

イロト イ部ト イヨト イヨト 二日

### Quantum Optimization Algorithms



#### Mohammad Ali Jafarizadeh

University of Tabriz

October 17, 2024

# Outline I

- Introduction to Quantum Optimization
- 2 Binary and Quadratic Optimization Problems
  - Examples of QUBO Formulation
    - The Max Cut Problem
    - The Number Partitioning Problem

#### 3 Creating QUBO Models Using Known Penalties

- Minimum Vertex Cover (MVC) Problem
- The Set Packing Problem
- The Graph Coloring Problem

#### 4 The Max 2-Sat Problem

- 5 Quantum Algorithms for Optimization
  - Introduction to Quantum Optimization Algorithms

# Outline II

- 6 Mapping Optimization Problems to Quantum Hardware
  - 7 Quantum Adiabatic Optimization
    - Quantum Adiabatic Algorithm
- 8 One Qubit Example
- 9 2-SAT on a Ring

4 Adiabatic Quantum Computation & Deutsch's Algorithm



## § 1: Introduction to Quantum Optimization

- Binary Optimization Problems:
  - Decision variables  $x_i \in \{0,1\}$  or  $x_i \in \{-1,1\}$ .
  - The goal is to maximize or minimize an objective function.
  - Subject to constraints (optional) or unconstrained.
- General Form:

$$\min_{x\in\{0,1\}^n}f(x)$$

Common applications: scheduling, portfolio optimization, set covering, etc.

- Combinatorial Optimization: Many real-world problems in logistics, finance, and machine learning involve binary optimization.
- Quantum Binary Optimization: Quantum computers are uniquely suited for exploring the exponentially large solution spaces of binary optimization problems.
- Quantum Speedup: Quantum algorithms can leverage superposition and entanglement to explore multiple states in parallel, offering potential speedups over classical methods.

## Classical vs. Quantum Binary Optimization

#### • Classical Methods:

- Brute Force: Exhaustive search of the solution space (exponential time).
- Branch-and-Bound: A divide-and-conquer approach, but can still be computationally expensive for large problems.
- Heuristic Methods: Simulated annealing, genetic algorithms (do not guarantee optimal solutions).
- Quantum Approaches:
  - Quantum Annealing: Uses quantum tunneling to escape local minima.
  - QAOA (Quantum Approximate Optimization Algorithm): Hybrid quantum-classical algorithm designed for combinatorial optimization problems.
- Advantages: Quantum approaches offer the potential to explore large solution spaces more efficiently than classical algorithms.

# Real-World Applications of Quantum Binary Optimization

- Logistics:
  - Vehicle routing problems.
  - Supply chain optimization.
- Finance:
  - Portfolio optimization.
  - Risk management.
- Machine Learning:
  - Feature selection.
  - Training of large models (e.g., neural networks).
- Artificial Intelligence: AI model tuning and optimization for decision-making tasks.

- Binary optimization problems are central to many real-world challenges in logistics, finance, and machine learning.
- Quantum binary optimization offers significant potential advantages due to the ability of quantum systems to explore large solution spaces in parallel.
- Quantum algorithms like quantum annealing and QAOA are promising methods for solving complex binary optimization problems, especially in the context of NP-hard problems.

## § 2: Binary and Quadratic Optimization Problems

- Binary Optimization Problems involve decision variables  $x_i \in \{0, 1\}$  or  $x_i \in \{-1, 1\}$ .
- The goal is to minimize or maximize an objective function subject to constraints.
- General Form:

$$\min_{x\in\{0,1\}^n}f(x)$$

- Examples: Max-Cut, Knapsack, Set Covering Problems.
- Challenges:
  - NP-hard: The number of possible solutions grows exponentially with the size of the problem.
  - Complex solution landscapes require advanced strategies for finding global optima.

- Exponential Search Space: With *n* binary variables, the solution space has 2<sup>*n*</sup> possibilities.
- Classical Approaches:
  - Heuristics (e.g., simulated annealing, genetic algorithms).
  - Exact methods like branch-and-bound or brute-force search are often impractical for large problems.
- Quantum Potential: Quantum algorithms can search large spaces more efficiently through superposition and entanglement.

- QUBO is a specific class of binary optimization where the objective function is quadratic and unconstrained.
- Problem Formulation:

$$\min_{x\in\{0,1\}^n} x^T Q x + c^T x$$

where:

- Q is an  $n \times n$  matrix representing interactions between variables.
- c is a vector of linear coefficients.

• QUBO models a wide range of combinatorial optimization problems.

• Flexibility: QUBO can represent many types of problems, including:

- Portfolio optimization in finance.
- Feature selection in machine learning.
- Resource allocation in telecommunications.
- Standard Form: The QUBO formulation is widely used because it can easily be mapped to quantum systems such as quantum annealers and gate-based models.
- Optimization Task: By solving QUBO efficiently, many real-world problems can be addressed.

#### • Classical Approaches:

- Heuristic methods (e.g., simulated annealing, genetic algorithms) are often used to approximate solutions.
- Exact methods (e.g., brute force, branch-and-bound) are computationally expensive.
- Quantum Approaches:
  - Quantum Annealing: Solves QUBO by evolving the system to the ground state of a quantum system.
  - QAOA (Quantum Approximate Optimization Algorithm): A hybrid quantum-classical algorithm designed for combinatorial problems.
  - Advantage: Quantum algorithms explore multiple states in parallel, offering speedups for large QUBO problems.

- Parallelism: Quantum systems can explore a large number of possible solutions simultaneously due to superposition.
- Potential Speedups: In theory, quantum approaches like annealing or QAOA can outperform classical methods for certain NP-hard problems.
- Scalability: Quantum algorithms have the potential to scale more effectively for high-dimensional QUBO problems.
- Real-world applications of quantum optimization are still in the early stages but showing promise.

- Binary Optimization Problems involve decision variables restricted to binary values and are often NP-hard.
- QUBO provides a flexible framework for a wide range of combinatorial optimization problems.
- Quantum algorithms offer the potential to solve large-scale QUBO problems faster than classical approaches through parallel exploration of solution spaces.

