Quantum Computing for Drug Discovery

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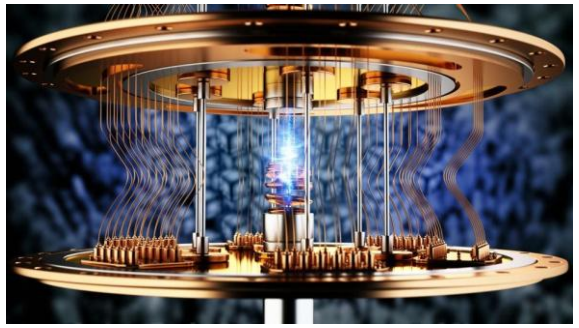
https://youtu.be/UqrfxJBg3cA

Clearing Up Things

- “quant” does NOT mean “quantum”
- “quant” refers to “quantitative (financial) analysis”
- The term captures people who use mathematical models to make predictions on various markets, using logic and reasoning to navigate investments
- Quantum computing is currently being explored in quant, but they are NOT the same



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What is Quantum Computing

- quantum computing – “emergent field of cutting-edge computer science harnessing the unique qualities of quantum mechanics to solve problems beyond the ability of even the most powerful classical computers” (IBM)
- Advantage: have the potential to solve problems that conventional computers can’t due to…
  - Impractical run-times
  - Significant computational complexity
- Reality: still a young field; don’t deliver on their promises yet

Necessary Definitions

- Superposition – state in which a quantum particle can represent a combination of multiple possibilities; a qubit can be in multiple states at once
- Entanglement – when qubits have some relationship that prevents them from acting independently
  - occurs when quantum particle has a state (i.e. spin, charge) that's linked to another quantum particle's state
- Decoherence – process where quantum particles and systems can decay, collapse or change, losing its quantum state
- Interference – when entangled quantum states can interact and produce more/less likely probabilities

Qubits

- Qubit – the quantum version of a classical computer's most basic form of information, bits
- Created by manipulating and measuring quantum particles (e.g. photons, electrons, atoms, etc.)
- Can store zero, one, or weighted combination of zero and one (superposition) → more data than bits → better computational ability
- Qubit can only output single bit of information at end of computation

How Qubits are Created

- Scientists find spot in material where quantum properties can be accessed/controlled
- Use light or magnetic fields to create superposition, entanglement, and other properties
- One way is manipulating the spin of individual electrons
  - Electron spin is either up (highest energy state), down (lowest energy state), or combination of both
  - Microwaves and magnets applied to manipulate spin and control qubit

Different Types of Qubits

- Superconducting
- Trapped ions
- Quantum dots
- Photons
- Neutral atoms

Challenges with Qubits

- Qubits need to be cooled to temperatures a fraction of a degree higher than absolute zero to guarantee spin state (coherence)
  - If not, there is too much energy and the qubit will just randomly fluctuate between states
- Qubits sensitive to environment and don’t maintain state for long
  - Bad because that means information can change randomly
  - Even under the right conditions, qubits can fail due to decoherence
- Quantum states can interfere with one another to either amplify correct answers (good) or push wrong answers (bad)
  - Problem increases in scale as number of qubits used increases

How Quantum Computing Works

- Initialization
  - Set up qubits in a well-defined initial state
  - Different depending on what problem you are trying to solve and the input
- Computation
  - Apply a series of quantum operations (quantum gates, etc) to manipulate the qubits
  - Such operations will leverage superposition and entanglement to explore a large computational space, allowing quantum computers to surpass limitations of classical computers
- Measurement
  - Record the final state of qubits
  - The measurement process will collapse the superposition of qubits into either state 0 or 1
  - This stage is general done multiple times to ensure that the answer returned is accurate

Applications of Quantum Computing

- AI and ML
  - Enhance ML algorithms and enable stronger AI models due to quantum computers' greater computational capability
- Optimization problems
  - Can find optimal solutions for problems in logistics, finance, etc.
  - E.g. portfolio optimization, financial modeling, warehouse logistics
- Cryptography
  - Can break current encryptions fast, but also create stronger ones
- Drug discovery
  - *(will expand on in next slides)*

What is Drug Discovery?

- Drug discovery is a field in the medical industry that involves discovering new medications
  - How cures to diseases (e.g. COVID-19) are found
- Traditionally done using physical testing of compounds
  - Put experimental compound on trays with each of the testing compounds → wait → record results → repeat
  - This is a very time-consuming process
- Technological evolutions moved physical process to software
  - Virtual screening and docking allows for faster experimentation (a few seconds)
  - However, there are over 10^{16} compounds out there → lots of time overall
- GPU computing and AI can help, but both have limitations

Drug Discovery in Quantum Computing

- Heart of drug discovery is to understand molecular behavior
  - How do molecules interact? What is their stability? Energy state? Etc.
  - Notice that these questions are fundamental traits of a quantum computing problem
- Simulating molecules and materials at unprecedented levels of detail via quantum computing can lead to discovery of new drugs not possible with GPU and/or AI
- Applications
  - Calculating ground state energies to identify most stable configuration(s)
  - Identify binding energies between a drug and target protein
  - Predict reaction rates to different candidate drugs
- The more simulations and results we get, the faster, cheaper, and more successful drug design will be

