Developing QUBOs: The Graph Partitioning Example

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Problem Specifications

Given:

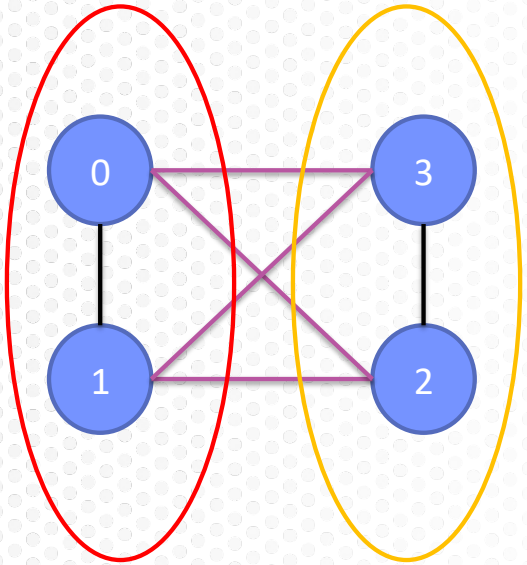
- A graph G

What do we want:

- Split the graph into two subsets such that:

  The subsets are the same size.

  There are as few edges as possible between the two subsets.



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QUBO Development Process

1. Write out your objective and constraints in your problem domain.

2. Convert your objective and constraints to math statements with binary variables.

3. Make your objective and constraints "QUBO appropriate".
   - Objective is a minimization function
   - Constraints are satisfied at their minimum values

4. Combine your objective and constraints.

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QUBO Step 1

Objective:

– Minimize the number of edges between subsets.

Constraints:

– The two subsets have equal size.

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QUBO Step 2: Binary Variables

Binary Variables:

– We need to split our nodes into two subsets, *A* and *B*.

– We can use the binary variables to "label" our nodes.

– $x_i = \begin{cases} 1, \text{if node } i \text{ is in set } A \\ 0, \text{if node } i \text{ is in set } B \end{cases}$

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QUBO Step 2: Objective

Objective:

Minimize the number of edges between subsets.

Let's look at what we want for one edge's cost.

If the qubits are the same, they're in the same set.

If the qubits are different, they're in different sets.

We want the qubits to be in the same set, to minimize the number in different sets.

x1	*x2*	Cost of edge (1, 2)
0	0	0
0	1	1
1	0	1
1	1	0

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QUBO Step 2: Objective

Objective:

- Thus, we want all edges to have the "2 qubits equal" solution
- We've seen this before – in the QUBO unit – 2 qubits equal – (1, 1, -2)
- Thus, for qubits x_1 and x_2, we will have $x_1 + x_2 - 2x_1x_2$
- For an arbitrary edge, we will have $x_i + x_j - 2x_ix_j$

- Cost of all edges: $\sum_{(i,j)\in E}(x_i + x_j - 2x_ix_j)$
- Objective function: $\min \sum_{(i,j)\in E}(x_i + x_j - 2x_ix_j)$

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QUBO Step 2: Constraint

Constraint:

- The two subsets have equal size.
- Equivalent statement: subset A has size $|V|/2$
- Size of subset A: $\sum_i^{|V|} x_i$

Constraint: $\sum_i^{|V|} x_i = \frac{|V|}{2}$

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QUBO Step 3

- Objective: $\min \sum_{(i,j)\in E}(x_i + x_j - 2x_i x_j)$

- Constraint: $\sum_i^{|V|} x_i = \frac{|V|}{2}$
  - Make QUBO-appropriate:
  - Move to one side: $\frac{|V|}{2} - \sum_i^{|V|} x_i$
  - Square to avoid negative values: $\left(\frac{|V|}{2} - \sum_i^{|V|} x_i\right)^2$
  - Simplify: $\frac{|V|^2}{4} - |V| \cdot \sum_i^{|V|} x_i + \left(\sum_i^{|V|} x_i\right)^2$
  - Remove constants for now: $-|V| \cdot \sum_i^{|V|} x_i + \left(\sum_i^{|V|} x_i\right)^2$

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QUBO Step 4

- QUBO:

$$min \sum_{(i,j)\in E} (x_i + x_j - 2x_i x_j) + \gamma \left(-|V| \cdot \sum_{i}^{|V|} x_i + \left(\sum_{i}^{|V|} x_i \right)^2 \right)$$

We'll need to multiply this out too, for sending to the QPU.

