# Intro to QUBOs

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# Session Outline

- Review relevant quantum annealing concepts
- Problem formulation
- Writing a QUBO
- Example: set partitioning

**Session Goals**

1. Develop an approach for thinking about problems in QUBO form
2. Formulate QUBO problems

# Review

# Quantum Annealing

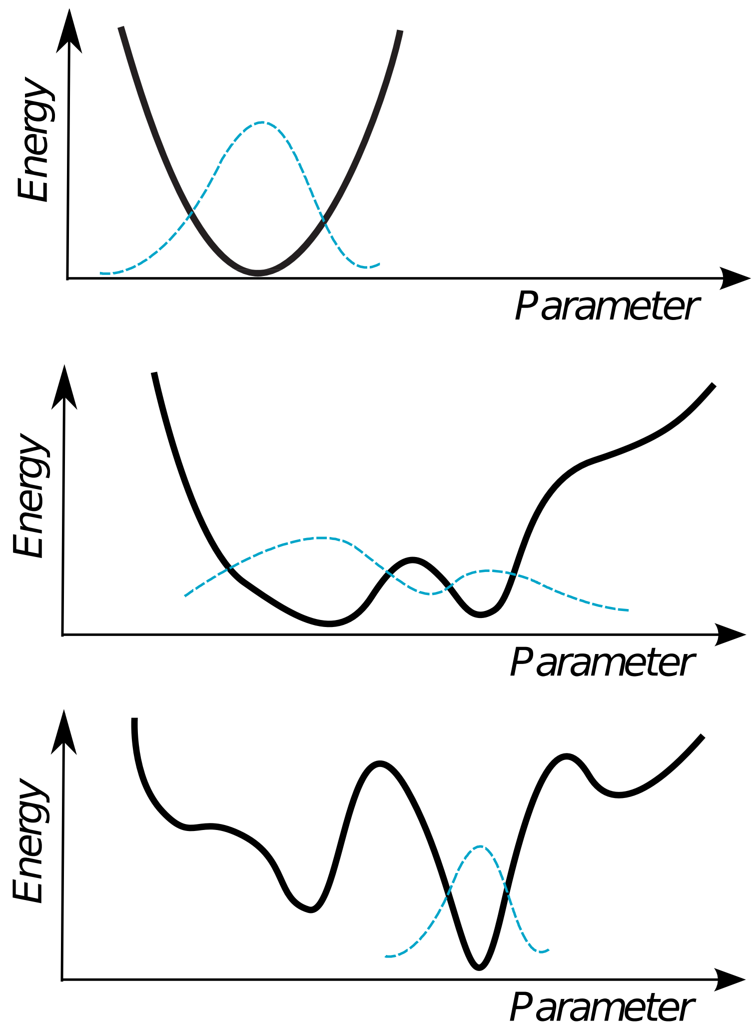
Start from $H_i$ and anneal slowly to $H_f$:

$$H_i = -\sum_i \sigma_x^{(i)}$$

- The ground state of $H_i$ will be superposition state of spin up and spin down
- This term drives quantum tunneling/spin flipping

$$H_f = -\sum_i h_i\,\sigma_z^{(i)} + \sum_{i,j>i} J_{ij}\,\sigma_z^{(i)}\sigma_z^{(j)}$$

Classical term representing the problem (ground state is the solution)



# Problem Formulations

# Problem Formulations

## Binary Quadratic Model (BQM)

- General class of problems that can be mapped to the QPU

### Ising Model

$$E_{ising} = \sum_{i} h_i \, s_i + \sum_{i>j} J_{i,j} s_i s_j$$

Binary variables:
$s_i \in \{-1,1\}$

### Quadratic Unconstrained Binary Optimization (QUBO)

$$E_{qubo} = \sum_{i} a_i \, q_i + \sum_{i>j} b_{i,j} q_i q_j$$

Binary variables:
$q_i \in \{0,1\}$

Converting between Ising and QUBO: $q_i = \dfrac{1+s_i}{2}$

# Examples: QUBO & Otherwise

One-variable QUBO:

$$3x + 4$$

Two-variable QUBO:

$$11 + 2.7x - 3y + 9.3\,xy$$

Three-variable QUBO:

$$xy + xz \; - yz$$

Another QUBO:

