Introduction To Developing QUBOs

D-Wave
The Quantum Computing Company™

Copyright © D-Wave Systems Inc.

Basic Problem: Turn on 1 of 3 variables

Suppose we have to assign one color to a region on a map.
It can be red, green or blue.

This is an example of an "*exactly one*" or "*one-hot*" problem.

Binary Variables: *r, g, b*
Each will equal 1 if the region has that color; 0 otherwise

How do we write a function which is minimized when exactly one of {*r, g, b*} is turned on?

Copyright © D-Wave Systems Inc.

Basic Problem: Turn on 1 of 3 variables

The QUBO: $(1 - r - g - b)$ ** 2 { or: $(r + g + b - 1)$ ** 2 }

Why squared? We don't want 0 turned on
We don't want 2 turned on…

Picture a parabola – the problem landscape

Reduced QUBO: $1 - r - g - b + 2br + 2gr + 2bg$

Remember the "Enemies" relationship from last unit?
Where did the squared terms go?

Copyright © D-Wave Systems Inc.

Sample Output from this QUBO

{'blue': 0, 'green': 0, 'red': 1} -1.0
{'blue': 0, 'green': 1, 'red': 0} -1.0
{'blue': 1, 'green': 0, 'red': 0} -1.0
{'blue': 0, 'green': 0, 'red': 0} 0.0
{'blue': 0, 'green': 1, 'red': 1} 0.0
{'blue': 1, 'green': 1, 'red': 0} 0.0
{'blue': 1, 'green': 0, 'red': 1} 0.0
{'blue': 1, 'green': 1, 'red': 1} 3.0

Ground states

Excited states

Are these the expected solutions?
Is this the expected number of ground state solutions?
Do the excited states show the expected energies?

Copyright © D-Wave Systems Inc.

QUBO Process

Copyright © D-Wave Systems Inc.

Developing an Ising or QUBO model

We start with a problem in the real world (**problem domain**)

Write a minimization function that incorporates:

- **Constraints**: The rules that we have to follow
- **Objective**: What we want to minimize

General form:

Ising or QUBO = min (**objective** + γ(**constraints**))

Copyright © D-Wave Systems Inc.

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.

Copyright © D-Wave Systems Inc.

Basic Problem
Using QUBO Process

Problem:

Pick the pair of boxes with the smallest sum.

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

Objective:
Minimize the sum of the boxes chosen

Constraints:
Pick exactly two boxes

Copyright © D-Wave Systems Inc.

Basic Problem
Using QUBO Process

Problem:

Pick the pair of boxes with the smallest sum.

Copyright © D-Wave Systems Inc.

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

Variables:
$x_i = 1$ if box i is selected, 0 otherwise

Objective:
$min(17x_1 + 21x_2 + 19x_3)$

Constraints:
$x_1 + x_2 + x_3 = 2$

D:wave

Basic Problem
Using QUBO Process

Problem:

Pick the pair of boxes with the smallest sum.

3. Make your objective and constraints "QUBO appropriate".

Variables:
$x_i = 1$ if box i is selected, 0 otherwise

Objective:
$\min(17x_1 + 21x_2 + 19x_3)$

Constraints:
$(x_1 + x_2 + x_3 - 2)^2$

Copyright © D-Wave Systems Inc.

D:wave

Basic Problem Using QUBO Process

Problem:

Pick the pair of boxes with the smallest sum.

4. Combine your objective and constraints.

Variables:

$x_i = 1$ if box i is selected, 0 otherwise

QUBO:

$$\min(17x_1 + 21x_2 + 19x_3) + \gamma(x_1 + x_2 + x_3 - 2)^2$$

Copyright © D-Wave Systems Inc.

D:wave

Here’s another QUBO to develop…

Copyright © D-Wave Systems Inc.

QUBO Development

Problem:

You have the set $A = \{1, 2, 3, 4, 5\}$. Find 3 numbers in A that add up to 8.

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.

Copyright © D-Wave Systems Inc.

Sample Output from this QUBO

{1: 1, 2: 0, 3: 1, 4: 1, 5: 0} -73.0
{1: 1, 2: 1, 3: 0, 4: 0, 5: 1} -73.0
{1: 1, 2: 1, 3: 0, 4: 1, 5: 0} -72.0
{1: 0, 2: 0, 3: 1, 4: 0, 5: 1} -72.0
{1: 1, 2: 0, 3: 1, 4: 0, 5: 1} -72.0
{1: 0, 2: 1, 3: 1, 4: 1, 5: 0} -72.0
{1: 0, 2: 0, 3: 1, 4: 1, 5: 0} -71.0
{1: 0, 2: 1, 3: 0, 4: 0, 5: 1} -71.0
{1: 0, 2: 0, 3: 0, 4: 1, 5: 1} -71.0

Ground states

Excited states

Are these the expected solutions?
Is this the expected number of ground state solutions?
Do the excited states show the expected energies?
Can you explain the energies of the ground states?

Copyright © D-Wave Systems Inc.

Summary

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.

Copyright © D-Wave Systems Inc.