Five Starter Problems: Solving Quadratic Unconstrained Binary Optimization Models on Quantum Computers

https://github.com/arulrhikm/Solving-QUBOs-on-Quantum-Computers

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Overview: Table of Contents[1]

[1] The animations on slides 19, 28, 33 were created using the `animate` package. It is only visible in PDF viewers that support animated PDF features, such as Adobe Acrobat Reader.

Section 1

Quadratic Unconstrained Binary Optimization

The QUBO Model

The Universal Language for Optimization

QUBO Model: Definition and Universality

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- **Universality:** QUBO provides a unified framework for representing combinatorial optimization, including many NP-hard problems.

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  - These methods offer competitive performance against specialized algorithms in practice.

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- **4. Quantum-Inspired Algorithms:**
  - Classical algorithms (like Quantum Particle Swarm Optimization) that incorporate principles from quantum mechanics to enhance performance without using quantum hardware.

Section 2

Canonical QUBO Formulation

The Number Partitioning Problem

Balancing the Binary Partition

Canonical Problem: Number Partitioning (NP)

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Modeling with Binary Variables

Decision Variable $x_i \in \{0, 1\}$:

- $x_i = 1 \implies s_i$ belongs to set A.
- $x_i = 0 \implies s_i$ belongs to set $S \setminus A$.

Let c be the total sum of all elements in S.

Number Partitioning QUBO

- **Sums of the Two Partitions:**

$$\text{Sum}(A) = \sum_{i=1}^{n} s_i x_i \qquad \text{Sum}(S \setminus A) = c - \sum_{i=1}^{n} s_i x_i$$

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- **The Difference (d):** The difference d between these two sums:

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- **QUBO Objective:** Since we want to minimize the absolute difference $|d|$, the equivalent unconstrained binary optimization is to minimize the square of the difference:

$$\min_{\mathbf{x} \in \{0,1\}^n} d^2 = \left(2 \sum_{i=1}^{n} s_i x_i - c \right)^2$$

Number Partitioning QUBO (continued)

- **Goal:** Express the squared difference as the QUBO quadratic form, $\min \mathbf{x}^\mathsf{T}\mathbf{Q}\mathbf{x}$ (ignoring the constant term c^2 from expansion).

$$\left(2\sum_{i=1}^{n} s_i x_i - c\right)^2 \propto \mathbf{x}^\mathsf{T}\mathbf{Q}\mathbf{x}$$

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- **QUBO Matrix Coefficients (q_{ij}):** The coefficients are derived from the squared objective function, where $\mathbf{Q}$ is a symmetric matrix.

$$q_{ij} = \begin{cases} \mathbf{s_i(s_i - c)} & \text{if } i = j \quad \text{(Diagonal, linear term in } x_i\text{)} \\ \mathbf{2s_is_j} & \text{if } i \neq j \quad \text{(Off-diagonal, quadratic term } x_i x_j\text{)} \end{cases}$$

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- **Significance:** This matrix $\mathbf{Q}$ is the input for all subsequent algorithms (SA, QA, QAOA).

Section 3

Practical QUBO Formulation

Cancer Genomics Pathways

Identifying Driver Mutations from TCGA Data

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- **Data Modeling: Hypergraph**
  - Genes (g_i) are the vertices.
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  - Modeled by the **Incidence Matrix (B)** where $b_{ij} = 1$ if gene i is mutated in patient j.

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- **Graph Laplacian:** The gene-gene correlation matrix is derived:

$$\mathbf{L}^{+} = \mathbf{B}\mathbf{B}^{T} = \mathbf{D} + \mathbf{A}$$

- The Graph Laplacian is decomposed into two matrices corresponding to two key combinatorial criteria for identifying "driver" mutations:

Cancer Genomics: Criteria for Driver Genes

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- **1. Coverage (Maximize $\mathbf{x}^T\mathbf{D}\mathbf{x}$):**
  - We seek genes that are prevalent across a large patient cohort.
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- **2. Exclusivity (Minimize $x^T Ax$):**
  - Multiple mutations are unlikely in a single patient for the same pathway.
  - Modeled by the **Adjacency Matrix (A)**: a_{ij} is the number of patients affected by both gene i and gene j.