$5x^3 - 2y$

Would require different interactions between qubits

Not QUBOs:

$$11 + 2.7x - 3 + 9.3\,x/y$$

$$xyz$$

Would require 3-local coupling

# Writing a QUBO

# Building Blocks of QUBOs

**To construct a QUBO for a particular problem you need to define a few things about that problem**

**Binary Variables**
Each state of the binary variables must be assigned a meaning

**Objective**
The overall goal of the problem – what we're trying to minimize or maximize

**Constraints**
Rules that define what solutions are acceptable and which are not

# Parts of a QUBO

$$E_{qubo} = \sum_i a_i\, q_i + \sum_{i>j} b_{i,j} q_i q_j$$

Another way to think about a QUBO:

$$\boxed{E_{qubo} = \min(objective) + \gamma(constraints)}$$

What we're minimizing

Rules we're enforcing

# Process for Constructing a QUBO

1. Write out the objective and constraints in your problem domain
2. Define the binary variables
3. Write out objective in QUBO form
4. Write out constraints in QUBO form
5. Combine objectives and constraints
6. Solve and interpret results
7. Tune your QUBO to get better results

# Example: Set Partitioning

## Set partitioning problem

- Partition numbers into two sets based on some criteria

## Applications

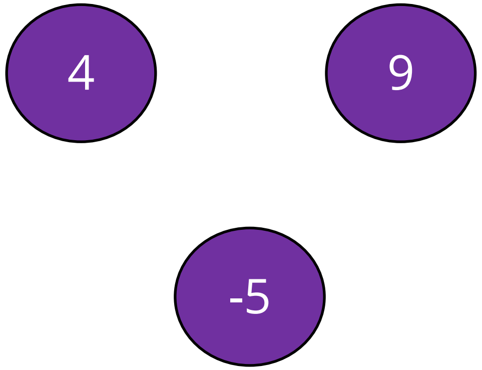
- Social networks (marketing, peace and conflict studies)
- Truck delivery management
- Task Scheduling
- Minimization of VLSI circuit size and delay
- Voting manipulation
- Bin packing

# Set Partitioning

# Set Partitioning Example - Introduction

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**



# Set Partitioning Example - Introduction

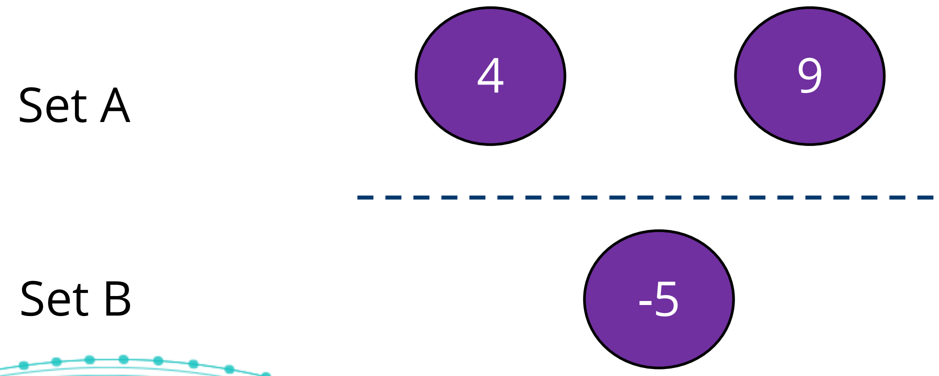
**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