IBM Qiskit

- IBM Qiskit – an open-source SDK for working with quantum computers at level of circuits, pulses, and application modules
- Allows building of quantum circuits, simulation (locally or cloud), executing on real quantum hardware (cloud), and post-analysis
- Contains various libraries for specific applications
  - qiskit-algorithms → algorithms like Grover (search) and VQE
  - qiskit-nature →many methods for chemistry and physics problems
  - qiskit-primitives
  - qiskit-circuit → collection of circuits and building blocks for algorithms or benchmarks (e.g. EfficientSU2)

Demo: Estimating Electronic Ground State Energy of H_2 using VQE

- Goal: find electronic ground state energy (lowest possible energy) of Hydrogen molecule H_2
- Why:
  - Electronic ground state energy helps determine molecule's stability, reactivity, and binding affinity which helps predict its behavior in the body and its potential as a drug candidate
  - Electronic ground state energy of H_2 can be easily calculated classically, but H_2 is the "hello world" of molecules
  - Electronic ground state energy of more complex molecules cannot be calculated as easily
  - Demo shows process that can be applied to other, more complex, molecules
- What is VQE?
  - Variational quantum eigensolver (VQE)
  - A hybrid quantum-classical algorithm
  - Hybrid part → prepared parameterized trial wavefunction (ansatz) and measures its energy
  - Classical part → optimizes parameters of the ansatz to find lowest energy

Demo: High-Level Explanation

- #1 Create Hamiltonian for H_2
  - Hamiltonian describes the energy of the molecule
  - H_2 at ~0.735 Angstrom can have its energy operator represented using 2 qubits
- #2 Initialize Ansatz circuit
  - Ansatz circuit is a parametrized quantum circuit that creates our trial wavefunction
  - EfficientSU2 used for demo; hardware-efficient ansatz suitable for chemistry problems
  - Other ansatz circuits include UCC and UCCSD
  - When fed to the VQE, VQE will try to find the best parameters for the ansatz
- #3 Initialize optimizer and estimator
  - Sequential least squares programming (SLSQP) optimizer commonly used with VQE; SPSA is another option
  - Estimator primitive computes expectation values of observables with respect to states prepared by quantum circuits
- #4 Initialize and run VQE algorithm to find electronic ground state energy
  - VQE initialized with ansatz, optimizer, and estimator as parameters
  - VQE prepares state, measures energy, and adjusts settings until lowest possible energy found
  - Minimum eigenvalue of VQE computed and dictates calculated electronic ground state energy of H_2 molecule

Demo: Create Fermionic Hamiltonian for H_2

- H_2 atoms and x-, y-, z-coordinates initialized in arrays
- Saved to Molecule object with charge 0, multiplicity 1, and Angstrom distance
  - Charge – the total charge of the molecule
  - Multiplicity – the multiplicity of the molecule (= 2*spin + 1)
  - Units – distance unit for xyz coordinates; angstrom (10^{-10} meter) used
- PySCFDriver used to get properties of H_2 molecule using classical calculations; good for obtaining reference values
- Classical calculations fine for H_2, but what about when molecules grow too complex to be solved using classical computation?

Demo: Convert fermionic Hamiltonian to qubit

- Goal: represent molecule energy in a way that a quantum computer can process; involves mapping fermionic Hamiltonian to qubit Hamiltonian
- Different types of mapping algorithms:
  - Jordan-Wigner
    - Intuitive for small systems, but inefficient for large-scale simulations due to linear scaling
  - Parity
    - Good for simplifying Hamiltonians in molecules with spatial symmetries
  - Bravyi-Kitaev
    - Good for large-scale simulations due to logarithmic scaling

Demo: Initialize Ansatz Circuit, Optimizer, Estimator

- EfficientSU2 ansatz circuit initialized with 2 qubits, linear entanglement, and 2 reps
  - Entanglement – linear entanglement connects qubits sequentially
  - Reps – # of layers of rotation and entanglement blocks; higher → more complex states
  - Other ansatz circuits include UCC, UCCSD
- Sequential least squares programming (SLSQP) optimizer commonly used with VQE
  - Other optimizers include SPSA
- Estimator – quantum primitive used to calculate expected value of the qubit Hamiltonian for a given ansatz state

Demo: Initialize VQE

- Built using ansatz, optimizer, and estimator
- A hybrid algorithm with a quantum and classical component
  - Quantum part – prepares a trial quantum state (AKA guess for molecule's electron configuration) on a quantum computer (simulator here) using an ansatz, then measures its energy using qubit Hamiltonian
  - Classical part – takes the measured energy and adjusts the parameters of the ansatz to try and find a lower energy
  - Both components repeat until a lower energy cannot be found

Demo: Running VQE

- Minimum eigenvalue of VQE is found over various iterations
- The result is the estimated electronic ground state energy of H_2
- Comparing the estimated value to that the classically calculated value shows nearly identical results
  - VQE performed well!
- Plots shows convergence of estimated energy over the iterations

What's the Big Deal?

- Shown that quantum computing can be leveraged to compute the electronic ground state energy of a molecule
- Classical calculations are fine for simple molecules like H_2, but will take prolonged periods of time for complex molecules
- Quantum computing can help solve this problem
- Electronic ground state energy helps determine molecule's stability, reactivity, and binding affinity which helps predict its behavior in the body and its potential as a drug candidate
- Quantum computing can accelerate drug discovery process and help scientists/researchers quickly, cheaply, and reliably produce new cures to detrimental diseases

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