Cancer Genomics: The QUBO Formulation

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- **Penalty Factor α:** The weight $\alpha \geq 1$ reflects that the coverage criterion (the linear term) is more important than exclusivity.

Section 4

Building Blocks of Quantum Computation

Circuits and the Ising Model

Bridging QUBO to Quantum Hardware

Qubits and Superposition

- **Qubits (Quantum Bits):** The fundamental unit of quantum information, analogous to a classical bit. They have two basis states,

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- **Born's Rule:** Measurement forces the qubit to collapse to a basis state ($|0\rangle$ or $|1\rangle$) with probabilities:

$$P(0) = |\alpha|^2, \quad P(1) = |\beta|^2, \quad \text{where } |\alpha|^2 + |\beta|^2 = 1$$

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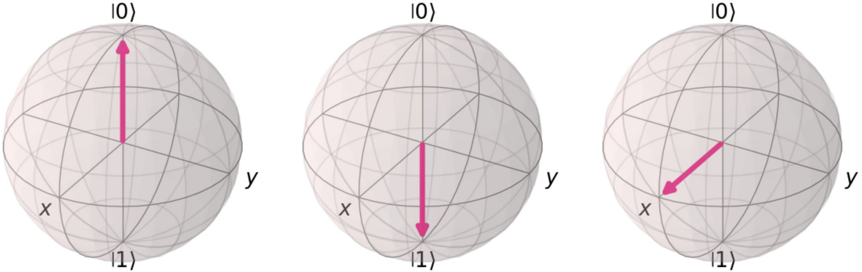

Figure: Bloch Sphere representations of $|0\rangle, |1\rangle$, and $|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$

Single-Qubit Gates

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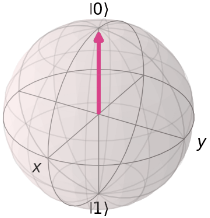
  - **Rotation Gates ($R_X(\theta), R_Y(\theta), R_Z(\theta)$):** Implement arbitrary **parameterized rotations** around the axes.
    - ★ These parameterized gates are the core components optimized by the classical loop in Variational Quantum Algorithms (VQAs) like QAOA.

Visualizing Single-Qubit Gates

Animations of key single-qubit gates acting on the Bloch sphere



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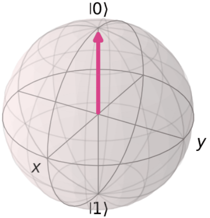
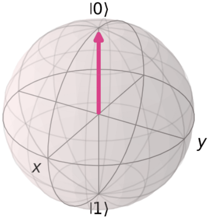


Pauli-X (σ_X)



Rotation $R_X(\pi/2)$

Naturally all gates are reversible (except measurement!).

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  - **Controlled-Z (CZ):** Flips the phase of the target qubit only if the control qubit is $|1\rangle$.
- **QUBO Interaction Gate ($R_{ZZ}(\theta)$):**
  - This gate applies a phase shift based on the correlation (or alignment) of the two qubits' Z-states.
  - It is essential for implementing the Cost Hamiltonian in quantum optimization algorithms, as it directly models the two-body interaction terms ($x_i x_j$) present in QUBOs.

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- **Tensor Product of States:** When multiple quantum states (each in different Hilbert spaces $\mathcal{H}_i$) or registers are combined, such as $|\psi_1\rangle \in \mathcal{H}_1$, $|\psi_2\rangle \in \mathcal{H}_2$, ..., the joint system is described by:

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle = |\psi_1 \psi_2 \cdots \psi_n\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0 \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

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- This circuit transforms $|00\rangle$ into a specific entangled state.