For example,

- Set A = {4, 9}, $\sum$Set A = 13
- Set B = {-5}, $\sum$Set B = -5

- Difference between the sums of the sets = 18



# Set Partitioning Example - Introduction

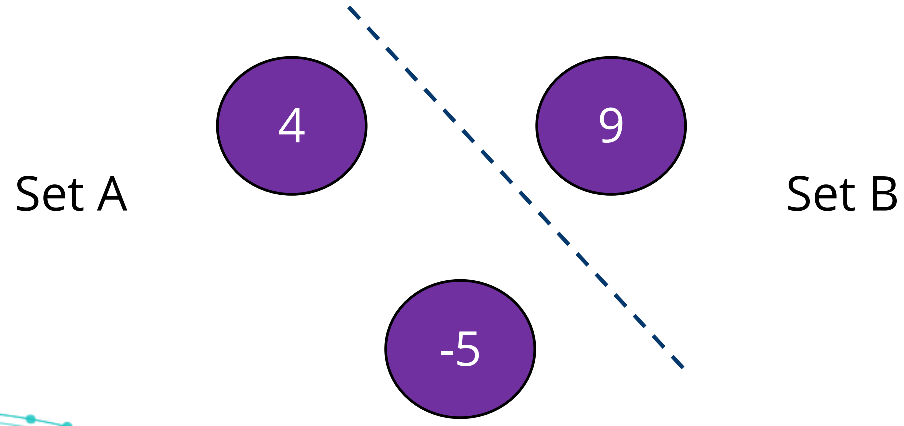
**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

For example,

- Set A = {4, -5}, $\sum$Set A = -1
- Set B = {9}, $\sum$Set B = 9

- Difference between the sums of the sets = 8



# Set Partitioning Example - Introduction

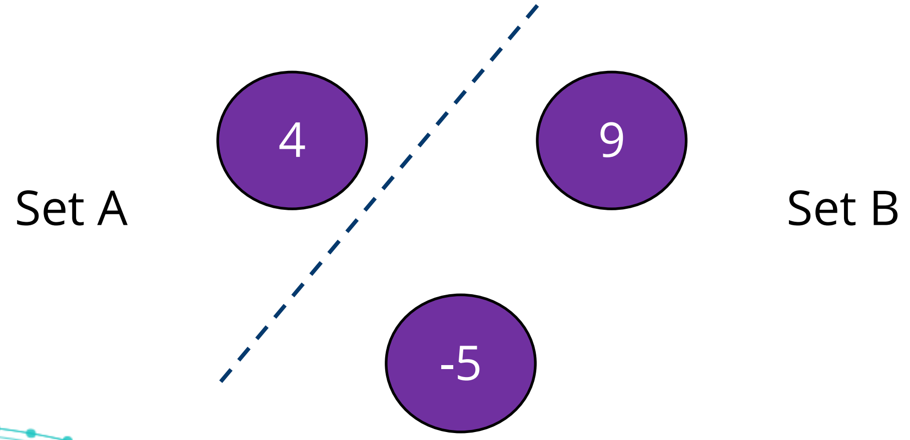
**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

For example,

- Set A = {4}, $\sum$Set A = 4
- Set B = {-5, 9}, $\sum$Set B = 4

- Difference between the sums of the sets = 0



# QUBO Formulation

# Example: Set Partitioning

## Problem

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 1.** Write out the objective and constraints in your problem domain

**Objective**:
We aren't trying to minimize anything so we don't have an objective

**Constraints:**
The difference between the sums of the partitioned sets needs to be 0.

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 2.** Define the binary values

$$E_{qubo} = \sum_i a_i\, x_i + \sum_i b_{i,j} x_i x_j$$

We're working in QUBO so our binary variables are $x_i \in \{0, 1\}$

Let's define them as

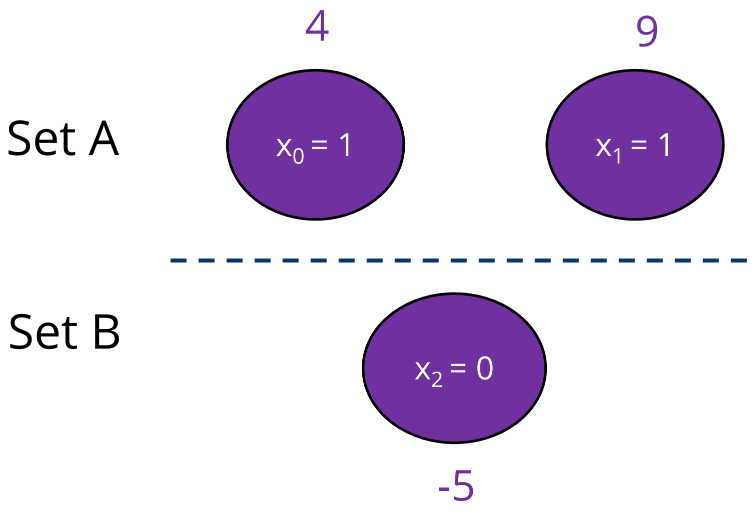
$$x_i = \begin{cases} 1 & if\ i\ is\ in\ Set\ A \\ 0 & if\ i\ is\ in\ Set\ B \end{cases}$$