• The Unconstrained Quadratic Binary Optimization problem (QUBO) is:

optimize 
$$H(x) = x^T Q x$$

- Where:
  - x is an *n*-vector of binary variables,
  - Q is an  $n \times n$  symmetric matrix of constants,
  - H(x) is called the energy of a QUBO solution x.

• The objective function in QUBO (i.e., the energy of a QUBO solution *x*) can be expanded as:

$$H(x) = \sum_{i=1}^{n} Q_{ii} x_i^2 + 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij} x_i x_j$$

This shows the quadratic and pairwise interaction terms in the QUBO problem.

## Some well-known applications of QUBO

- The QUBO model is highly flexible and can be applied to a wide variety of optimization problems.
- Some well-known applications include:
  - Maximum cut (Max-Cut)
  - SAT and Max Sat Problems
  - Spin Glass Problems
  - Graph Coloring Problems
  - Number Partitioning Problems
  - Maximum Independent Set Problems
  - Machine learning feature selection
  - Set Packing Problems
  - Graph partitioning
  - Quadratic Assignment Problems
  - Capital Budgeting Problems
  - Multiple Knapsack Problems
  - Task Allocation Problems (distributed computer systems)
  - Maximum Diversity Problems
  - P-Median Problems
  - Asymmetric and Symmetric Assignment Problems

- The matrix Q in QUBO is symmetric, meaning that  $Q_{ij} = Q_{ji}$  for all i and j.
- This property simplifies the representation and computation of the QUBO objective function.

### Basic QUBO Problem Formulation

- Minimize/Maximize  $H(x) = x^T Q x$ : x binary
- For a symmetric matrix Q

$$x^{T}Qx = \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij}x_{i}x_{j}$$

where  $x_i \in \{0, 1\}$ .

• In linear + quadratic form:

$$H(x) = x^{T} Q x = \sum_{i=1}^{n} Q_{ii} x_{i} + \sum_{i=1}^{n} \sum_{j=i+1}^{n} 2Q_{ij} x_{i} x_{j}$$

- The QUBO formulation is widely used in combinatorial optimization.
- The binary nature of x simplifies many optimization problems.

- The QUBO formulation involves minimizing or maximizing H(x) = x<sup>T</sup>Qx where x is a binary vector and Q is a symmetric matrix.
- Binary optimization problems have wide applications in combinatorial optimization and can be tackled using both classical and quantum approaches.

# § 2.1: Examples of QUBO Formulation

Image: Image:

æ

### § 2.1.1: The Max Cut Problem

æ

< □ > < 同 > < 回 > < 回 > < 回 >

- Given an undirected graph G(V, E), the Max Cut problem seeks to partition V into two sets such that the number of edges between the two sets (the cut) is as large as possible.
- We can model this problem by introducing binary variables x<sub>i</sub>, where:

$$x_i = \begin{cases} 1 & \text{if vertex } i \text{ is in one set,} \\ 0 & \text{if vertex } i \text{ is in the other set.} \end{cases}$$

• The quantity  $(1 - x_i)(1 - x_j)$  identifies whether the edge (i, j) is in the cut.

• The problem of maximizing the number of edges in the cut can be formulated as:

maximize 
$$\sum_{(i,j)\in E} \frac{1-x_i x_j}{2}$$

• This is an instance of a QUBO (Quadratic Unconstrained Binary Optimization) problem:

maximize 
$$H(x) = x^T Q x$$

• Consider an undirected graph with 5 vertices and 6 edges:

- Vertices: 1, 2, 3, 4, 5
- Edges: (1,2), (1,3), (2,3), (3,4), (4,5), (2,5)
- The objective is to partition the vertices into two sets such that the number of edges between the sets is maximized.



## QUBO Representation of Max Cut Problem

• Explicitly taking into account all edges in the graph gives the following formulation:

$$Q = egin{bmatrix} 0 & 1 & 1 & 0 & 1 \ 1 & 0 & 1 & 0 & 1 \ 1 & 1 & 0 & 1 & 0 \ 0 & 0 & 1 & 0 & 1 \ 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

• This takes the desired form of a QUBO problem: maximize  $H(x) = x^T Q x$ .

• Solving the QUBO model gives the optimal binary vector:

$$x = [0, 1, 1, 0, 0]$$

- Hence, vertices 2 and 3 are in one set, while vertices 1, 4, and 5 are in the other set.
- The maximum cut value for this problem is 5.

## § 2.1.2: The Number Partitioning Problem

æ

- Partition a set of numbers into two subsets such that the subset sums are as close to each other as possible.
- We model this problem as a QUBO instance as follows:
- Consider a set of numbers  $S = \{s_1, s_2, ..., s_n\}$ .
- Let  $x_i = 1$  if  $s_i$  is assigned to subset 1; 0 otherwise.
- The sum for subset 1 is given by  $\sum_{i} x_i s_i$  and the sum for subset 2 is given by  $\sum_{i} (1 x_i) s_i$ .

### The Number Partitioning Problem

• We aim to minimize the difference between the sums of the two subsets:

$$\left(\sum_i x_i s_i - \sum_i (1-x_i) s_i\right)^2$$

• Simplifying the expression leads to:

$$\left(2\sum_i x_i s_i - \sum_i s_i\right)^2$$

Dropping the additive and multiplicative constants, our QUBO optimization problem becomes:

QUBO: min 
$$H(x) = \sum_{i,j} Q_{ij} x_i x_j$$

#### Numerical Example: The Number Partitioning Problem

• Consider the set of eight numbers:

$$S = \{25, 7, 13, 31, 42, 17, 21, 10\}$$

• From the previous development, the QUBO problem is:

$$\min H(x) = \sum_{i,j} Q_{ij} x_i x_j$$

with

	F −3525	175	325	775	1050	425	525	ך 250
<i>Q</i> =	175	-1113	91	217	294	119	147	70
	325	91	-1989	403	546	221	273	130
	775	217	403	-4185	1302	527	651	310
	1050	294	546	1302	-5208	714	882	420
	425	119	221	527	714	-2533	357	170
	525	147	273	651	882	357	-3045	210
	L 250	70	130	310	420	170	210	—1560 <b>」</b>
- Solving the QUBO gives x = (00011001), yielding perfectly matched subset sums of 83.
- The development employed here can be expanded to address other forms of the number partitioning problems as discussed in Alidaee, et.al. (2005)

# § 3: Creating QUBO Models Using Known Penalties

- A penalty function is a Valid Infeasible Penalty (VIP) if:
  - It is zero for feasible solutions.
  - It is positive for infeasible solutions.
- Including quadratic VIPs in the objective function for each constraint yields a transformed QUBO model.