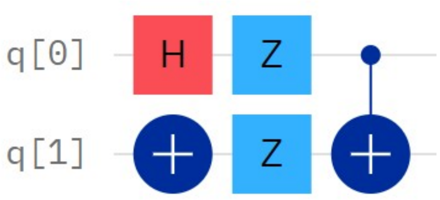

Figure: Quantum circuit represents: $[(\text{CX}) \times (Z \otimes Z) \times (X \otimes H)]|00\rangle$.

Hamiltonian and Quantum Evolution

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- **Relevance to QA:** This continuous time evolution is the basis for Quantum Annealing (QA), where the system is slowly steered from a known initial state to the problem's ground state.

Ising Model and QUBO

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- **The Critical Link: QUBO-Ising Equivalence**
  - QUBO (binary variables $x_i \in \{0, 1\}$) is directly convertible to the Ising Model (spin variables $\sigma_i \in \{-1, 1\}$).
  - The substitution is: $x_i = \frac{1+\sigma_i}{2}$.

Section 5

Optimization Landscape

Algorithms: Simulated Annealing (SA) - Classical

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- **Key Feature: Escaping Local Minima**
  - If the neighbor is better ($\Delta E < 0$), accept it deterministically.
  - If the neighbor is worse ($\Delta E > 0$), accept it **probabilistically**. This resistance to sticking to local minima is what sets SA apart.

Simulated Annealing: Temperature Schedule and Cooling

- **Acceptance Probability:** The likelihood of accepting a worse solution $\mathbf{x}'$ ($\Delta E = f(\mathbf{x}') - f(\mathbf{x}) > 0$) is given by the formula derived from thermal annealing:

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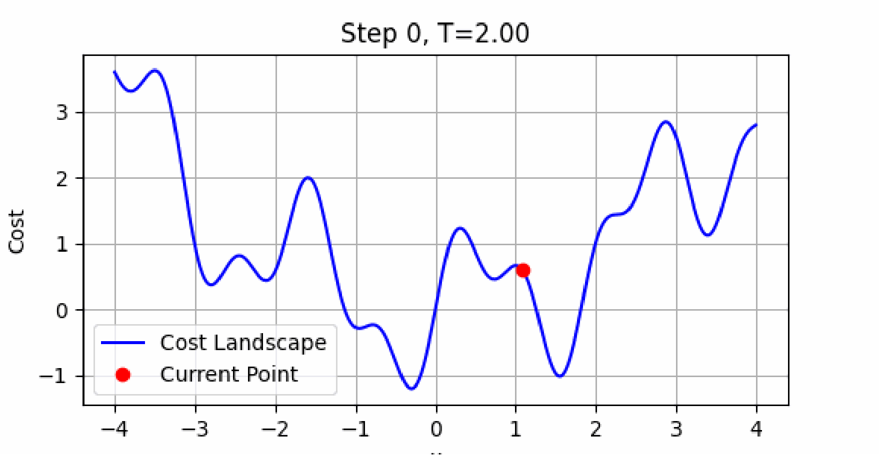
- **Trade-offs:**
  - **Advantage:** Simple and effective at escaping local minima.
  - **Limitation:** Performance is highly dependent on careful tuning of parameters (initial T, α, iterations per temperature).

Simulated Annealing Visualization



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Mapping the Problem

The QUBO problem $\mathbf{x}^T\mathbf{Q}\mathbf{x}$ is mapped to the equivalent **Ising Hamiltonian** H_C, where the variables are quantum spins $\sigma_i \in \{-1, 1\}$.

Quantum Annealing: The Adiabatic Theorem

- **Core Principle:** A quantum system initially in the ground state of a time-dependent Hamiltonian $\mathbf{H}(t)$ will **remain in its instantaneous ground state** throughout the evolution, provided the evolution is **sufficiently slow** (adiabaticity).

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- **Implication:** A smaller min gap requires a much longer annealing time T to avoid exciting the system into a non-optimal state.