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 2.** Define the binary values




$$x_i = \begin{cases} 1 & if\ i\ is\ in\ Set\ A \\ 0 & if\ i\ is\ in\ Set\ B \end{cases}$$

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 3.** Write out the objective in QUBO form

There's no objective in this problem so we skip this step

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

In math terms, *the difference between the sums of the partitioned sets needs to be 0* can be expressed as

$$(\sum Set\ A - \sum Set\ B) = 0$$

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

In math terms, *the difference between the sums of the partitioned sets needs to be 0* can be expressed as

$$\left(\sum Set\ A - \sum Set\ B\right) = 0$$

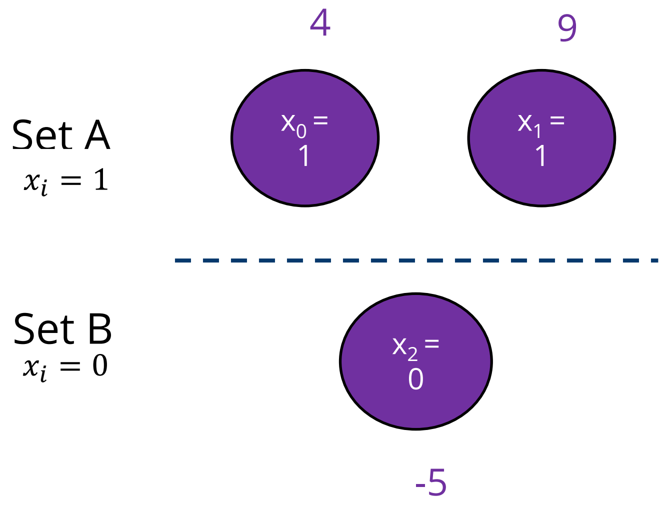
How can we write $\sum Set\ A$ and $\sum Set\ B$ in terms of our binary variables?

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i}\,\boldsymbol{x_i}}$$

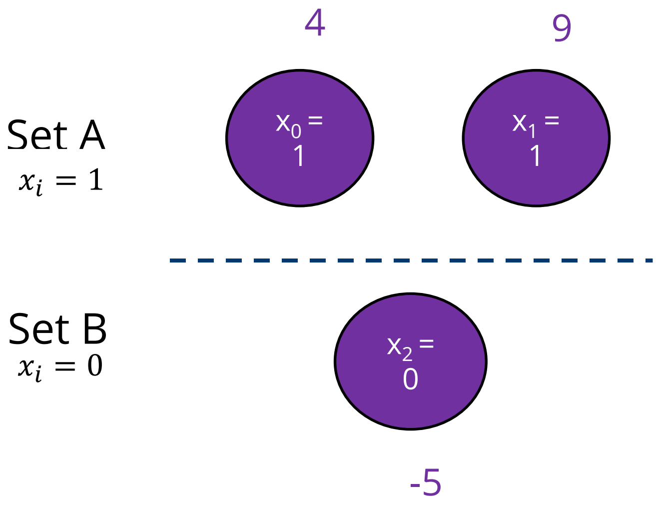
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i}\, \boldsymbol{x_i}}$$

