1]
```

Experimental part

To plot the state on the basis of Pauli matrices:

```
plot_state(bell_rho, 'paulivec')
```

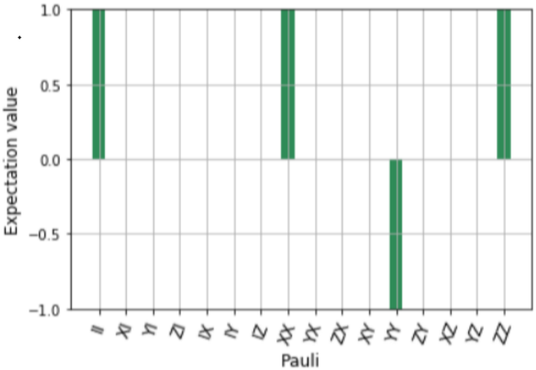


Figure: Representation of the $\frac{1}{2}(|00\rangle + |11\rangle)$ state on the Pauli basis.

Experimental part

To specify the quantum state tomography experiment:

```
bell_tomo_set = tomo.state_tomography_set([0,1])
```

Onto reconstructing the maximum likelihood estimate Smolin et al. 2011 of the state:

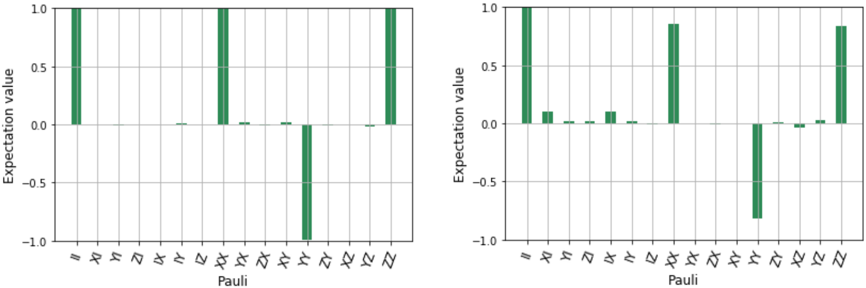
```
rho_fit = tomo.fit_tomography_data(bell_tomo_data)
```

It's also possible to compare the reconstruction with the ideal state through the Fidelity function, given by $F = sqrt(\langle\psi|\,\rho\,|\psi\rangle$

```
target = np.array([1., 0., 0., 1.]/np.sqrt(2.))
F_fit = state_fidelity(rho_fit, target)
```

Experimental part

The program can be run on both the offline simulator and the quantum computer:



A) Fidelity = 0.9977073180512603

B) F = 0.937599059667

Figure: Reconstruction of the Bell state through maximum likelihood quantum tomography, and fidelity function, for the A) mathematical simulator, and B) IBMqx2.

Summary

- For local quantum systems, a digital quantum simulator provides an exponential boost in efficiency over a classical simulator;
- While quantum tomography methods successfully reconstruct a quantum state, they're too resource intensive for larger systems;
- Quantum interactive proofing and blind quantum computation are promising developments into verifying quantum computations and simulations;
- QISKit allows for the successful use of simple quantum state and process tomography techniques.

Future work: implement other tomography protocols and/or higher-complexity (QIP, BQP) verifying protocols, further contributing to the development of the QISKit libraries.

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