# Creating QUBO using Known Penalties

• Many constrained problems can be re-formulated as QUBO models by introducing quadratic penalties with a positive scalar *P*.

Classical Constraint	Equivalent Penalty
$x + y \le 1$	P(xy)
$x + y \ge 1$	P(1-x-y+xy)
x + y = 1	P(1-x-y+2xy)
$x \leq y$	P(x-xy)
$x_1 + x_2 + x_3 \le 1$	$P(x_1x_2 + x_1x_3 + x_2x_3)$
x = y	P(x+y-2xy)

Table: Simple examples: Known constraint/penalty pairs

- Certain types of constraints can be represented by quadratic penalty functions.
- For example, consider binary variables x and y with a constraint  $x + y \le 1$ .
- A quadratic infeasibility penalty for this constraint is:

#### Pxy

where P is a large positive scalar.

## § 3.0.1: Minimum Vertex Cover (MVC) Problem

Creating QUBO Models Using Known Penalties

∃ > October 17, 2024 42/130

æ

- A vertex cover is a subset of vertices such that every edge is incident to at least one vertex in the subset.
- The Minimum Vertex Cover (MVC) problem seeks to find the smallest such subset.
- The objective is to minimize the number of vertices in the cover.

$$egin{array}{lll} {
m min} & \sum_{j\in V} x_j \ x_i+x_j\geq 1 & {
m for all} & (i,j)\in E \end{array}$$

• The constraints in MVC can be represented by a penalty function:

$$P(1-x-y+xy)$$

• This transforms the constrained problem into an unconstrained QUBO model as follows

min 
$$H(x) = \sum_{j \in V} x_j + P\left(\sum_{(i,j) \in E} 1 - x_i - x_j + x_i x_j\right)$$

• we can write this as minimize  $\mathbf{x}^T Q \mathbf{x}$  plus a constant term

# MVC Numerical Example

- Consider a graph with 6 edges and 5 nodes.
- The QUBO model is written as:

$$\min Qx = x_1 + x_2 + x_3 + x_4 + x_5 + P(1 - x_1 - x_2 + x_1x_2) + P(1 - x_1 - x_3 + x_1x_3) + P(1 - x_2 - x_4 + x_2x_4) + P(1 - x_3 - x_4 + x_3x_4) + P(1 - x_3 - x_5 + x_3x_5) + P(1 - x_4 - x_5 + x_45)$$

where Q is a matrix. Qx can be written as  $Qx = (1 - 2P)x_1 + (1 - 2P)x_2 + (1 - 3P)x_3 + (1 - 3P)x_4 + (1 - 2P)x_5 + Px_1x_2 + Px_1x_3 + Px_2x_4 + Px_3x_4 + Px_3x_5 + Px_4x_5 + 6P$ 

# MVC Solution Example

• Arbitrarily choosing P = 8 and dropping the additive constant gives a QUBO model, with the Q matrix given by

$$\begin{bmatrix} -15 & 4 & 4 & 0 & 0 \\ 4 & -15 & 0 & 4 & 0 \\ 4 & 0 & -23 & 4 & 4 \\ 0 & 4 & 4 & -23 & 4 \\ 0 & 0 & 4 & 4 & -15 \end{bmatrix}$$

• The solution to the QUBO model is:

$$x = (01101), \quad x^T Q x = -45$$

• The minimum vertex cover consists of nodes 2, 3, and 5.

Solving this QUBO model gives: H(x) = x<sup>T</sup>Qx = -45 at x = (0,1,1,0,1) for which H(x) = 48 - 45 = 3, meaning that a minimum cover is given by nodes 2, 3, and 5.



### § 3.0.2: The Set Packing Problem

Creating QUBO Models Using Known Penalties

< ∃⇒ October 17, 2024 48/130

Image: Image:

æ

- The Set Packing Problem maximizes the number of selected disjoint subsets.
- This can be formulated as:

$$\max \sum w_i x_i$$
 subject to  $\sum a_{ij} x_i \leq 1$ 

where  $x_i$  are binary variables, and  $w_i$  and  $a_{ij}$  are weights and coefficients.

 By applying penalties, we can reformulate the Set Packing problem as a QUBO:

$$\max H(x) = x^T Q x$$

where the matrix Q is constructed using penalties for violating the disjoint constraint.

#### Set Packing Numerical Example

• Consider a small example of a set packing problem:

 $\max x_1 + x_2 + x_3 + x_4 \\ s.t. x_1 + x_3 + x_4 \le 1, \ x_1 + x_2 \le 1$ 

Re-casting as QUBO via the penalties of previous Table.

max 
$$x_1 + x_2 + x_3 + x_4 - Px_1x_3 - Px_1x_4 - Px_3x_4 - Px_1x_2$$

This has our customary QUBO form max H(x) = x<sup>T</sup>Qx, where the Q matrix, with P arbitrarily chosen to be 6, is given by

• The solution of this QUBO model is:

$$x = (0, 1, 1, 0), \quad y = 2$$

- All penalty terms are equal to zero in the solution.
- Remark: Set packing problems with thousands of variables and constraints have been efficiently reformulated and solved in Alidaee, et. al. (2008) using the QUBO reformulation illustrated in this example.