$$= 4x_0 + 9x_1 - 5x_2$$

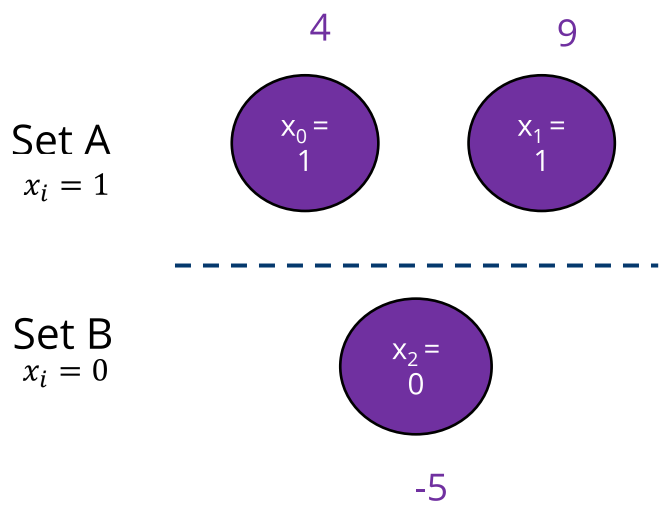
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i}\, \boldsymbol{x_i}}$$

$$= 4x_0 + 9x_1 - 5x_2$$

$$= 4*1 + 9*1 + -5*0$$

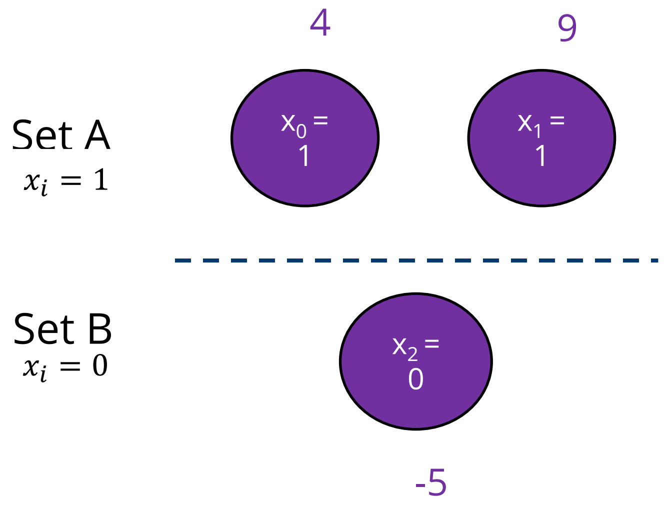
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i x_i}}$$

$= 4x_0 + 9x_1 - 5x_2$

$= 4*1 + 9*1 + -5*0$

$= 13$

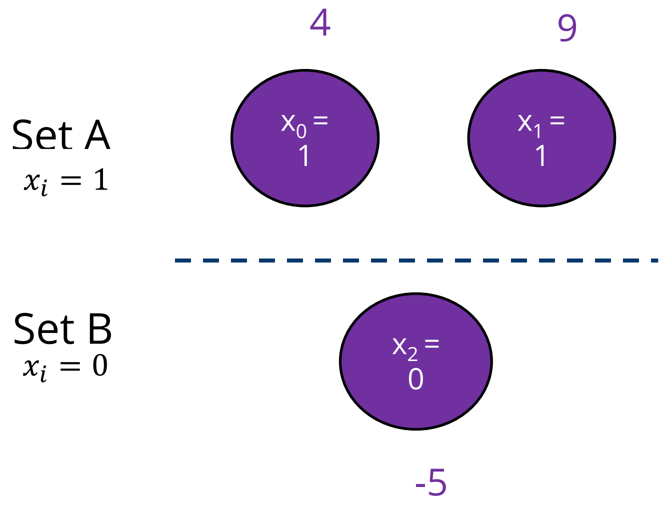
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i}\,\boldsymbol{x_i}}$$

$$= 4x_0 + 9x_1 - 5x_2 = \quad 13$$

$$\boxed{\sum Set\ B = \sum_i \boldsymbol{a_i}\,(\mathbf{1} - \boldsymbol{x_i})}$$

