Building Quantum Bridges: Advancing Drug Discovery with QAOA and Explaining Quantum Computing with Building Blocks

Using quantum computers to solve combinatorial optimization problems

PRESENTER:
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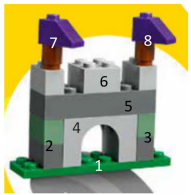
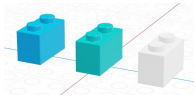
BACKGROUND: Pharmaceutical companies like Novo Nordisk and Johnson & Johnson have begun exploring quantum computers to advance Drug Design and Discovery. Optimization problems are a class of problems which quantum computers are starting to rival their classical counterparts. To demonstrate an example we describe and solve an optimization problem using "interlocking bricks"!

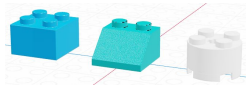
Problem: We have a database of every brick in a box of "interlocking bricks" and want to build a castle. We want to generate multiple castle designs for different conditions. We first divide the castle into regions. Every brick is associated with a region and has the properties:



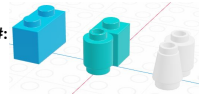
Color:



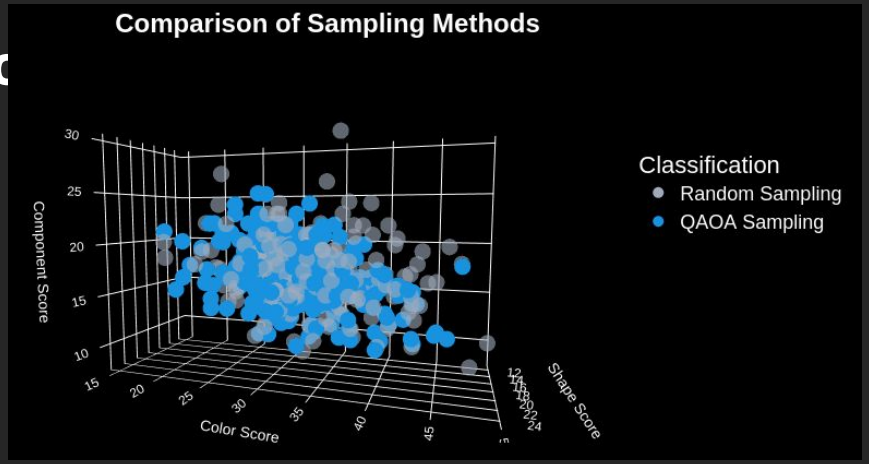
Brick Shape:



Components #:



Quantum Computers are effective at generating a Pareto front of solutions for large combinatorial pro



Take a picture to **find** the **github repo!**

METHODS:

1. Generate hamiltonians for one brick per region constraint, property constraints, and mixer.
2. Optimize parameters for a 2-layer QAOA circuit.
3. Using the optimal parameters run the QAOA circuit
4. Postprocess results from quantum computer

Results:
Using a database of 48 bricks and a castle with 6 regions quantum sampling with the IBM Eagle was better finding optimal solutions compared to random sampling.

Translating to Chemistry:
Fragment-based drug design involves identifying small chemical fragments that bind to a target protein and optimizing them to develop potent and selective drug candidates. Follow this QR code to learn how PolarisQB achieves quantum utility accelerating the drug design process

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QuADD
Quantum-Aided Drug Design from POLARIS qb