# § 3.0.3: The Graph Coloring Problem

Image: Image:

æ

- Vertex coloring problems seek to assign colors to nodes of a graph such that adjacent nodes receive different colors.
- These problems can be modeled as satisfiability problems as follows:
- Let  $x_{ij} = 1$  if node *i* is assigned color *j* and 0 otherwise.
- Each node must be assigned a color, so we have the constraints:

$$\sum_{j=1}^{K} x_{ij} = 1 \quad \text{for all nodes } i$$

• For adjacent nodes *i* and *j*, the constraints ensure that they receive different colors.

- A feasible coloring where adjacent nodes are assigned different colors is assured by imposing adjacency constraints.
- This problem can be recast into a QUBO model using:
  - Transformation #1 on the node assignment constraints.
  - Transformation #2 on the adjacency constraints.
- The resulting QUBO model is optimized to find the feasible coloring.

### Numerical Example: Graph Coloring with 3 Colors

- Consider the problem of finding a feasible coloring of the graph using K = 3 colors.
- The goal is to find a solution to the system:

$$\sum_{j=1}^{3} x_{ij} = 1$$
 for all adjacent nodes  $i$  and  $j$ 

such that  $x_{ip} + x_{jp} \le 1$  for p = 1, ..., 3 for all adjacent nodes *i* and *j*. • Graph structure:



56 / 130

#### Solving the QUBO Model for Graph Coloring

• The problem is formulated as a QUBO problem:

minimize  $H(x) = x^T Q x$  where x is binary



#### Solving the QUBO Model for Graph Coloring

• Solving this model yields a feasible coloring:

$$x_2 = x_4 = x_9 = x_{11} = x_{15} = 1$$

with all other variables equal to zero.

- In this example, the solution means:
  - Nodes 1 and 4 get color #2.
  - Node 2 gets color #1.
  - Nodes 3 and 5 get color #3.



#### § 4: The Max 2-Sat Problem

< □ > < 同 > < 回 > < 回 > < 回 >

æ

- Satisfiability problems are used in many settings and represented in terms of clauses in conjunctive normal form (CNF).
- Max 2-Sat problems consist of clauses with two literals, and a clause is satisfied if either or both literals are true.
- The goal is to maximize the number of satisfied clauses.

- There are three types of clauses in Max 2-Sat, each associated with a quadratic penalty:
  - **1** No negations:  $x_i \lor x_j$

Constraint:  $x_i + x_j \ge 1$ , Penalty:  $1 - x_i - x_j + x_i x_j$ 

**2** One negation:  $x_i \vee \overline{x}_j$ 

Constraint: 
$$x_i + (1 - x_j) \ge 1$$
, Penalty:  $x_j - x_i x_j$ 

**3** Two negations:  $\overline{x}_i \vee \overline{x}_j$ 

Constraint:  $(1 - x_i) + (1 - x_j) \ge 1$ , Penalty:  $x_i x_j$ 

イロト 不得 トイヨト イヨト

- The problem is recast into a Quadratic Unconstrained Binary Optimization (QUBO) model by minimizing the number of unsatisfied clauses.
- The penalty function is:

$$\min H(x) = x^T Q x$$

• Example: A Max 2-Sat instance with 4 variables and 12 clauses gives the QUBO model:

$$\min H(x) = 3 + x_1 - 2x_4 - x_2x_3 + x_2x_4 + 2x_3x_4$$

Clause #	Clause	Quadratic Penalty
1	$x_1 \lor x_2$	$1 - x_1 - x_2 + x_1 x_2$
2	$x_1 \vee \overline{x}_2$	$x_2 - x_1 x_2$
3	$\overline{x}_1 \lor x_2$	$x_1 - x_1 x_2$
4	$\overline{x}_1 \vee \overline{x}_2$	<i>x</i> <sub>1</sub> <i>x</i> <sub>2</sub>
5	$\overline{x}_1 \lor x_3$	$x_1 - x_1 x_3$
6	$\overline{x}_1 \lor \overline{x}_3$	<i>x</i> <sub>1</sub> <i>x</i> <sub>3</sub>
7	$x_2 \vee \overline{x}_3$	$x_3 - x_2 x_3$
8	$x_2 \lor x_4$	$1 - x_2 - x_4 + x_2 x_4$
9	$\overline{x}_2 \lor x_3$	$x_2 - x_2 x_3$
10	$\overline{x}_2 \vee \overline{x}_3$	<i>x</i> <sub>2</sub> <i>x</i> <sub>3</sub>
11	$x_3 \lor x_4$	$1 - x_3 - x_4 + x_3 x_4$
12	$\overline{x}_3 \vee \overline{x}_4$	X3X4

#### Table: Penalties for the 12 Clauses

The Max 2-Sat Problem

October 17, 2024

Image: A matrix

æ

∃ →

The QUBO model can be represented in matrix form as:

$$\min H(x) = 3 + x^T Q x$$

where the Q matrix is:

$$Q = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 1 \\ 0 & \frac{1}{2} & 1 & -2 \end{pmatrix}$$

Image: Image:

э

- Solving the QUBO model minimizes the number of unsatisfied clauses.
- Example solution: H(x) = 1 when  $x_1 = x_2 = x_3 = 0$  and  $x_4 = 1$ , meaning all but one clause is satisfied.
- The QUBO approach is scalable and has been used to solve Max 2-Sat problems with hundreds of variables.

- The QUBO model size is independent of the number of clauses and depends only on the number of variables.
- Max 2-Sat problems with hundreds of variables and thousands of clauses can be efficiently solved using the QUBO approach.