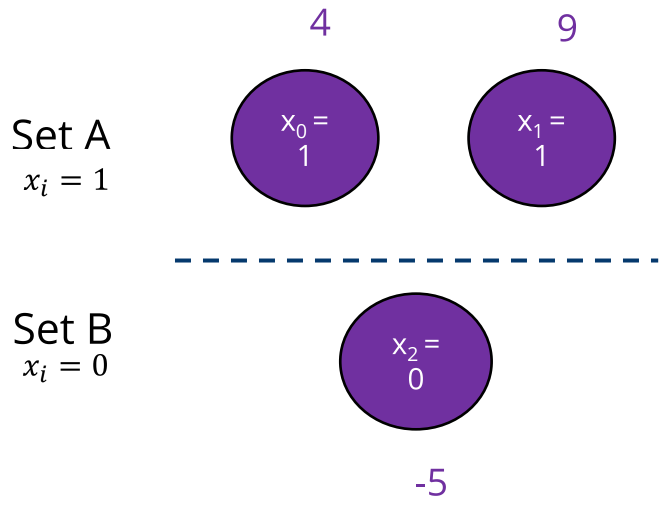
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i x_i}}$$

$= 4x_0 + 9x_1 – 5x_2 = \ \ 13$

$$\boxed{\sum Set\ B = \sum_i \boldsymbol{a_i\,(1\ -\ x_i)}}$$

$= 4(1 - x_0) + 9(1 - x_1) - 5(1 - x_2)$

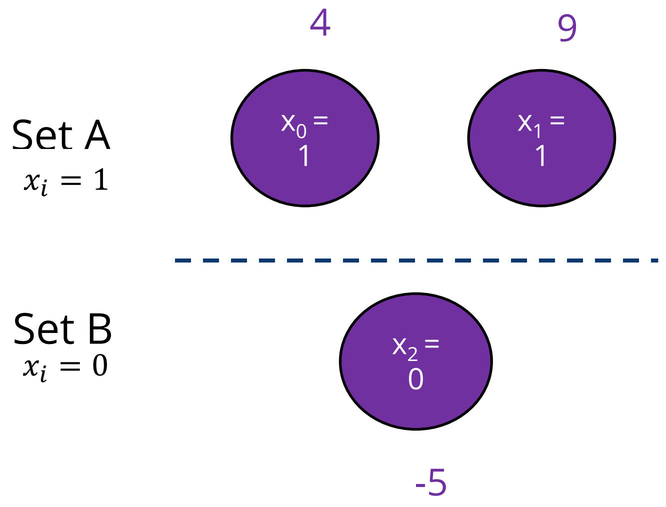
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i x_i}}$$

$= 4x_0 + 9x_1 - 5x_2 =\ \ 13$

$$\boxed{\sum Set\ B = \sum_i \boldsymbol{a_i} (\mathbf{1} - \boldsymbol{x_i})}$$

$= 4(1 - x_0) + 9(1 - x_1) - 5(1 - x_2)$

$= 4\,(1 - 1) + 9(1 - 1) - 5(1 - 0)$

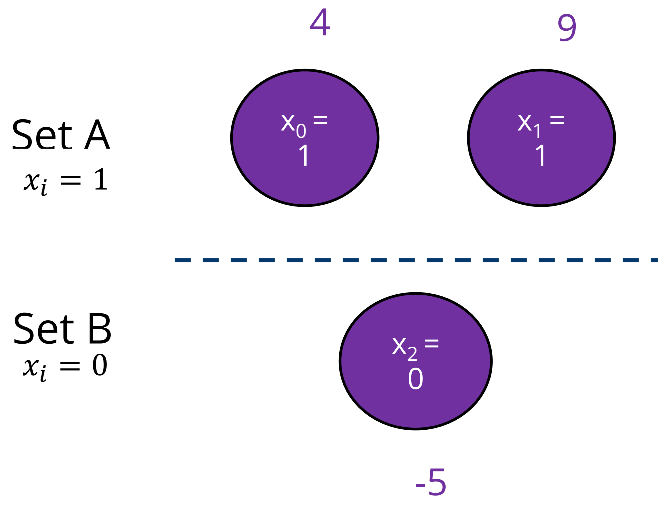
*$a_i$ = the numbers in the set*

# Example: Set Partitioning

## Problem

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form




$$\boxed{\sum Set\ A = \sum_i \boldsymbol{a_i\, x_i}}$$

$= 4x_0 + 9x_1 - 5x_2 = \quad 13$

$$\boxed{\sum Set\ B = \sum_i \boldsymbol{a_i\, (1 - x_i)}}$$

$= 4(1 - x_0) + 9(1 - x_1) - 5(1 - x_2)$

$= 4\,(1 - 1) + 9(1 - 1) - 5(1 - 0)$

$= -5$

*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

In math terms, *the difference between the sums of the partitioned sets needs to be 0* can be expressed as