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QUBO Step 4: Algebra

$$\left(\sum_i^{|V|} x_i\right)^2 = ?$$

$$= x_1\,(x_1 + x_2 + x_3 + \dots) + x_2\,(x_1 + x_2 + x_3 + \dots) + x_3\,(x_1 + x_2 + x_3 + \dots) + \dots$$

$$= {x_1}^2 + {x_2}^2 + {x_3}^2 + \dots + 2\,x_1\,x_2 + 2\,x_1\,x_3 + 2\,x_1\,x_4 + 2\,x_2\,x_3 + 2\,x_2\,x_4 + \dots$$

$$= x_1 + x_2 + x_3 + \dots. + \sum_i^{|V|} \sum_{j>i} 2x_i x_j$$

$$= \sum_i^{|V|} x_i + \sum_i^{|V|} \sum_{j>i} 2x_i x_j$$

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QUBO Step 4 (Finally)

- General Graph Partitioning QUBO:
  $\min \sum_{(i,j)\in E}(x_i + x_j - 2x_i x_j) \; + \; \gamma\left(-|V| \cdot \sum_i^{|V|} x_i + \sum_i^{|V|} x_i + \sum_i^{|V|} \sum_{j>i} 2x_i x_j\right)$

- Simplifying for Clique (Fully Connected Graph):
  $$\min \;\; (2\gamma \; - 2) \sum_{(i,j)\in E} x_i x_j \; + \sum_{(i,j)\in E}(x_i + x_j) \; + \; \gamma\left(-|V| \cdot \sum_i^{|V|} x_i + \sum_i^{|V|} x_i\right)$$

- Simplifying a little more for Clique:
  $$\min \;\; (2\gamma \; - 2) \sum_{(i,j)\in E} x_i x_j \; + \sum_{(i,j)\in E}(x_i + x_j) \; + \gamma(1 - |V|)\left(\sum_i^{|V|} x_i\right)$$

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Sample Output from this QUBO with γ = 1.5

{0: 1, 1: 1, 2: 0, 3: 0} -2.0
{0: 0, 1: 1, 2: 1, 3: 0} -2.0
{0: 1, 1: 0, 2: 1, 3: 0} -2.0
{0: 0, 1: 0, 2: 1, 3: 1} -2.0
{0: 0, 1: 1, 2: 0, 3: 1} -2.0
{0: 1, 1: 0, 2: 0, 3: 1} -2.0
{0: 1, 1: 0, 2: 0, 3: 0} -1.5
{0: 0, 1: 1, 2: 0, 3: 0} -1.5

Ground states

Excited states

6 ground state solutions

Let's analyze these solutions and their energies…

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The First Solution

Qubit 0: 1

Qubit 1: 1

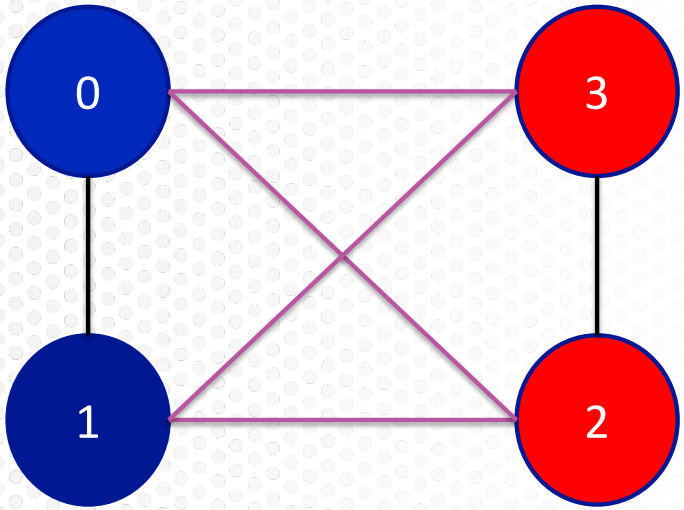
Qubit 2: 0

Qubit 3: 0

Are the partitions the same size?