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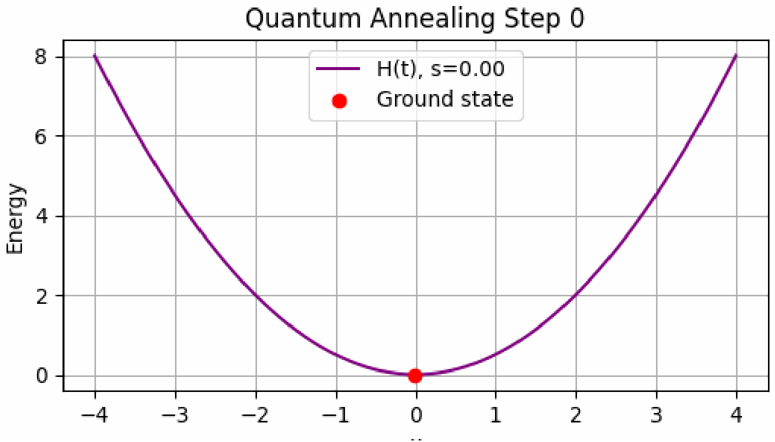
- **Final State ($s = 1$):** The Hamiltonian is dominated by $\mathbf{H}_C$ (Pauli-Z terms). The qubits collapse to the configuration that minimizes this energy, yielding the optimal QUBO solution.

Quantum Annealing Visualization



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- **Workflow:** A quantum circuit generates a state, and a optimizer tunes the circuit's parameters to minimize the expected cost.

QAOA: The Parametrized Quantum Circuit

- **Initial State Preparation:** The circuit begins by applying a Hadamard gate (H) to all n qubits, creating a uniform superposition of all 2^n possible solutions:

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- **The Ansatz (U):** The quantum state after p layers is:

$$|\psi(\vec{\beta}, \vec{\gamma})\rangle = \prod_{i=1}^{p} e^{-i\beta_i H_D} e^{-i\gamma_i H_C} |\psi(0)\rangle$$

- Parameterized by **2p** angles: $\vec{\beta} = \{\beta_1, \ldots, \beta_p\}$ and $\vec{\gamma} = \{\gamma_1, \ldots, \gamma_p\}$.

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- **Implementation:** It is approximated (via Trotterization) using a series of single-qubit Z-rotations and two-qubit U_{ZZ} gates:

$$e^{-i\gamma H_C} \approx \prod_{i<j} e^{-i\gamma J_{ij} \sigma_Z^{(i)} \sigma_Z^{(j)}} \prod_i e^{-i\gamma h_i \sigma_Z^{(i)}}$$

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QAOA Visualization

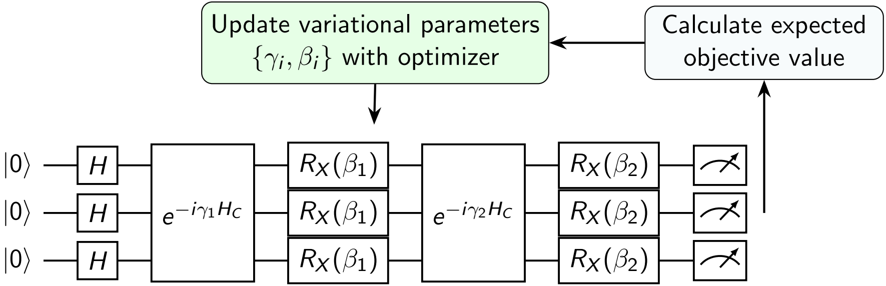

Figure: QAOA Circuit: Each layer alternates between a problem-specific cost unitary $e^{-i\gamma H_C}$ and a mixing unitary $R_X(\beta)$. The parameters $(\gamma_1, \beta_1), (\gamma_2, \beta_2)$ are optimized classically.

Section 6

Implementation and Workflow

Solving QUBOs in Code

From QUBO Matrix to Algorithm Output

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  The rotation angles are directly proportional to the γ parameter and the respective QUBO coefficients.