$$(\sum Set\ A - \sum Set\ B) = 0$$

The sum of set A can be expressed as

$$\boxed{\sum Set\ A = \sum_i a_i\, x_i}$$

And the sum of set B is

$$\boxed{\sum Set\ B = \sum_i a_i\,(1 - x_i)}$$

*$a_i$ = the numbers in the set*

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i x_i - \sum_i a_i (1 - x_i) = 0$

# Example: Set Partitioning

**Problem**

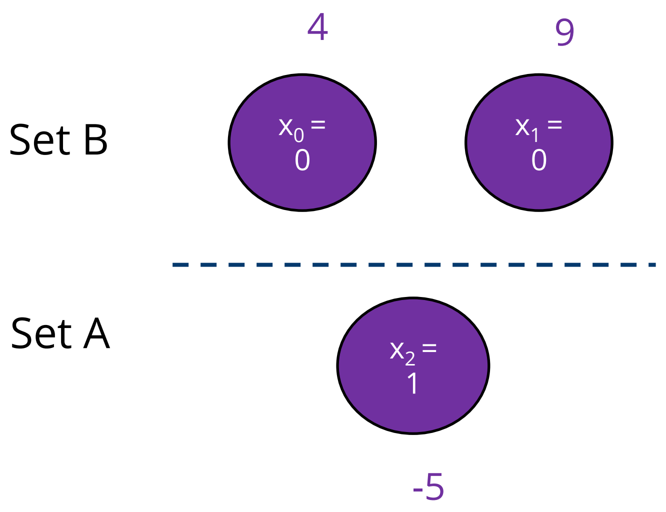
**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i x_i - \sum_i a_i (1 - x_i) = 0$

-5 - 13 = -18



# Example: Set Partitioning

## Problem

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

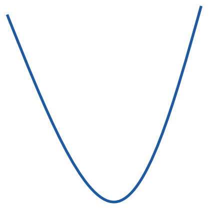
**Step 4.** Write out the constraints in QUBO form

$$(\sum Set\ A - \sum Set\ B) = 0$$

$$\sum_i a_i\, x_i - \sum_i a_i\,(1 - x_i) = 0$$

$$(\sum_i a_i\, x_i - \sum_i a_i\,(1 - x_i))^2 = 0$$

← Square the constraints to force a parabolic shape



# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i\, x_i$ - $\sum_i a_i\, (1 - x_i) = 0$

$(\sum_i a_i\, x_i - \sum_i a_i\, (1 - x_i))^2 = 0$

← Square the constraints to force a parabolic shape

Sub in numbers for $a_i$ and simplify

$[2(-5x_0 + 9x_1 + 4x_2) - 8]^2 = 0$

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i\, x_i - \sum_i a_i\, (1 - x_i) = 0$

$(\sum_i a_i\, x_i - \sum_i a_i\, (1 - x_i))^2 = 0$

← Square the constraints to force a parabolic shape

Sub in numbers for $a_i$ and simplify

$[2(-5x_0 + 9x_1 + 4x_2) - 8]^2 = 0$

$100\, x_0^2 + 324\, x_1^2 + 64\, x_2^2 - 360\, x_0\, x_1 - 160\, x_0\, x_2 + 288\, x_1\, x_2 + 160\, x_0 - 288\, x_1 - 128\, x_2 + 64 = 0$

# Example: Set Partitioning

## Problem

## Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i\, x_i - \sum_i a_i\, (1 - x_i) = 0$

$(\sum_i a_i\, x_i - \sum_i a_i\, (1 - x_i))^2 = 0$

← Square the constraints to force a parabolic shape

Sub in numbers for $a_i$ and simplify

$[\,2(-5x_0 + 9x_1 + 4x_2) - 8]^2 = 0$

$100\, x_0^2 + 324\, x_1^2 + 64\, x_2^2 - 360\, x_0\, x_1 - 160\, x_0\, x_2 + 288\, x_1\, x_2 + 160\, x_0 - 288\, x_1 - 128\, x_2 + 64 = 0$

Binary variables: $0^2 = 0,\ \ 1^2 = 1$

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 4.** Write out the constraints in QUBO form

$(\sum Set\ A - \sum Set\ B) = 0$

$\sum_i a_i x_i - \sum_i a_i (1 - x_i) = 0$

$(\sum_i a_i x_i - \sum_i a_i (1 - x_i))^2 = 0$ ← Square the constraints to force a parabolic shape

Sub in numbers for $a_i$ and simplify

$[\,2(-5x_0 + 9x_1 + 4x_2) - 8]^2 = 0$ ← trick: $x_i{}^2 = x_i$

$$\boxed{260x_0 + 36\,x_1 - 64x_2 - 360x_0\,x_1 + 288x_1x_2 - 160x_0\,x_2 + 64 = 0}$$

# Example: Set Partitioning

## Problem

Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal

**Step 5.** Combine objectives and constraints

$$E_{qubo} = \min(objective) + \gamma(constraints)$$

$$E_{qubo} = 260x_0 + 36\,x_1 - 64x_2 - 360x_0\,x_1 + 288x_1x_2 - 160x_0\,x_2 + \cancel{64}$$

Remove the constant since it just shifts the E

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

**Step 6.** Solve and interpret results

A solution consists of values {0, 1} for $x_0, x_1$, and $x_2$

How many solutions are there?

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

$$E_{qubo} = 260x_0 + 36\,x_1 - 64x_2 - 360x_0\,x_1 + \,288x_1x_2 - 160x_0\,x_2$$

| $x_0$ | $x_1$ | $x_2$ | **E** |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | -64 |
| 0 | 1 | 0 | 36 |
| 0 | 1 | 1 | 260 |
| 1 | 0 | 0 | 260 |
| 1 | 0 | 1 | 36 |
| 1 | 1 | 0 | -64 |
| 1 | 1 | 1 | 0 |

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

$$\boxed{E_{qubo} = 260x_0 + 36\,x_1 - 64x_2 - 360x_0\,x_1 + \,288x_1x_2 - 160x_0\,x_2}$$

| $x_0$ | $x_1$ | $x_2$ | E |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | -64 |
| 0 | 1 | 0 | 36 |
| 0 | 1 | 1 | 260 |
| 1 | 0 | 0 | 260 |
| 1 | 0 | 1 | 36 |
| 1 | 1 | 0 | -64 |
| 1 | 1 | 1 | 0 |

Set A = [4]
Set B = [-5, 9]

$$x_i = \begin{cases} 1 & if\ i\ is\ in\ Set\ A \\ 0 & if\ i\ is\ in\ Set\ B \end{cases}$$

Set A = [-5, 9]
Set B = [4]

# Example: Set Partitioning

**Problem**

**Partition the numbers in [-5, 9, 4] into two sets such that the sum of each set is equal**

$$\boxed{E_{qubo} = 260x_0 + 36\,x_1 - 64x_2 - 360x_0\,x_1 + 288x_1x_2 - 160x_0\,x_2}$$

| $x_0$ | $x_1$ | $x_2$ | **E** |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | -64 |
| 0 | 1 | 0 | 36 |
| 0 | 1 | 1 | 260 |
| 1 | 0 | 0 | 260 |
| 1 | 0 | 1 | 36 |
| 1 | 1 | 0 | -64 |
| 1 | 1 | 1 | 0 |

Classical Energy Gap

Ground States

Energy Spectrum

# Recap

# Session Review

- **The QPU naturally minimizes an objective**
- **Formulated a QUBO for a set partitioning problem**
- **Learned two tricks**
  - Square expressions to create an equality constraint
  - Squared binary variables reduce to linear variables

**Session Goals**

1. Develop an approach for thinking about problems in QUBO form
2. Formulate QUBO problems