# § 5: Quantum Algorithms for Optimization

æ

# Contents I

- Introduction
- Adiabatic Quantum Computing
- Quantum Supremacy in the Adiabatic Setting and Computational Efficiency of Quantum Annealing
  - Types of Quantum Speedups
  - Weak Strong Clustering
- Adiabatic Quantum Algorithms
  - Adiabatic Grover's Search
  - Adiabatic Quantum Linear Systems Solver
- Combinatorial Optimization
  - Weighted MAX-SAT
  - QUBO
  - Ising Minimization Problem
  - Optimization Algorithms
    - Simulated Annealing
    - Quantum Annealing

- Quantum Monte Carlo
- Parallel Tempering
- Tabu Search
- Experimental Implementations of Quantum Annealers

э

# § 5.1: Introduction to Quantum Optimization Algorithms

# Introduction to Quantum Optimization Algorithms

- Quantum Optimization Algorithms aim to solve complex optimization problems by utilizing the principles of quantum mechanics.
- Quantum Adiabatic Optimization (AQO):
  - A form of optimization where the system evolves slowly from an initial simple Hamiltonian  $H_B$  to a final Hamiltonian  $H_P$  that encodes the problem solution.
  - The system stays in its ground state, finding the global minimum, provided the evolution is slow enough.
- Other quantum optimization techniques:
  - Quantum Annealing (QA): A practical implementation of AQO used in hardware like D-Wave to solve optimization problems.
  - Variational Quantum Algorithms (VQA): Combines quantum state preparation with classical optimization methods (e.g., VQE, QAOA).
- **Applications**: Used for solving problems like **Max-Cut**, and other combinatorial optimization problems.

< ロ > < 同 > < 回 > < 回 > < 回 >

# § 6: Mapping Optimization Problems to Quantum Hardware

Mapping Optimization Problems to Quantum Hardware
- QUBO (Quadratic Unconstrained Binary Optimization) is a mathematical formulation of optimization problems that can be efficiently mapped to quantum hardware.
- Ising Model: A physical model used in quantum systems to represent binary variables as spins s<sub>i</sub> ∈ {−1, 1}.
- Transformation: The mapping of QUBO to the Ising model is done via the relation:

$$x_i = \frac{1+s_i}{2}$$

where  $x_i \in \{0, 1\}$  represents binary variables, and  $s_i \in \{-1, 1\}$  represents spin variables.

## Significance of the Ising Model in Quantum Hardware

- The Ising model serves as a bridge between optimization problems and quantum systems.
- Hamiltonian Formulation: The Ising model is expressed as a Hamiltonian:

$$H = \sum_{i,j} J_{ij} s_i s_j + \sum_i h_i s_i$$

where  $J_{ij}$  represents the interaction between spins and  $h_i$  represents an external magnetic field. Both  $J_{ij}$  and  $h_i$  can be derived in terms of  $Q_{ii}$  and  $Q_{ij}$ .

• Substituting  $s_i$  with  $\sigma_z^{(i)} = I_{2i-1} \otimes \sigma_z \otimes I_{2n-i}$ , the Ising problem is converted to quantum Ising Hamiltonian.

• The Hamiltonian is often expressed as an Ising Hamiltonian:

$$H = \sum_{i < j} J_{ij} \sigma_i^z \sigma_j^z + \sum_i h_i \sigma_i^z$$

•  $\sigma^z$  is the Pauli Z operator

- Many quantum optimization algorithms, such as Quantum Adiabatic Optimization, and Quantum Annealing, operate by finding the ground state of this Ising Hamiltonian.
- The Ising model is used in quantum hardware like D-Wave to solve optimization problems.

### § 7: Quantum Adiabatic Optimization

æ

- Quantum computations can be implemented by the adiabatic evolution of a system's Hamiltonian.
- The system is initialized in the ground state of a simple Hamiltonian and adiabatically evolved to a Hamiltonian that encodes the solution.
- Adiabatic quantum computation (AQC) evolves Hamiltonians rather than applying quantum gates.

- Adiabatic theorem: A quantum system remains in its ground state if the Hamiltonian evolves slowly.
- Evolution starts with  $H_{initial}$ , transitioning to  $H_{final}$  which encodes the solution.
- System evolution:

$$H(t) = (1 - s(t))H_{\text{initial}} + s(t)H_{\text{final}}$$

• Steps: Initialize in ground state of  $H_{initial}$ , slowly evolve to  $H_{final}$ , measure to obtain the solution.

- Effective in solving NP-hard problems such as Max-Cut, Traveling Salesman, and Graph Coloring.
- Real-world applications: logistics (vehicle routing, supply chain), finance (portfolio optimization), and machine learning (feature selection).
- Implementations: D-Wave quantum systems perform adiabatic optimization.
- Challenges: Decoherence, noise, scalability, and time constraints (slow evolution required).

#### The Adiabatic Theorem

• Schrodinger equation:

$$i\hbarrac{d}{dt}|\psi(t)
angle=H(t)|\psi(t)
angle$$

Instantaneous eigenstate:

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

Initial condition:

$$|\psi(0)
angle = |\mathit{n}(0)
angle$$

• If evolution is slow enough, the system remains in its instantaneous eigenstate.

$$|\psi(t)
angle pprox e^{i heta(t)}|\psi(0)
angle, \qquad |\psi_n(t)
angle = U(t)|\psi(0)
angle, \ U_l(t) = \sum_{q=0}^{\infty} (-1)^q \int_0^t dt_q \cdots \int_0^{t_2} dt_1 H_l(t_q) \cdots H_l(t_1)$$

#### Adiabatic Theorem (Born and Folk 1928)

- A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.
- Under a slowly changing Hamiltonian H(t), with instantaneous eigenstate  $|n(t)\rangle$  and the corresponding energy  $E_n(t)$ , a quantum system evolves from an initial state  $|n(0)\rangle$  to the final state  $|n(t)\rangle$ .

$$|\psi(0)\rangle = \sum_{n} c_{n}(0)|n(0)\rangle \xrightarrow{\text{Final}} |\psi(t)\rangle = \sum_{n} c_{n}(t)|n(t)\rangle$$

$$c_n(t) = c_n(0)e^{i\theta_n(t)}e^{i\gamma_n(t)}$$

• Dynamical Phase:  $\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt'$ 

• Geometrical Phase:  $\gamma(t) = i \int_0^t \langle n(t') | \dot{n}(t') \rangle dt'$ 

• The rate of change of Hamiltonian  $\frac{dH(t)}{dt}$  is small, and there is a finite gap  $E_m(t) - E_n(t) \neq 0$  between energies  $m \neq n \rightarrow$ 

$$\langle n(t')|\dot{n}(t')\rangle = -\frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_m(t) - E_n(t)} \to 0$$

•  $|c_n(t)|^2 = |c_n(0)|^2$  so if the system begins in an eigenstate of H(0), it remains in an eigenstate of H(t) during the evolution, with a change of phase only.

