Introduction to QUBO

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The Quantum Computing Company™

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QUBO & synonyms

Highest power of variable appearing is two

No constraint is applied to the variables

Variables take their values from $\{0,1\}$

Minimize or Maximize an objective function

Q	Quadratic
U	Unconstrained
B	Binary
O	Optimization

AKA…

B	Binary
Q	Quadratic
M	Model

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Background: Magnetism in Materials

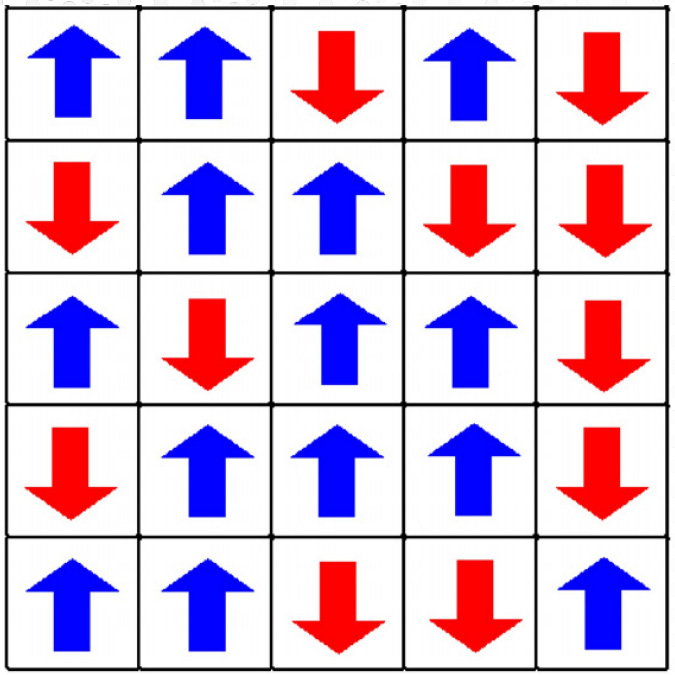
Magnetic behavior can be understood by thinking of each atom as a *spin*, which can be pointing up or down

Spins can want to line up against, or with a magnetic field

Neighboring spins affect each other, but not those further away

Try the most basic interactions:

- Linear term, for magnetic field
- Pairwise quadratic, for couplers



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Ising Model (Physics)

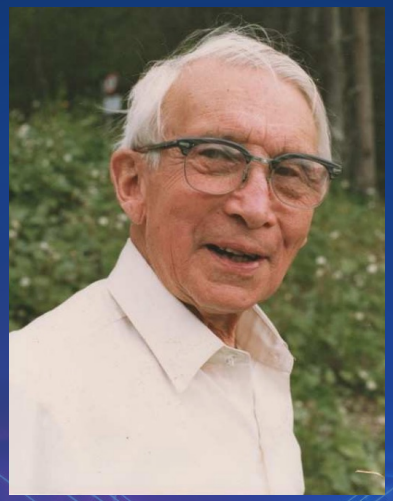
The objective function – the energy - of the Ising Model is defined to be (S is spin):

$$E = -\sum_{i} h_i S_i + \sum_{ij} J_{ij} S_i S_j$$

Where the spins assume values:

$$S_i \in \{-1, +1\}$$

The h's and J's are adjustable constants.
One h for each spin.
One J for each interacting pair of spins.



Ernst Ising

From Wikipedia, the free encyclopedia

Ernst Ising (German: [ˈiːzɪŋ]; May 10, 1900 in Cologne, Rhine, Germany – May 11, 1998 in Peoria, Illinois, USA) was a German physicist, who is best remembered for the development of the Ising model. He was a professor of physics at Bradley University until his retirement in 1976.[1]

Photo credit: https://arxiv.org/abs/1706.01764
Wiki: https://en.wikipedia.org/wiki/Ernst_Ising

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QUBO and Relation to Ising Model

QUBO:

$$\boldsymbol{Obj(c, a_i, b_{ij}; q_i) = c + \sum_i a_i\, q_i + \sum_{i<j} b_{ij} q_i\, q_j}$$

q's are qubit variables – 0 and 1, instead of -1 and 1
a's and **b**'s are adjustable constants

Convert between 0/1 variables (QUBO) and spins (Ising) via:

$$q_i = \frac{1 + S_i}{2}$$

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Examples: QUBO & otherwise

One-variable QUBO:

$$3x + 4$$

Two-variable QUBO:

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

Three-variable QUBO:

$$xy + xz - yz$$

Not QUBOs:

$$3x + 4 + x^3$$

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

$$xyz$$

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How Does This Relate to D-Wave?

The D-Wave Quantum Processing Unit (QPU) solves QUBO or Ising Model problems

We send Quantum Machine Instructions (QMI) to the QPU; a QMI is a set of all the a's and b's

The QPU finds the lowest-energy solution – the values of q which minimize the objective function

We set the a's and b's to take our specific problem into account

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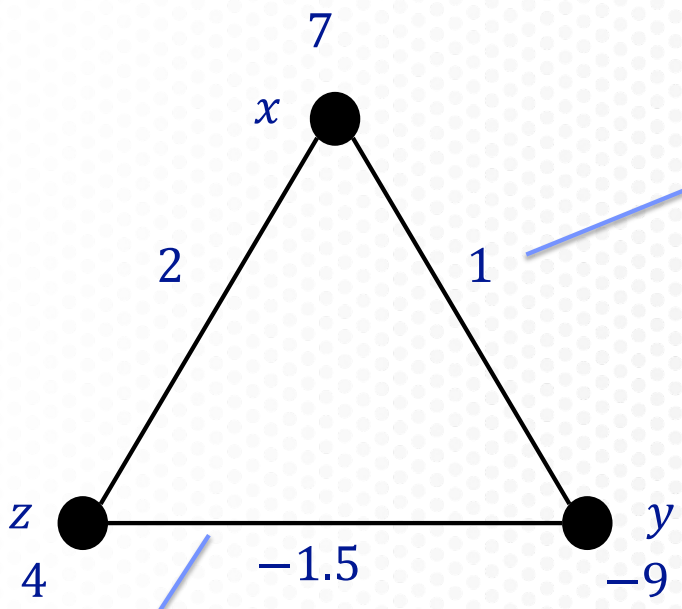
Graphical representation of a QUBO



7x-9y+4z+xy+2xz-1.5yz

Quadratic terms appear on edges

Constant term and variable names are generally omitted in this representation (but shown here)

Linear terms appear on nodes

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Matrix representation

7	1	2
	-9	-1.5
		4

7x-9y+4z+xy+2xz-1.5yz

Quadratic terms appear on off-diagonals

Upper diagonal is sufficient for Ocean

Constant term and variable names are generally omitted in this representation

Linear terms appear on diagonal

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Another Example

Minimize the following equation with binary variables:

Minimize $y = -5x_1 - 3x_2 - 8x_3 - 6x_4 + 4x_1x_2 + 8x_1x_3 + 2x_2x_3 + 10x_3x_4$

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Another Example

Minimize $y = \boxed{-5x_1 - 3x_2 - 8x_3 - 6x_4} \boxed{- 4x_1x_2 + 8x_1x_3 + 2x_2x_3 + 10x_3x_4}$

$-5x_1 - 3x_2 - 8x_3 - 6x_4$

Linear Terms

$4x_1x_2 + 8x_1x_3 + 2x_2x_3 + 10x_3x_4$

Quadratic Terms

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Another Example

$$-5x_1 - 3x_2 - 8x_3 - 6x_4$$

$$\boxed{-5x_1 - 3x_2 - 8x_3 - 6x_4} \quad \begin{pmatrix} -5 & & & \\ & -3 & & \\ & & -8 & \\ & & & -6 \end{pmatrix}$$

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Another Example

$$4x_1x_2 + 8x_1x_3 + 2x_2x_3 + \mathbf{10}x_3x_4$$

Quadratic Terms

$$\begin{pmatrix} -5 & & & \\ & -3 & & \\ & & -8 & \\ & & & -6 \end{pmatrix}$$

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Another Example

Filling in the Rest

$$\begin{pmatrix} -5 & 4 & 8 & 0 \\ 0 & -3 & 2 & 0 \\ 0 & 0 & -8 & 10 \\ 0 & 0 & 0 & -6 \end{pmatrix}$$

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Question?

Which “Example” is the real QUBO?

All of them!
They are different representations,
some in code,
some in equations,
some in pictures,
all of the same underlying thing.

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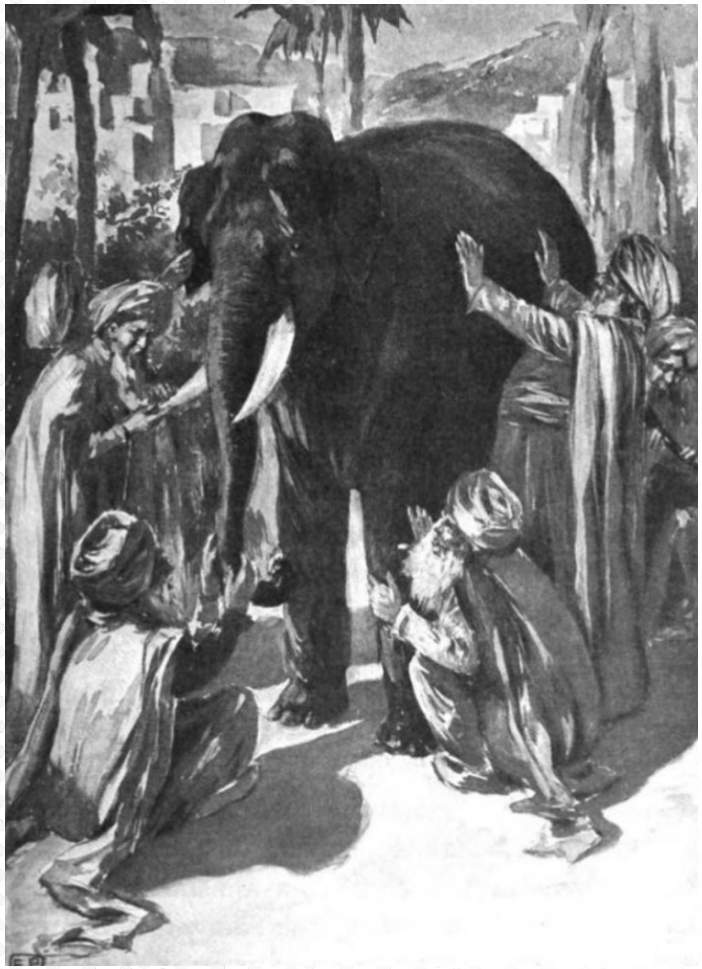

The Blind Men and the Elephant
http:// https://en.wikipedia.org/wiki/Blind_men_and_an_elephant

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Is it possible to express problems as QUBOs?

- Partitioning Problems
  - Number Partitioning
  - Graph Partitioning
  - Cliques
  - Reducing N TO logN Spins in Some Constraints
- Binary Integer Linear Programming
- Covering and Packing Problems
  - Exact Cover
  - Set Packing
  - Vertex Cover
  - Satisfiability
  - Minimal Maximal Matching
- Problems with Inequalities
  - Set Cover
  - Knapsack with Integer Weights
- Coloring Problems
  - Graph Coloring
  - Clique Cover
  - Job Sequencing with Integer Lengths
- Hamiltonian Cycles
  - Hamiltonian Cycles and Paths
  - Traveling Salesman
- Tree Problems
  - Minimal Spanning Tree with a Maximal Degree Constraint
  - Steiner Trees
  - Directed Feedback Vertex Set
  - Undirected Feedback Vertex Set
  - Feedback Edge Set
- Graph Isomorphisms

frontiers in PHYSICS

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Ising formulations of many NP problems

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We provide Ising formulations for many NP-complete and NP-hard problems, including all of Karp's 21 NP-complete problems. This collects and extends mappings to the Ising model from partitioning, covering, and satisfiability. In each case, the required number of spins is at most cubic in the size of the problem. This work may be useful in designing adiabatic quantum optimization algorithms.

Keywords: spin glasses, complexity theory, adiabatic quantum computation, NP, algorithms

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Understanding Two-Qubit Problems

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Problem One

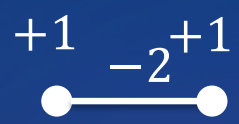
Favor: Qubits with same value

Penalize: Qubits with different values

x	y	$ax + by + cxy + d$
0	0	0
0	1	1
1	0	1
1	1	0

Most general QUBO

1 is arbitrary choice



$const = 0$

$a = +1$
$b = +1$
$c = -2$
$d = 0$

$0 = \boldsymbol{d}$
$\mathbf{1} = \boldsymbol{b} + \boldsymbol{d}$
$\mathbf{1} = \boldsymbol{a} + \boldsymbol{d}$
$0 = \boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c} + \boldsymbol{d}$

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Spectrum & gap for this two-qubit problem

x	y	objective
0	0	0
0	1	1
1	0	1
1	1	0

Ground state

Ground state

Spectrum

objective = $x + y - 2xy$

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Problem Two

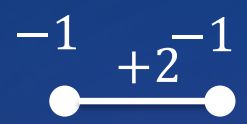
Favor: Qubits with different values

Penalize: Qubits with same values

x	y	$ax + by + cxy + d$
0	0	1
0	1	0
1	0	0
1	1	1

Most general QUBO

1 is arbitrary choice



$const = 1$

$a = -1$
$b = -1$
$c = +2$
$d = 1$

$1 = \boldsymbol{d}$
$\mathbf{0} = \boldsymbol{b} + \boldsymbol{d}$
$\mathbf{0} = \boldsymbol{a} + \boldsymbol{d}$
$\mathbf{1} = \boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c} + \boldsymbol{d}$

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Spectrum & gap for this two-qubit problem

x	y	objective
0	0	1
0	1	0
1	0	0
1	1	1

Ground state

Ground state

Spectrum

objective = $2xy - x - y + 1$

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Solutions to a Three-Qubit Problem

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Spectrum & gap for a three-qubit problem

x	y	z	objective
0	0	0	0
0	0	1	4
0	1	1	-6.5
0	1	0	-9
1	0	0	7
1	0	1	13
1	1	0	-1
1	1	1	3.5

First excited state

Ground state

Bigger gap = better QPU performance

Spectrum

objective = $7x - 9y + 4z + xy + 2xz - 1.5yz$

gap = first excited state – ground state = 2.5

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Summary

- QUBOs are a form of optimization problem that have been studied in the Operations Research (OR) community.
- Many common OR problems can be formulated as a QUBO and these formulations can be very efficient.
- There is a close similarity between the D-Wave QMI and a QUBO.
- So- it makes sense for D-Wave to provide tools that allow users to run QUBOs on the D-Wave system (e.g., Ocean, Simulated Annealing, …)
- And users need to learn techniques for converting problems of interest into QUBOs to map them to the D-Wave System.

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