How many links between partitions?

Is this a valid solution?



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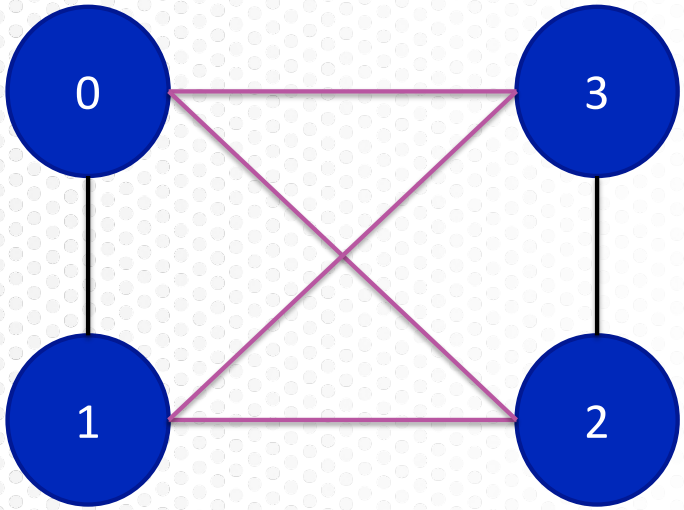
Understanding the Results

For our graph, the full mesh with four qubits, how many lowest-energy solutions did we get?

Can you explain why we got that many?



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Understanding the Results - Energy Analysis

- The problem is a competition between two requirements:
  - Minimizing the number of edges between subsets (”0 connected to 1”)
    - Each such edge costs an energy of 1 (that’s how we set the problem up)
  - The subsets of 0 and 1 should be the same size
    - The γ term raises the energy if the subsets are not the same size
- Can a solution satisfy both requirements?
- Choose one of our solutions, and assess the following:
  - How many edges between subsets are there?
  - Are the subsets the same size?
- What total energy did you get?
- Does it agree with the program’s results?

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Understanding the Results - Energy Analysis (continued)

- We forgot the constant: $\gamma \frac{|V|^2}{4}$
- If we add the observed energies to the constant, do we get the expected total energy?

- Interesting: change γ to some other number > 1
- Do we observe the same total energy?

- Interesting: set γ = 1
- Any idea what happened?
- Let's write this out for γ = 1:

$$\min \ (2\gamma - 2) \sum_{(i,j)\in E} x_i x_j + \sum_{(i,j)\in E} (x_i + x_j) + \gamma(1 - |V|)\left(\sum_{i}^{|V|} x_i\right)$$

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Just for fun – understanding these results for γ = 1

- We saw that Q = 0 for γ = 1 – what does this mean?
- The QUBO has nothing to say about the problem – it doesn't favor any partition
- Given that it is completely random – what do we expect?
- Consider first qubit – coin flip – 50% up, 50% down
- Consider second qubit – also 50% up, 50% down…
- So this is equivalent to: choose any 2 from 4
- Does this explain our observations?

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

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Does this explanation work for $\gamma > 1$?

- Even for γ close to 1, I observe the same number of equal-energy solutions
- Note that if we reduce the number of 0-1 edges, which decreases the energy, then we have an unequal number of nodes in the subsets, and that increases the energy
- Extra credit: can you make a mathematical argument why these solutions appear for any $\gamma > 1$?
- Extra credit: can you write an expression for the number of 0-1 edges, in terms of *N*, the number of nodes? (If you can, you're writing an expression for the *energy*)

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Summary

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