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

• Assume  $m \neq n$  and perform the inner product with  $\langle m(t) |$ :

$$H(t)|m(t)
angle = E_m(t)|m(t)
angle, \qquad \langle m(t)|n(t)
angle \ \langle m(t)|\dot{n}(t)
angle = -rac{\langle m(t)|\dot{H}(t)|n(t)
angle}{E_m(t) - E_n(t)}$$

• Adiabatic approximation: The rate of change in the Hamiltonian  $\frac{dH(t)}{dt}$  is small, and there is a finite gap  $E_m(t) - E_n(t)$ .

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \rightarrow |\psi(t)\rangle = \sum_{n} c_{n}(t)|n(t)\rangle$$
$$i\hbar\dot{c}_{m}(t) + i\hbar\sum_{n} c_{n}(t)\langle m(t)|\dot{n}(t)\rangle = c_{m}(t)E_{m}(t)$$

• In the Adiabatic limit  $\langle m(t)|n(t)\rangle \approx 0$  for  $m \neq n$ :

$$egin{aligned} &i\hbar\dot{c}_m(t)+i\hbar c_m(t)\langle m(t)|\dot{m}(t)
angle &=c_m(t)E_m(t)\ &rac{\dot{c}_m(t)}{c_m(t)}=-rac{i}{\hbar}E_m(t)+ii\langle m(t)|\dot{m}(t)
angle \end{aligned}$$

Image: Image:

æ

• In the Adiabatic limit  $\langle m(t)|n(t)\rangle \approx 0$  for  $m \neq n$ :

$$c_m(t) = c_m(0)e^{i\theta_m(t)}e^{i\gamma_m(t)}$$

• Dynamical phase:

$$\theta_m(t) = -\frac{1}{\hbar} \int_0^t E_m(t') dt',$$

• Geometrical phase:

$$\gamma(t) = i \int_0^t \langle m(t') | \dot{m}(t') \rangle dt'$$

э

# § 7.1: Quantum Adiabatic Algorithm

æ

- The Quantum Adiabatic Algorithm (QAA) can be used on a quantum computer as an optimization method for finding the global minimum of a classical cost function f : {0,1}<sup>n</sup> → ℝ.
- The cost function is encoded in a problem Hamiltonian  $H_P$ , which acts on the Hilbert space of n spin- $\frac{1}{2}$  particles.

$$H_P = \sum_{z \in \{0,1\}^n} f(z) |z\rangle \langle z|$$

where for QUBO we have  $H_p = \sum_{i < j} J_{ij} \sigma_i^z \sigma_j^z + \sum_i h_i \sigma_i^z$ .

• The system is initialized in the ground state of the beginning Hamiltonian  $H_B$ :

$$H_B = \sum_{i=1}^n \left(\frac{1-\sigma_i^x}{2}\right)$$

• The ground state of *H*<sub>B</sub> is the uniform superposition of computational basis states:

$$|\psi_{\mathsf{init}}
angle = rac{1}{\sqrt{2^n}}\sum_{z\in\{0,1\}^n}|z
angle$$

• The system evolves according to:

$$H(t) = (1 - t/T)H_B + (t/T)H_P$$

• Alternatively, using a parameter s = t/T, we write:

$$H(s) = (1-s)H_B + sH_P$$

• Start in the ground state of  $H_B$  at t = 0 and evolve to t = T, where the state will be very close to the ground state of  $H_P$ , which gives the solution.

• The minimum gap  $g_{\min}$  is defined as:

$$g_{\min} = \min_{0 \le s \le 1} \left( E_1(s) - E_0(s) \right)$$

- If  $g_{min} > 0$ , the system evolves adiabatically, and the ground state is preserved.
- To ensure the system evolves correctly, the total evolution time *T* must satisfy:

$$T \gg \frac{E}{g_{\min}^2}$$

where:

$$E = \max_{0 \le s \le 1} \left| \langle 1; s | \frac{dH}{ds} | 0; s 
angle 
ight|$$

• For a problem instance with a unique minimizing string *w*, the success probability at time *t* = *T* is:

$$P(T) = |\langle w | \psi(T) \rangle|^2$$

October 17, 2024 92 / 130

э

→ < ∃ →</p>

Image: Image:

- The strategies presented, including evolving more rapidly, initializing in excited states, and using modified evolution paths, consistently increased success probabilities in all hard instances tested.
- Future work will involve testing these strategies on larger problem instances using quantum hardware.

# § 8: One Qubit Example

Image: A matrix

æ

- Consider a one-bit problem where the clause is satisfied if  $z_1 = 1$ .
- The problem Hamiltonian is given by:

$$H_P = rac{1}{2} + rac{1}{2}\sigma_z^{(1)}$$

• The ground state of  $H_P$  is  $|z_1 = 1\rangle$ .

• The initial Hamiltonian  $H_B$  is chosen as:

$$H_B=\frac{1}{2}-\frac{1}{2}\sigma_x^{(1)}$$

• The smooth interpolating Hamiltonian H(s) is:

$$H(s) = (1-s)H_B + sH_P$$

#### Eigenvalues of the Interpolating Hamiltonian

• The eigenvalues of H(s) are given by:

$$\lambda_{\pm}(s) = rac{1}{2} \left(1 \pm \sqrt{1-2s+2s^2}
ight)$$

 These eigenvalues are plotted in the following figure, showing a modest minimum gap:



97 / 130

• Suppose we replace  $H_B$  with:

$$\mathcal{H}_B^\prime = rac{1}{2} - rac{1}{2} \sigma_z^{(1)}$$

• Now H(s) is diagonal in the z-basis for all s, and the eigenvalues cross at s = 0.5:

$$\lambda_1 = s, \quad \lambda_2 = 1 - s$$

• This symmetry causes a level crossing and a minimum gap of zero.