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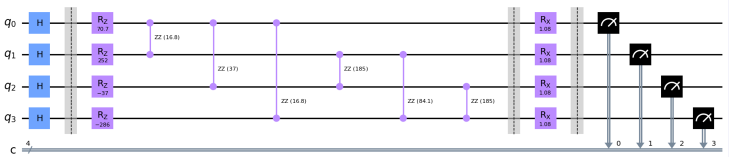
Qiskit Circuit (Example for $p = 1$)



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Workflow Summary

QAOA alternates between quantum measurements (to evaluate cost) and classical optimization (to improve parameters).

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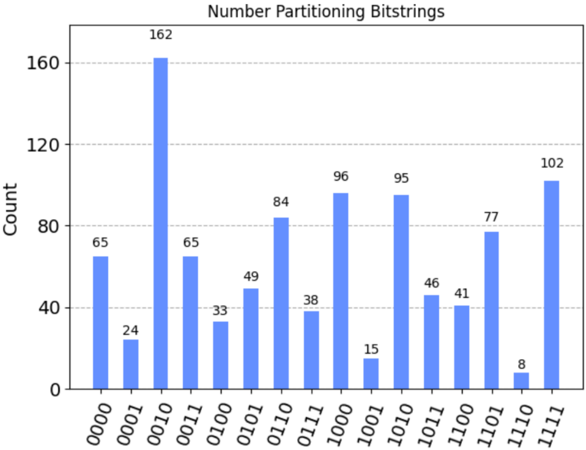

Interpreting the Output

Most probable bitstring (e.g., 0010) $\Rightarrow$ Partition $\{1, 5, 5\}$ vs. $\{11\}$ in the number partitioning problem.

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Input Data

Mutation data is sourced from databases like cBioPortal (TCGA AML study) to establish a Patient-Gene dictionary.

QA Preprocessing: Constructing **D** and **A**

- **1. Degree Matrix (D):** Defines the linear terms ($\mathbf{x}^T \mathbf{D} \mathbf{x}$).
  - **Role:** Measures Coverage (gene prevalence across patients).
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```
Patient-Gene Dictionary:
TCGA-AB-2802
['IDH1', 'PTPN11', 'NPM1', 'MT-ND5', 'DNMT3A']
TCGA-AB-2804
['PHF6']
TCGA-AB-2805
['IDH2', 'RUNX1']
TCGA-AB-2806
['KDM6A', 'PLCE1', 'CROCC']
```

Figure 15: Sample of Patient-Gene Dictionary (Mapping patients to mutated gene lists)

QA Workflow: BQM and Embedding

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- **Embedding (Minor Embedding):** This is the crucial step where the abstract BQM graph is mapped onto the fixed physical topology of the Quantum Processing Unit (QPU).
  - D-Wave's `EmbeddingComposite` often handles this automatic placement and chaining of logical variables onto physical qubits.

QA Execution and Solution

1. **Sampling:** Submit BQM to D-Wave with multiple reads.
2. **Annealing:** System evolves toward the ground state.
3. **Results:** Returns bitstrings with associated energies.
4. **Selection:** Choose lowest-energy bitstring as optimal pathway.
5. **Mapping:** Convert binary solution to gene IDs.
6. **Validation:** Analyze pathway properties (e.g., coverage, exclusivity).

```
['ASXL1', 'BRINP3', 'DNMT3A']
coverage: 61.0
coverage/gene: 20.33
indep: 4.0
measure: 5.08
```

Example of a Discovered Cancer Gene Pathway

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- **Algorithmic Synthesis:** QUBO links classical and quantum solvers by acting as the common input format:

Algorithm	**Platform**	**Mechanism**
Simulated Annealing (SA)	Classical	Thermal Fluctuation
Quantum Annealing (QA)	Quantum Hardware	Quantum Tunneling
QAOA	Hybrid/Gate Model	Parameterized Ansatz

Table: QUBO Solver Comparison

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- **Near-Term Solutions:** Continued development of **Quantum-Inspired** classical methods while fault-tolerant hardware matures.