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Quadratic Unconstrained Binary Optimization

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INVESTING IN YOUR FUTURE

Quadratic Unconstrained Binary Optimization

$$\text{minimize/maximize} \quad f(x) = x^T Q x$$

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

Quadratic Unconstrained Binary Optimization

- Wide range
- Quantum annealing

Quantum Bridge Analytics I: A Tutorial on Formulating and Using QUBO Models

Fred Glover, Gary Kochenberger, Yu Du
November 2019, arXiv:1811.11538

Combinatorial Optimization

- Polynomial-time problems
- NP-hard problems
  - Polynomial time for special cases
  - Approximation algorithms

Problem-specific solution algorithms

Quadratic Unconstrained Binary Optimization

- general framework to formulate optimization problems
- QUBO solvers can efficiently solve important problems
- two-step process
  1. re-cast the original model into QUBO form
  2. solve with an appropriate QUBO solver
- using modern meta-heuristic methods help to find optimal solutions in acceptable time

Known QUBO problems

- SAT Problems
- Graph Coloring Problems
- Maximum Cut Problems
- Maximum Clique Problems
- Number Partitioning Problems
- Constraint Satisfaction Problems (CSPs)
- Quadratic and Multiple Knapsack Problems
- Capital Budgeting Problems
- Warehouse Location Problems
- Discrete Tomography Problems
- etc.

General QUBO form

$$\text{minimize/maximize} \quad f(x) = x^T Q x$$

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

- symmetric Q
- upper-triangular Q

QUBO as an objective function

$$\text{minimize/maximize } f(x) = \sum_{i,j} Q_{ij} x_i x_j$$

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

QUBO as an objective function

$$\text{minimize/maximize } f(x) = \sum_i Q_{ii} x_i + \sum_{i \neq j} Q_{ij} x_i x_j$$

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

containing linear and quadratic terms

Symmetric Q

$$\sum_{i} Q_{ii} x_i + \sum_{i<j} (Q_{ij} + Q_{ji}) x_i x_j$$

Transformation

$$\forall i \neq j : Q'_{ij} := \frac{(Q_{ij} + Q_{ji})}{2}$$

Upper-triangular Q

$$\sum_i Q_{ii} x_i + \sum_{i<j} (Q_{ij} + Q_{ji}) x_i x_j$$

Transformation

$$\forall i, j : Q'_{i,j} := \begin{cases} Q_{i,j} + Q_{j,i}, & \text{if } i < j \\ 0, & \text{if } i > j \end{cases}$$

Equivalence to Ising model

Configuration energy:

$$H(s) = -\sum_{i<j} J_{ij} s_i s_j - \mu \sum_i h_i s_i$$

where $s_i \in \{-1, 1\}$

Conversion to QUBO:

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

Number Partitioning Problem

Partition the set $S = \{v_1, v_2, \dots v_m\}$ of numbers into S_0 and S_1 such that $\sum S_0$ and $\sum S_1$ are as close as possible.

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$$\text{diff} = \left| \sum_{i=1}^{m} v_i - 2 \sum_{i=1}^{m} v_i x_i \right| = \left| c - 2 \sum_{i=1}^{m} v_i x_i \right|$$

Number Partitioning Problem as QUBO

$$\text{diff}^2 = \left(c - 2\sum_{i=1}^{m} v_i x_i\right)^2$$

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where $Q_{ii} = v_i(v_i - c)$ and $Q_{ij} = Q_{ji} = v_i v_j$.

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$$\text{minimize } x^T Q x$$

Formulating constrained problems as QUBO

minimize $y = f(x_1, x_2)$
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- Penalty P is large enough constant
- Penalty P is not too large

Quadratic penalties

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

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- MVC: find a cover with a minimum number of vertices
- formulated as:

$$\text{minimize} \sum_{j \in V} x_j$$

$$\text{subject to } \forall uv \in E : x_u + x_v \geq 1$$

$$\text{where } x_v = 1 \text{ iff vertex } v \text{ is in the cover}$$

Minimum Vertex Cover (MVC) Problem

- the problem can be re-cast to QUBO by adding penalty to the objective function
- the penalty (as per the table) is $P(1 - x - y + xy)$
- hence the unconstrained version of the problem is:

$$\text{minimize} \sum_{j \in V} x_j + P \sum_{(i,j) \in E} (1 - x_i - x_j + x_i x_j)$$

- which can be written as minimize $x^T Qx + C$, where C is constant term
- since C has no impact in the optimization, it can be dropped, leaving us with the QUBO form

Summary

- Many optimization problems can be turned to QUBO
- Quadratic penalties
- Uniform solution with successful meta-heuristics
- Applications in Machine Learning
- Equivalence to Ising model
- Quantum annealing
- Hybrid solvers

Set partitioning problem (SPP)

- partition a set of items into subsets so that:
  - each item appears in exactly one subset and
  - the cost of the subsets chosen is minimized
- appears in many settings including the airline and other industries
- traditionally formulated in binary variables:

$$\text{minimize} \sum_{j=1}^{n} c_j x_j$$

$$\text{subject to: } \forall i \in [1..m] : \sum_{j=1}^{n} a_{ij} x_j = 1$$

Set partitioning problem (SPP)

- an SPP can be re-cast into QUBO problem by adding the quadratic penalties:

$$P\sum_i\left(\sum_{j=1}^{n} a_{ij}x_j - b_i\right)^2$$

- where the outer sum is taken over all original constrains
- expanding the sums and dropping the additive constant from the objective function will give the form:

$$\text{minimize } x^T Qx, \;\; x \in \{0, 1\}$$

Unsupervised Machine Learning

- clustering can be represented as set partitioning problem solvable by QUBO
- clique partitioning problem offers a general model for correlation clustering modularity maximization
- application of QUBO based quantum computers are also a filed of study

Supervised Machine Learning

- the Ising model is useful for any representation of neural function
- QUBO based processing units could be used with convolutional neural networks and constraint satisfaction problems

ML to Improve QUBO Solution Processes

- mainly pre-processing techniques
- identify relationships such as values (or bounds) that can be assigned to variables
- identify inequalities that can constrain feasible spaces more tightly
- up to 45% reduction in problem size is possible