• Adding a small off-diagonal term to break the symmetry:

$$H_\epsilon(s) = egin{pmatrix} s & \epsilon(1-s) \ \epsilon(1-s) & 1-s \end{pmatrix}$$

• The minimum gap  $g_{\min}$  is now  $\epsilon$ , ensuring no level crossing.

# § 9: 2-SAT on a Ring

2-SAT on a Ring

October 17, 2024 100 / 130

Ξ.

<ロト < 四ト < 三ト < 三ト

- Consider an *n*-bit problem with *n* clauses, each acting on adjacent bits.
- Clause  $C_j$  acts on bits j and j + 1.
- The boundary condition is cyclic: bit n + 1 is identified with bit 1.
- Clauses can either be "agree" (00 and 11 are satisfying) or "disagree" (01 and 10 are satisfying).
- The problem is restricted to an even number of disagree clauses so that a satisfying assignment exists.

- Given the list of clauses, constructing the satisfying assignment is trivial.
- If  $w_1, w_2, \ldots, w_n$  is a satisfying assignment, so is  $\overline{w}_1, \overline{w}_2, \ldots, \overline{w}_n$ .
- There are exactly two satisfying assignments.

• The quantum version of the problem is described by the Hamiltonian:

$$H_P = H_{12}^{C_1} + H_{23}^{C_2} + \dots + H_{n1}^{C_n}$$

- Each  $C_j$  is either an "agree" or "disagree" clause.
- The ground states of  $H_P$  are  $|w_1\rangle|w_2\rangle\cdots|w_n\rangle$  and  $|\overline{w}_1\rangle|\overline{w}_2\rangle\cdots|\overline{w}_n\rangle$ .

• Define the unitary transformation:

$$egin{aligned} &z_1 
angle |z_2 
angle \ldots |z_n 
angle 
ightarrow |z_1' 
angle |z_2' 
angle \ldots |z_n' 
angle \ &z_j' = egin{cases} &z_j & ext{if } w_j = 1 \ & \overline{z}_j & ext{if } w_j = 0 \end{aligned}$$

• Under this transformation,  $H_P$  becomes:

$$H_P = H_{12}^{\text{agree}} + H_{23}^{\text{agree}} + \dots + H_{n1}^{\text{agree}}$$

• We choose the initial Hamiltonian  $H_B$  as:

$$H_B = \sum_{j=1}^n \left(1 - \sigma_j^x\right)$$

- $H_B$  is invariant under the transformation described earlier.
- The ground state of  $H_B$  is:

$$|x=0\rangle = \frac{1}{2^{n/2}} \sum_{z_1, z_2, \dots, z_n} |z_1 z_2 \dots z_n\rangle$$

• The adiabatic evolution Hamiltonian is given by:

$$H(s) = (1-s)\sum_{j=1}^{n} (1-\sigma_{j}^{x}) + s\sum_{j=1}^{n} \frac{1}{2}(1-\sigma_{j}^{z}\sigma_{j+1}^{z})$$

• This Hamiltonian is diagonalized in the space of symmetric states.

• Define the fermion operators for  $j = 1, \ldots, n$ :

$$b_{j} = \sigma_{1}^{x} \sigma_{2}^{x} \dots \sigma_{j-1}^{x} \sigma_{j}^{-}$$
$$b_{j}^{\dagger} = \sigma_{1}^{x} \sigma_{2}^{x} \dots \sigma_{j-1}^{x} \sigma_{j}^{+}$$

• These operators satisfy the anticommutation relations:

$$\{b_j, b_k^{\dagger}\} = \delta_{jk}, \quad \{b_j, b_k\} = 0$$

• The ground state energy  $E_{-}(s)$  is given by:

$$E_{-}(s) = 2 - s - \sqrt{(2 - 3s)^2 + 4s(1 - s)(1 - \cos(\pi p/n))}$$

• The minimum gap occurs at s = 2/3 and is:

$$g_{\min} \approx \frac{4\pi}{3n}$$

• The required evolution time T scales as  $T \sim n^3$ .
- Quantum adiabatic evolution successfully solves the 2-SAT problem on a ring.
- The evolution time T scales polynomially with n, specifically  $T \sim n^3$ .
- This method is generalizable to other simple problems with structured constraints.

- The phenomenon of **level repulsion** ensures that in typical systems, level crossings are avoided.
- This behavior is common in more complicated systems.
- For small  $\epsilon$ , the gap  $g_{\min}$  prevents crossing, ensuring adiabatic evolution.

## § 10: Adiabatic Quantum Computation & Deutsch's Algorithm

Adiabatic Quantum Computation & Deutsch's Algorithm

- Quantum computation harnesses the principle of superposition in quantum mechanics for enhanced efficiency in problem-solving.
- Deutsch's algorithm is one of the earliest quantum algorithms, determining whether a function f : {0,1} → {0,1} is constant or balanced.
- The four possible outcomes for f are:

• 
$$f(0) = f(1) = 0$$
 (constant)

- f(0) = f(1) = 1 (constant)
- f(0) = 0, f(1) = 1 (balanced)
- f(0) = 1, f(1) = 0 (balanced)

- Adiabatic quantum computation replaces quantum gates with a Hamiltonian that evolves continuously with time.
- The system remains in its ground state throughout the evolution.
- Hamiltonians  $H_0$  and  $H_1$  are defined as:

$$H_0 = I - |\psi_0\rangle\langle\psi_0|$$
 and  $H_1 = I - |\psi_1\rangle\langle\psi_1|$ 

where

$$|\psi_0
angle=rac{1}{\sqrt{2}}(|0
angle+|1
angle)$$

and

$$|\psi_1\rangle = \alpha |\mathbf{0}\rangle + \beta |\mathbf{1}\rangle$$

• The coefficients  $\alpha$  and  $\beta$  are defined as:

$$\alpha = \frac{1}{2} \left| (-1)^{f(0)} + (-1)^{f(1)} \right|$$
$$\beta = \frac{1}{2} \left| (-1)^{f(0)} - (-1)^{f(1)} \right|$$

- If f is constant,  $\alpha = 1$  and  $\beta = 0$ .
- If f is balanced,  $\alpha = 0$  and  $\beta = 1$ .

• The time-dependent Hamiltonian is defined as:

$$H(t) = (1 - s(t))H_0 + s(t)H_1$$

where s(t) is a function of time such that s(0) = 0 and s(T) = 1.

• The system evolves adiabatically from the ground state of  $H_0$  to the ground state of  $H_1$ .

• The matrix elements of H(s) in the basis  $\{|0\rangle, |1\rangle\}$  are:

$$H(s) = \begin{pmatrix} 1/2 + s(\beta - 1/2) & -1/2(1 - s) \\ -1/2(1 - s) & 1/2 + s(\alpha - 1/2) \end{pmatrix}$$

• The corresponding eigenvalues are:

$$E_{\pm}(s)=rac{1}{2}\left(1\pm\sqrt{1-2s+2s^2}
ight)$$

116 / 130

• The minimum gap occurs at s = 1/2, and the minimum evolution time T is bounded by:

$$T \ge \frac{1}{\epsilon}$$

where  $\epsilon$  is the desired accuracy.

• For an accuracy of 90%, the minimum time is approximately  $T \approx$  4.4.

Adiabatic Quantum Computation & Deutsch's Algorithm

3

ヨト・モラト

< □ > < 同 >

- Similar to the circuit model Grover algorithm, the objective is to find the marked item in an unsorted database of *N* items with the fewest queries.
- Formally, one is allowed to call a function  $f : \{0,1\}^n \to \{0,1\}$ , where  $N = 2^n$ , with the promise that f(m) = 1 for the marked item m and f(x) = 0 for all  $x \neq m$ .

### Hamiltonian Setup

- The final Hamiltonian is  $H_1 = I |m\rangle \langle m|$ , where  $|m\rangle$  is the marked state.
- The initial Hamiltonian is  $H_0 = I |\phi\rangle\langle\phi|$ , where  $|\phi\rangle$  is the uniform superposition state:

$$|\phi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle$$

• The time-dependent Hamiltonian is:

$$H(s) = (1 - A(s))H_0 + A(s)H_1$$

where A(s) = s for a linear schedule.

#### Evolution in the Two-Dimensional Subspace

• The evolution is restricted to the subspace spanned by  $|m\rangle$  and  $|m^{\perp}\rangle$ , where:

$$|m^{\perp}\rangle = \frac{1}{\sqrt{N-1}}\sum_{i\neq m}|i\rangle$$

• In this subspace, the Hamiltonian can be written as:

$$H(s) = \frac{1}{2}I_{2\times 2} - \frac{\Delta(s)}{2} \begin{pmatrix} \cos\theta(s) & \sin\theta(s) \\ \sin\theta(s) & -\cos\theta(s) \end{pmatrix}$$

where  $\Delta(s)$  is the gap and  $\theta(s)$  is defined by:

$$\cos \theta(s) = rac{1-2s}{\Delta(s)}, \quad \sin \theta(s) = rac{2s\sqrt{N-1}}{\Delta(s)}$$

121 / 130

• The eigenvalues in the two-dimensional subspace are:

$$\epsilon_0(s)=rac{1}{2}(1-\Delta(s)), \quad \epsilon_1(s)=rac{1}{2}(1+\Delta(s))$$

• The minimum gap occurs at  $s = \frac{1}{2}$  and scales as:

$$\Delta_{\min} = \frac{1}{\sqrt{N}} = 2^{-n/2}$$

• The adiabatic condition requires that the total runtime t<sub>f</sub> satisfies:

$$t_f \gg 2 \max_s \frac{\|\dot{H}(s)\|}{\Delta^2(s)}$$

• For the Grover problem, this results in a runtime scaling as  $t_f \sim O(\sqrt{N})$ , matching the circuit model Grover's algorithm.

- The results generalize to the case where there are M ≥ 1 marked states.
- The final Hamiltonian is:

$$H_1 = I - \sum_{m \in M} |m
angle \langle m|$$

- The system evolves in an M + 1 dimensional subspace.
- The minimum gap is:

$$\Delta(s) = 1 - 2s^2 + \frac{4M}{N}s(1-s)$$

#### § 11: Quantum Annealing

∃ > October 17, 2024

æ

- Quantum Annealing is a quantum algorithm designed to solve optimization problems by evolving a quantum system towards its ground state.
- It is especially useful for solving combinatorial optimization problems.
- Compares closely with simulated annealing but leverages quantum superposition and tunneling to escape local minima more efficiently.

#### Simulated Annealing:

- Classical algorithm that mimics the annealing process in physics to find the global minimum.
- Uses thermal fluctuations to escape local minima.
- Quantum Annealing:
  - Uses quantum tunneling to move through energy barriers, potentially escaping local minima more efficiently.
  - Explores many solutions simultaneously due to superposition.
- Advantage: Quantum tunneling allows exploration of regions that classical algorithms may not reach efficiently.

• The core principle behind quantum annealing is adiabatic evolution, ensuring that the system reaches the minimum energy state.

- D-Wave Systems: The most well-known quantum annealer, used to solve optimization problems in various industries.
- Applications:
  - Logistics: Vehicle routing, supply chain optimization.
  - Finance: Portfolio optimization.
  - Artificial Intelligence: Feature selection and machine learning model training.
- D-Wave has demonstrated significant performance in specific types of optimization tasks.

# Thank You!

æ

글 에 에 글 어

Image: Image: