A Tutorial on Formulating and Using QUBO Models  
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Abstract

Recent years have witnessed the remarkable discovery that the Quadratic Unconstrained Binary Optimization (QUBO) model unifies a wide variety of combinatorial optimization problems, and moreover is the foundation of adiabatic quantum computing and a subject of study in neuromorphic computing. Through these connections, QUBO models lie at the heart of experimentation carried out with quantum computers developed by D-Wave Systems and neuromorphic computers developed by IBM and are actively being explored for their research and practical applications by Google and Lockheed Martin in the commercial realm and by Los Alamos National Laboratory, Oak Ridge National Laboratory and Lawrence Livermore National Laboratory in the public sector. Computational experience is being amassed by both the classical and the quantum computing communities that highlights not only the potential of the QUBO model but also its effectiveness as an alternative to traditional modeling and solution methodologies.

This tutorial discloses the basic features of the QUBO model that give it the power and flexibility to encompass the range of applications that have thrust it into prominence. We show how many different types of constraints arising in practice can be embodied within the “unconstrained” QUBO formulation in a very natural manner using penalty functions, yielding exact model representations in contrast to the approximate representations produced by customary uses of penalty functions. Each step of generating such models is illustrated in detail by simple numerical examples, to highlight the convenience of using QUBO models in numerous settings. We also describe recent innovations for solving QUBO models that offer a rich potential for integrating classical and quantum computing and for applying these models in machine learning.

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Acknowledgments
**Section 1: Introduction**

The field of Combinatorial Optimization (CO) is one of the most important areas in the general field of optimization, with important applications found in every industry, including both the private and public sectors. It is also one of the most active research areas pursued by the research communities of Operations Research, Computer Science and Analytics as they work to design and test new methods for solving real world CO problems.

Generally, these problems are concerned with making wise choices in settings where a large number of yes/no decisions must be made and each set of decisions yields a corresponding objective function value – like a cost or profit value. Finding good solutions in these settings is extremely difficult. The traditional approach is for the analyst to develop a solution algorithm that is tailored to the mathematical structure of the problem at hand. While this approach has produced good results in certain problem settings, it has the disadvantage that the diversity of applications arising in practice requires the creation of a diversity of solution techniques, each with limited application outside their original intended use.

In recent years, we have discovered that a mathematical formulation known as QUBO, an acronym for a Quadratic Unconstrained Binary Optimization problem, can embrace a large variety of important CO problems found in industry, science and government. Through special reformulation techniques that are easy to apply, the power of QUBO solvers can be used to efficiently solve many important problems once they are put into the QUBO framework.

This two-step process of first re-casting an original model into the form of a QUBO model and then solving it with appropriate software enables the QUBO model to become a unifying framework for combinatorial optimization. The alternative path that results for effectively modeling and solving many important problems is a new development in the field of combinatorial optimization. The significance of this situation is enhanced by the fact that the QUBO model can be shown to be equivalent to the Ising model that plays a prominent role in physics. Consequently, the broad range of optimization problems solved effectively by state-of-the-art QUBO solution methods are joined by an important domain of problems arising in physics applications.
The materials provided in the sections that follow illustrate the process of reformulating important optimization problems as QUBO models through a series of explicit examples. Collectively these examples highlight the application breadth of the QUBO model. We disclose the unexpected advantages of modeling a wide range of problems in a form that differs from the linear models classically adopted in the optimization community. As part of this, we provide techniques that can be used to recast a variety of problems that may not seem at first to fit within an unconstrained binary optimization structure, and perhaps existing in a classical mathematical form, into an equivalent QUBO model. We also discuss the underpinnings of today’s leading QUBO solution methods and the links they provide between classical and quantum computing.

As pointed out in Kochenberger and Glover (2006), the QUBO model embraces the following important optimization problems:

- Quadratic Assignment Problems
- Capital Budgeting Problems
- Multiple Knapsack Problems
- Task Allocation Problems (distributed computer systems)
- Maximum Diversity Problems
- P-Median Problems
- Asymmetric Assignment Problems
- Symmetric Assignment Problems
- Side Constrained Assignment Problems
- Quadratic Knapsack Problems
- Constraint Satisfaction Problems (CSPs)
- Discrete Tomography Problems
- Set Partitioning Problems
- Set Packing Problems
- Warehouse Location Problems
Maximum Clique Problems
Maximum Independent Set Problems
Maximum Cut Problems
Graph Coloring Problems
Number Partitioning Problems
Linear Ordering Problems
Clique Partitioning Problems
SAT problems

Details of such applications are elaborated more fully in Kochenberger et al. (2014).

In the following development we will show approaches that make it possible to model these and many other types of problems in the QUBO framework. In the concluding section we additionally provide information about recent developments linking QUBO to machine learning and quantum computing.

**Basic QUBO Problem Formulation**

We now give a formal definition of the QUBO model whose significance will be made clearer by numerical examples that give a sense of the diverse array of practical QUBO applications.

Definition: The QUBO model is expressed by the optimization problem:

\[ \text{QUBO: minimize } y = x^T Q x \]

where \( x \) is a vector of binary decision variables and \( Q \) is a square matrix of constants.

It is common to assume that the \( Q \) matrix is symmetric or in upper triangular form, which can be achieved without loss of generality simply as follows:

**Symmetric form:** For all \( i \) and \( j \) except \( i = j \), replace \( q_{ij} \) by \( (q_{ij} + q_{ji})/2 \).
Upper triangular form: For all $i$ and $j$ with $j > i$, replace $q_{ij}$ by $q_{ij} + q_{ji}$. Then replace all $q_{ij}$ for $j < i$ by 0. (If the matrix is already symmetric, this just doubles the $q_{ij}$ values above the main diagonal, and then sets all values below the main diagonal to 0).

Note: In the examples given in the following sections, we will work with the full, symmetric Q matrix rather than adopting the “upper triangular form.”

Section 2: Illustrative Examples and Definitions

Before presenting common practical applications, we first give examples and definitions to lay the groundwork to see better how these applications can be cast in QUBO form.

To begin, consider the optimization problem

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

where the variables, $x_j$, are binary. We can make several observations:

1. The function to be minimized is a quadratic function in binary variables with a linear part $-5x_1 - 3x_2 - 8x_3 - 6x_4$ and a quadratic part $4x_1x_2 + 8x_1x_3 + 2x_2x_3 + 10x_3x_4$.

2. Since binary variables satisfy $x_j = x_j^2$, the linear part can be written as $-5x_1^2 - 3x_2^2 - 8x_3^2 - 6x_4^2$.

3. Then we can re-write the model in the following matrix form:

$$
\text{Minimize } y = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}^T \begin{bmatrix} -5 & 2 & 4 & 0 \\ 2 & -3 & 1 & 0 \\ 4 & 1 & -8 & 5 \\ 0 & 0 & 5 & -6 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \mathbf{x}^T Q \mathbf{x}
$$

4. In turn, this can be written in the matrix notation introduced in Section 1 as

Minimize $y = \mathbf{x}^T Q \mathbf{x}$

where $\mathbf{x}$ is a column vector of binary variables. Note that the coefficients of the original linear terms appear on the main diagonal of the $Q$ matrix. In this case $Q$ is symmetric.
about the main diagonal without needing to modify the coefficients by the approach shown in Section 1.

5. Other than the 0/1 restrictions on the decision variables, QUBO is an unconstrained model with all problem data being contained in the Q matrix. These characteristics make the QUBO model particularly attractive as a modeling framework for combinatorial optimization problems, offering a novel alternative to classically constrained representations.

6. The solution to the model in (3) above is: $y = -11, \ x_1 = x_4 = 1, \ x_2 = x_3 = 0$.

Remarks:

- As already noted, the stipulation that Q is symmetric about the main diagonal does not limit the generality of the model.
- Likewise, casting the QUBO model as a minimization problem does not limit generality. A well-known observation permits a maximization problem to be solved by minimizing the negative of its objective function (and the negative of the minimized objective function value gives the optimum value for the maximization problem).
- As previously emphasized, a variety of optimization problems can naturally be formulated and solved as an instance of the QUBO model. In addition, many other problems that don’t appear to be related to QUBO problems can be re-formulated as a QUBO model. We illustrate this special feature of the QUBO model in the sections that follow.
Section 3: Natural QUBO Formulations

As mentioned earlier, several important problems fall naturally into the QUBO class. To illustrate such cases, we provide two examples of important applications whose formulations naturally take the form of a QUBO model.

3.1 The Number Partitioning Problem:

The Number Partitioning problem has numerous applications cited in the Reference section of these notes. A common version of this problem involves partitioning a set of numbers into two subsets such that the subset sums are as close to each other as possible. We model this problem as a QUBO instance as follows:

Consider a set of numbers \( S = \{s_1, s_2, s_3, ..., s_m\} \). Let \( x_j = 1 \) if \( s_j \) is assigned to subset 1; 0 otherwise. Then the sum for subset 1 is given by

\[
\text{sum}_1 = \sum_{j=1}^{m} s_j x_j
\]

and the sum for subset 2 is given by

\[
\text{sum}_2 = \sum_{j=1}^{m} s_j - \sum_{j=1}^{m} s_j x_j
\]

The difference in the sums is then

\[
diff = \sum_{j=1}^{m} s_j - 2 \sum_{j=1}^{m} s_j x_j = c - 2 \sum_{j=1}^{m} s_j x_j.
\]

We approach the goal of minimizing this difference by minimizing

\[
diff^2 = \left\{ c - 2 \sum_{j=1}^{m} s_j x_j \right\}^2 = c^2 + 4x^tQx
\]

where

\[
q_{ii} = s_i (s_i - c) \quad q_{ij} = q_{ji} = s_i s_j
\]

Dropping the additive and multiplicative constants, our QUBO optimization problem becomes:

\[
\text{QUBO}: \min \ y = x^tQx
\]
where the Q matrix is constructed with $q_{ii}$ and $q_{ij}$ as defined above.

**Numerical Example:** Consider the set of eight numbers

$$S = \{25, 7, 13, 31, 42, 17, 21, 10\}$$

By the development above, we have $c^2 = 27,556$ and the equivalent QUBO problem is

$$\min \ y = x'Qx \text{ with}$$

$$Q = \begin{bmatrix}
-3525 & 175 & 325 & 775 & 1050 & 425 & 525 & 250 \\
175 & -1113 & 91 & 217 & 294 & 119 & 147 & 70 \\
325 & 91 & -1989 & 403 & 546 & 221 & 273 & 130 \\
775 & 217 & 403 & -4185 & 1302 & 527 & 651 & 310 \\
1050 & 294 & 546 & 1302 & -5208 & 714 & 882 & 420 \\
425 & 119 & 221 & 527 & 714 & -2533 & 357 & 170 \\
525 & 147 & 273 & 651 & 882 & 357 & -3045 & 210 \\
250 & 70 & 130 & 310 & 420 & 170 & 210 & -1560
\end{bmatrix}$$

Solving QUBO gives $x = (0,0,0,1,1,0,0,1)$ for which $y = -6889$, yielding perfectly matched sums which equal 83. The development employed here can be expanded to address other forms of the number partitioning problem, including problems where the numbers must be partitioned into three or more subsets.

**3.2 The Max-Cut Problem**

The Max Cut problem is one of the most famous problems in combinatorial optimization. Given an undirected graph $G(V,E)$ with a vertex set $V$ and an edge set $E$, the Max Cut problem seeks to partition $V$ into two sets such that the number of edges between the two sets (considered to be severed by the cut), is a large as possible.

We can model this problem by introducing binary variables satisfying $x_j = 1$ if vertex $j$ is in one set and $x_j = 0$ if it is in the other set. Viewing a cut as severing edges joining two sets, to leave endpoints of the edges in different vertex sets, the quantity $x_i + x_j - 2x_i x_j$ identifies whether the edge $(i, j)$ is in the cut. That is, if $(x_i + x_j - 2x_i x_j)$ is equal to 1, then exactly one of $x_i$ and $x_j$
equals 1, which implies edge \((i, j)\) is in the cut. Otherwise \((x_i + x_j - 2x_ix_j)\) is equal to zero and the edge is not in the cut.

Thus, the problem of maximizing the number of edges in the cut can be formulated as

\[
\text{Maximize } y' = \sum_{(i,j) \in E} \left( x_i + x_j - 2x_ix_j \right)
\]

Sticking with our definition of QUBO in \textit{minimization} form, we write our model as:

\[
\text{Minimize } y = -y' = \sum_{(i,j) \in E} \left( 2x_i x_j - x_i - x_j \right)
\]

which is an instance of

\[
\text{QUBO: min } y = x'Qx
\]

The linear terms determine the elements on the main diagonal of \(Q\) and the quadratic terms determine the off-diagonal elements.

**Numerical Example:** To illustrate the Max Cut problem, consider the following undirected graph with 5 vertices and 6 edges.

Explicitly taking into account all edges in the graph gives the following formulation:

\[
\text{Minimize } y = (-x_1 - x_2 + 2x_1x_2) + (-x_1 - x_3 + 2x_1x_3) + (-x_2 - x_4 + 2x_2x_4) + (-x_3 - x_4 + 2x_3x_4) + (-x_3 - x_5 + 2x_3x_5) + (-x_4 - x_5 + 2x_4x_5)
\]
or

\[
\min y = -2x_1 - 2x_2 - 3x_3 - 3x_4 - 2x_5 + 2x_1x_2 + 2x_1x_3 + 2x_2x_4 + 2x_3x_4 + 2x_3x_5 + 2x_4x_5
\]

This takes the desired form

\[
QUBO : \min y = x'^TQx
\]

by writing the symmetric \(Q\) matrix as:

\[
Q = \begin{bmatrix}
-2 & 1 & 1 & 0 & 0 \\
1 & -2 & 0 & 1 & 0 \\
1 & 0 & -3 & 1 & 1 \\
0 & 1 & 1 & -3 & 1 \\
0 & 0 & 1 & 1 & -2
\end{bmatrix}
\]

Solving this QUBO model gives \(x = (0, 1, 1, 0, 0)\). Hence vertices 2 and 3 are in one set and vertices 1, 4, and 5 are in the other, with a maximum cut value of 5.

In the above examples, the problem characteristics led directly to an optimization problem in QUBO form. As previously remarked, many other problems require “re-casting” to create the desired QUBO form. We introduce a widely-used form of such re-casting in the next section.
Section 4: Creating QUBO Models Using Known Penalties

The “natural form” of a QUBO model illustrated thus far contains no constraints other than those requiring the variables to be binary. However, by far the largest number of problems of interest include additional constraints that must be satisfied as the optimizer searches for good solutions.

Many of these constrained models can be effectively re-formulated as a QUBO model by introducing quadratic penalties into the objective function as an alternative to explicitly imposing constraints in the classical sense. The penalties introduced are chosen so that the influence of the original constraints on the solution process can alternatively be achieved by the natural functioning of the optimizer as it looks for solutions that avoid incurring the penalties. That is, the penalties are formulated so that they equal zero for feasible solutions and equal some positive penalty amount for infeasible solutions. For a minimization problem, these penalties are added to create an augmented objective function to be minimized. If the penalty terms can be driven to zero, the augmented objective function becomes the original function to be minimized.

For certain types of constraints, quadratic penalties useful for creating QUBO models are known in advance and readily available to be used in transforming a given constrained problem into a QUBO model. Examples of such penalties for some commonly encountered constraints are given in the table below. Note that in the table, all variables are intended to be binary and the parameter P is a positive, scalar penalty value. This value must be chosen sufficiently large to assure the penalty term is indeed equivalent to the classical constraint, but in practice an acceptable value for P is usually easy to specify. We discuss this matter more thoroughly later.

<table>
<thead>
<tr>
<th>Classical Constraint</th>
<th>Equivalent Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x + y \leq 1$</td>
<td>$P(xy)$</td>
</tr>
<tr>
<td>$x + y \geq 1$</td>
<td>$P(1 - x - y + xy)$</td>
</tr>
<tr>
<td>$x + y = 1$</td>
<td>$P(1 - x - y + 2xy)$</td>
</tr>
<tr>
<td>$x \leq y$</td>
<td>$P(x - xy)$</td>
</tr>
<tr>
<td>$x_1 + x_2 + x_3 \leq 1$</td>
<td>$P(x_1x_2 + x_1x_3 + x_2x_3)$</td>
</tr>
<tr>
<td>$x = y$</td>
<td>$P(x + y - 2xy)$</td>
</tr>
</tbody>
</table>

Table of a few Known constraint/penalty pairs
To illustrate the main idea, consider a traditionally constrained problem of the form:

\[
\text{Min } y = f(x)
\]

subject to the constraint

\[
x_1 + x_2 \leq 1
\]

where \( x_1 \) and \( x_2 \) are binary variables. Note that this constraint allows either or neither \( x \) variable to be chosen. It explicitly precludes both from being chosen (i.e., both cannot be set to 1).

From the 1\textsuperscript{st} row in the table above, we see that a quadratic penalty that corresponds to our constraint is

\[
P x_1 x_2
\]

where \( P \) is a positive scalar. For \( P \) chosen sufficiently large, the unconstrained problem

\[
\text{minimize } y = f(x) + P x_1 x_2
\]

has the same optimal solution as the original constrained problem. If \( f(x) \) is linear or quadratic, then this unconstrained model will be in the form of a QUBO model. In our present example, any optimizer trying to minimize \( y \) will tend to avoid solutions having both \( x_1 \) and \( x_2 \) equal to 1, else a large positive amount will be added to the objective function. That is, the objective function incurs a penalty corresponding to infeasible solutions.

4.1 The Minimum Vertex Cover (MVC) Problem

In section 3.2 we saw how the QUBO model could be used to represent the famous Max Cut problem. Here we consider another well-known optimization problem on graphs called the Minimum Vertex Cover problem. Given an undirected graph with a vertex set \( V \) and an edge set \( E \), a vertex cover is a subset of the vertices (nodes) such that each edge in the graph is incident to at least one vertex in the subset. The Minimum Vertex Cover problem seeks to find a cover with a minimum number of vertices in the subset.
A standard optimization model for MVC can be formulated as follows. Let $x_j = 1$ if vertex $j$ is in the cover (i.e., in the subset) and $x_j = 0$ otherwise. Then the standard constrained, linear 0/1 optimization model for this problem is:

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

subject to

$$x_i + x_j \geq 1 \text{ for all } (i, j) \in E$$

Note the constraints ensure that at least one of the endpoints of each edge will be in the cover and the objective function seeks to find the cover using the least number of vertices. Note also that we have a constraint for each edge in the graph, meaning that even for modest sized graphs we can have many constraints. Each constraint will alternatively be imposed by adding a penalty to the objective function in the equivalent QUBO model.

Referring to our table above, we see that the constraints in the standard MVC model can be represented by a penalty of the form $P(1 - x - y + xy)$. Thus, an unconstrained alternative to the constrained model for MVC is

$$\text{Minimize } y = \sum_{j \in V} x_j + P\left( \sum_{(i, j) \in E} \left(1 - x_i - x_j + x_i x_j\right) \right)$$

where $P$ again represents a positive scalar penalty. In turn, we can write this as minimize $x^T Q x$ plus a constant term. Dropping the additive constant, which has no impact on the optimization, we have an optimization problem in the form of a QUBO model.

**Remark:** A common extension of this problem allows a weight $w_j$ to be associated with each vertex $j$. Following the development above, the QUBO model for the Weighted Vertex Cover problem is given by:

$$\text{Minimize } y = \sum_{j \in V} w_j x_j + P\left( \sum_{(i, j) \in E} \left(1 - x_i - x_j + x_i x_j\right) \right)$$
Numerical Example

Consider the graph of section 3.2 again but this time we want to determine a minimum vertex cover.

For this graph with $n = 6$ edges and $m = 5$ nodes, the model becomes:

Minimize \[
y = x_1 + x_2 + x_3 + x_4 + x_5 + \\
P(1 - x_1 - x_2 + x_1x_2) + \\
P(1 - x_1 - x_3 + x_1x_3) + \\
P(1 - x_2 - x_4 + x_2x_4) + \\
P(1 - x_3 - x_4 + x_3x_4) + \\
P(1 - x_3 - x_5 + x_3x_5) + \\
P(1 - x_4 - x_5 + x_4x_5)
\]

which can be written as

Minimize \[
y = (1 - 2P)x_1 + (1 - 2P)x_2 + (1 - 3P)x_3 + (1 - 3P)x_4 + (1 - 2P)x_5 \\
+ Px_1x_2 + Px_1x_3 + Px_2x_4 + Px_3x_4 + Px_3x_5 + Px_4x_5 + 6P
\]

Arbitrarily choosing $P$ to be equal to 8 and dropping the additive constant $(6P = 48)$ gives our QUBO model

\[QUBO : \min x'Qx\]
with the Q matrix given by

\[
\begin{bmatrix}
-15 & 4 & 4 & 0 & 0 \\
4 & -15 & 0 & 4 & 0 \\
4 & 0 & -23 & 4 & 4 \\
0 & 4 & 4 & -23 & 4 \\
0 & 0 & 4 & 4 & -15
\end{bmatrix}
\]

Note that we went from a constrained model with 5 variables and 6 constraints to an unconstrained QUBO model in the same 5 variables. Solving this QUBO model gives:

\[ x^T Q x = -45 \] at \( x = (0,1,1,0,1) \) for which \( y = 48 - 45 = 3 \), meaning that a minimum cover is given by nodes 2, 3, and 5. It’s easy to check that at this solution, all the penalty functions are equal to 0.

**Remarks about the Scalar Penalty P:**

As we have indicated, the reformulation process for many problems requires the introduction of a scalar penalty P for which a numerical value must be given. These penalties are not unique, meaning that many different values can be successfully employed. For a particular problem, a workable value is typically set based on domain knowledge and on what needs to be accomplished. Often, we use the same penalty for all constraints but there is nothing wrong with having different penalties for different constraints if there is a good reason to differentially treat various constraints. If a constraint must absolutely be satisfied, i.e., a “hard” constraint, then P must be large enough to preclude a violation. Some constraints, however, are “soft”, meaning that it is desirable to satisfy them but slight violations can be tolerated. For such cases, a more moderate penalty value will suffice.

A penalty value that is too large can impede the solution process as the penalty terms overwhelm the original objective function information, making it difficult to distinguish the quality of one solution from another. On the other hand, a penalty value that is too small jeopardizes the search for feasible solutions. Generally, there is a ‘Goldilocks region’ of considerable size that contains penalty values that work well. A little preliminary thought about the model can yield a ballpark estimate of the original objective function value. Taking P to be some percentage (75% to 150%) of this estimate is often a good place to start. In the end, solutions generated can always
be checked for feasibility, leading to changes in penalties and further rounds of the solution process as needed to zero in on an acceptable solution.

4.2 The Set Packing Problem

The Set Packing problem is a well-known optimization problem in binary variables with a general (traditional) formulation given by

\[
\max \sum_{j=1}^{n} w_j x_j \\
\text{st} \\
\sum_{j=1}^{n} a_{ij} x_j \leq 1 \quad \text{for } i = 1, \ldots, m
\]

where the \( a_{ij} \) are 0/1 coefficients, the \( w_j \) are weights and the \( x_j \) variables are binary. Using the penalties of the form shown in the first and fifth rows of the table given earlier, we can easily construct a quadratic penalty corresponding to each of the constraints in the traditional model. Then by subtracting the penalties from the objective function, we have an unconstrained representation of the problem in the form of a QUBO model. Keeping with our preference for stating QUBO as a minimization problem, we can multiply through by -1 and switch to minimization.

Numerical Example

Consider the following small example of a set packing problem:

\[
\max \ x_1 + x_2 + x_3 + x_4 \\
\text{st} \\
x_1 + x_3 + x_4 \leq 1 \\
x_1 + x_2 \leq 1
\]
Here all the objective function coefficients, the \( w_j \) values, are equal to 1. Using the penalties mentioned above, the equivalent unconstrained problem is:

\[
\max x_1 + x_2 + x_3 + x_4 - Px_1x_3 - Px_1x_4 - Px_3x_4 - Px_1x_2
\]

Switching to minimization we have

\[
\min y = -x_1 - x_2 - x_3 - x_4 + Px_1x_3 + Px_1x_4 + Px_3x_4 + Px_1x_2
\]

This has our customary QUBO form

\[
QUBO: \min x'Qx
\]

where the Q matrix, with P arbitrarily chosen to be 6, is given by

\[
\begin{bmatrix}
-1 & 3 & 3 & 3 \\
3 & -1 & 0 & 0 \\
3 & 0 & -1 & 3 \\
3 & 0 & 3 & -1 \\
\end{bmatrix}
\]

Solving the QUBO model gives \( y = -2 \) at \( x = (0,1,1,0) \). Note that at this solution, all four penalty terms are equal to zero.

**Remark:** Set covering problems with thousands of variables and constraints have been efficiently reformulated and solved using the QUBO reformulation illustrated in this example.

### 4.3 The Max 2-Sat Problem

Satisfiability problems, in their various guises, have applications in many different settings. Often these problems are represented in terms of clauses, in conjunctive normal form, consisting of several true/false literals. The challenge is to determine the literals so that as many clauses as possible are satisfied.
For our optimization approach, we’ll represent the literals as 0/1 values and formulate models that can be re-cast into the QUBO framework and solved with QUBO solvers. To illustrate the approach, we consider the category of satisfiability problems known as Max 2-Sat problems.

For Max 2-Sat, each clause consists of two literals and a clause is satisfied if either or both literals are true. There are three possible types of clauses for this problem, each with a traditional constraint that must be satisfied if the clause is to be true. In turn, each of these three constraints has a known quadratic penalty given in our previous table.

The three clause types along with their traditional constraints and associated penalties are:

1. **No negations**: Example \((x_i \lor x_j)\)
   
   Traditional constraint: \(x_i + x_j \geq 1\)
   
   Quadratic Penalty: \((1 - x_i - x_j + x_i x_j)\)

2. **One negation**: Example \((x_i \lor \overline{x}_j)\)
   
   Traditional constraint: \(x_i + \overline{x}_j \geq 1\)
   
   Quadratic Penalty: \((x_j - x_i x_j)\)

3. **Two negations**: Example \((\overline{x}_i \lor \overline{x}_j)\)
   
   Traditional constraint: \(\overline{x}_i + \overline{x}_j \geq 1\)
   
   Quadratic Penalty: \((x_i x_j)\)

(Note that \(x_j = 1\) or 0 denoting whether literal \(j\) is true or false. The notation \(\overline{x}_j\), the complement of \(x_j\), is equal to \((1 - x_j)\). )

For each clause type, if the traditional constraint is satisfied, the corresponding penalty is equal to zero, while if the traditional constraint is not satisfied, the quadratic penalty is equal to 1. Given this one-to-one correspondence, we can approach the problem of maximizing the number of clauses satisfied by equivalently minimizing the number of clauses not satisfied. This perspective, as we will see, gives us a QUBO model.

For a given Max 2-Sat instance then, we can add the quadratic penalties associated with the problem clauses to get a composite penalty function which we want to minimize. Since the penalties are all quadratic, this penalty function takes the form of a QUBO model,
\min y = x'Qx. Moreover, if \( y \) turns out to be equal to zero when minimizing the QUBO model, this means we have a solution that satisfies all of the clauses; if \( y \) turns out to equal 5, that means we have a solution that satisfies all but 5 of the clauses; and so forth.

This modeling and solution procedure is illustrated by the following example with 4 variables and 12 clauses where the penalties are determined by the clause type.

<table>
<thead>
<tr>
<th>Clause #</th>
<th>Clause</th>
<th>Quadratic Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( x_1 \lor x_2 )</td>
<td>((1 - x_1 - x_2 + x_1x_2))</td>
</tr>
<tr>
<td>2</td>
<td>( x_1 \lor \bar{x}_2 )</td>
<td>((x_2 - x_1x_2))</td>
</tr>
<tr>
<td>3</td>
<td>( \bar{x}_1 \lor x_2 )</td>
<td>((x_1 - x_1x_2))</td>
</tr>
<tr>
<td>4</td>
<td>( \bar{x}_1 \lor \bar{x}_2 )</td>
<td>((x_1x_2))</td>
</tr>
<tr>
<td>5</td>
<td>( \bar{x}_1 \lor x_3 )</td>
<td>((x_1 - x_1x_3))</td>
</tr>
<tr>
<td>6</td>
<td>( \bar{x}_1 \lor \bar{x}_3 )</td>
<td>((x_1x_3))</td>
</tr>
<tr>
<td>7</td>
<td>( x_2 \lor \bar{x}_3 )</td>
<td>((x_3 - x_2x_3))</td>
</tr>
<tr>
<td>8</td>
<td>( x_2 \lor x_4 )</td>
<td>((1 - x_2 - x_4 + x_2x_4))</td>
</tr>
<tr>
<td>9</td>
<td>( \bar{x}_2 \lor x_3 )</td>
<td>((x_2 - x_2x_3))</td>
</tr>
<tr>
<td>10</td>
<td>( \bar{x}_2 \lor \bar{x}_3 )</td>
<td>((x_2x_3))</td>
</tr>
<tr>
<td>11</td>
<td>( x_3 \lor x_4 )</td>
<td>((1 - x_3 - x_4 + x_3x_4))</td>
</tr>
<tr>
<td>12</td>
<td>( \bar{x}_3 \lor \bar{x}_4 )</td>
<td>((x_3x_4))</td>
</tr>
</tbody>
</table>

Adding the individual clause penalties together gives our QUBO model

\[
\min \quad y = 3 + x_1 - 2x_4 - x_2x_3 + x_2x_4 + 2x_3x_4
\]

or,

\[
\min \quad y = 3 + x'Qx
\]
where the Q matrix is given by

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & -1/2 & 1/2 \\
0 & -1/2 & 0 & 1 \\
0 & 1/2 & 1 & -2 \\
\end{bmatrix}
\]

Solving QUBO gives: \( y = 3 - 2 = 1 \) at \( x_1 = x_2 = x_3 = 0, x_4 = 1 \), meaning that all clauses but one are satisfied.

Remarks:

1. The QUBO approach illustrated above has been successfully used to solve Max 2-sat problems with hundreds of variables and thousands of clauses.

2. An interesting feature of this approach for solving Max 2-sat problems is that the size of the resulting QUBO model to be solved is independent of the number of clauses in the problem and is determined only by the number of variables at hand. Thus, a Max 2-Sat problem with 200 variables and 30,000 clauses can be modeled and solved as a QUBO model with just 200 variables.
Section 5: Creating QUBO Models: A General Purpose Approach

In this section, we illustrate how to construct an appropriate QUBO model in cases where a QUBO formulation doesn’t arise naturally (as we saw in section 3) or where useable penalties are not known in advance (as we saw in section 4). It turns out that for these more general cases, we can always “discover” useable penalties by adopting the procedure outlined below.

For this purpose, consider the general 0/1 optimization problem of the form:

$$\min \ y = x^t C x$$

s.t. $\ A x = b, \ x \ binary$ 

This model accommodates both quadratic and linear objective functions since the linear case results when $C$ is a diagonal matrix (observing that $x_j^2 = x_j$ when $x_j$ is a 0-1 variable). Under the assumption that $A$ and $b$ have integer components, problems with inequality constraints can always be put in this form by including slack variables and then representing the slack variables by a binary expansion. (For example, this would introduce a slack variable $s$ to convert the inequality $4x_1 + 5x_2 - x_3 \leq 6$ into $4x_1 + 5x_2 - x_3 + s = 6$, and since clearly $s \leq 7$ (in case $x_3 = 1$), $s$ could be represented by the binary expansion $s_1 + 2s_2 + 4s_3$ where $s_1, s_2,$ and $s_3$ are additional binary variables. If it is additionally known that at not both $x_1$ and $x_2$ can be 0, then $s$ can be at most 3 and can be represented by the expansion $s_1 + 2s_2$. A fuller treatment of slack variables is given subsequently.) These constrained quadratic optimization models are converted into equivalent unconstrained QUBO models by converting the constraints $Ax = b$ (representing slack variables as $x$ variables) into quadratic penalties to be added to the objective function, following the same re-casting as we illustrated in section 4.

Specifically, for a positive scalar $P$, we add a quadratic penalty $P(Ax - b)^t (Ax - b)$ to the objective function to get
\[ y = x' Cx + P (Ax - b)' (Ax - b) \]
\[ = x' Cx + x' Dx + c \]
\[ = x' Qx + c \]

where the matrix D and the additive constant c result directly from the matrix multiplication indicated. Dropping the additive constant, the equivalent unconstrained version of the constrained problem becomes

\[ \text{QUBO: min } x' Qx, \ x \text{ binary} \]

Remarks:

1. A suitable choice of the penalty scalar P, as we commented earlier, can always be chosen so that the optimal solution to QUBO is the optimal solution to the original constrained problem. Solutions obtained can always be checked for feasibility to confirm whether or not appropriate penalty choices have been made.

2. For ease of reference, the preceding procedure that transforms the general problem into an equivalent QUBO model will be called **Transformation #1**. The mechanics of Transformation #1 can be employed whenever we need to convert linear constraints of the form \( Ax = b \) into usable quadratic penalties in our efforts to re-cast a given problem with equality constraints into the QUBO form.

For realistic applications, a program will need to be written implementing Transformation #1 and producing the Q matrix needed for the QUBO model. Any convenient language, like C++, Python, Matlab, etc., can be used for this purpose. For small problems, or for preliminary tests preceding large-scale applications, we can usually proceed manually as we’ll do in these notes.

3. Note that the additive constant, c, does not impact the optimization and can be ignored during the optimization process. Once the QUBO model has been solved, the constant c can be used to recover the original objective function value. Alternatively, the original objective function value can always be determined by using the optimal \( x \), found when QUBO is solved.
Transformation #1 is the “go to” approach in cases where appropriate quadratic penalty functions are not known in advance. In general, it represents an approach that can be adopted for any problem. Due to this generality, Transformation #1 has proven to be an important modeling tool in many problem settings.

Before moving on to applications in this section, we want to single out another constraint/penalty pair for special recognition that we worked with before in section 4:

$$(x_i + x_j \leq 1) \rightarrow P(x_i, x_j)$$

Constraints of this form appear in many important applications. Due to their importance and frequency of use, we refer to this special case as Transformation #2. We’ll have occasion to use this as well as Transformation #1 later in this section.

5.1 Set Partitioning

The set partitioning problem (SPP) has to do with partitioning a set of items into subsets so that each item appears in exactly one subset and the cost of the subsets chosen is minimized. This problem appears in many settings including the airline and other industries and is traditionally formulated in binary variables as

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

$$st$$

$$\sum_{j=1}^{n} a_{ij} x_j = 1 \quad for \ i = 1, \ldots, m$$

$x_j$ where denotes whether or not subset $j$ is chosen, $c_j$ is the cost of subset $j$, and the $a_{ij}$ coefficients are 0 or 1 denoting whether or not variable $x_j$ explicitly appears in constraint $i$.

Note that this model has the form of the general model given at the beginning of this section where, in this case, the objective function matrix $C$ is a diagonal matrix with all off-diagonal elements equal to zero and the diagonal elements are given by the original linear objective.
function coefficients. Thus, we can re-cast the model into a QUBO model directly by using Transformation # 1. We illustrate this with the following example.

**Numerical Example**

Consider a set partitioning problem

\[
\min y = 3x_1 + 2x_2 + x_3 + x_4 + 3x_5 + 2x_6
\]

subject to

\[
\begin{align*}
x_1 + x_3 + x_6 &= 1 \\
x_2 + x_3 + x_5 + x_6 &= 1 \\
x_3 + x_4 + x_5 &= 1 \\
x_1 + x_2 + x_4 + x_6 &= 1
\end{align*}
\]

and \(x\) binary. Normally, Transformation # 1 would be embodied in a supporting computer routine and employed to re-cast this problem into an equivalent instance of a QUBO model. For this small example, however, we can proceed manually as follows: The conversion to an equivalent QUBO model via Transformation # 1 involves forming quadratic penalties and adding them to the original objective function. In general, the quadratic penalties to be added (for a minimization problem) are given by

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

where the outer summation is taken over all constraints in the system \(Ax = b\).

For our example we have

\[
\begin{align*}
\min y &= 3x_1 + 2x_2 + x_3 + x_4 + 3x_5 + 2x_6 \\
&\quad + P(x_1 + x_3 + x_6 - 1)^2 + P(x_2 + x_3 + x_5 + x_6 - 1)^2 \\
&\quad + P(x_3 + x_4 + x_5 - 1)^2 + P(x_1 + x_2 + x_4 + x_6 - 1)^2
\end{align*}
\]
Arbitrarily taking $P$ to be 10, and recalling that $x_j^2 = x_j$ since our variables are binary, this becomes

$$
\min y = -17x_1^2 - 18x_2^2 - 29x_3^2 - 19x_4^2 - 17x_5^2 - 28x_6^2 + 20x_1x_2 + 20x_1x_3 + 20x_1x_4 + 40x_1x_6 \\
+ 20x_2x_3 + 20x_2x_4 + 20x_2x_5 + 40x_2x_6 + 20x_3x_4 + 40x_3x_5 + 40x_3x_6 + 20x_4x_5 \\
+ 20x_4x_6 + 20x_5x_6 + 40
$$

Dropping the additive constant (40), we then have our QUBO model

$$
\min x'Qx, \ x binary
$$

where the $Q$ matrix is

$$
Q = \begin{bmatrix}
-17 & 10 & 10 & 10 & 0 & 20 \\
10 & -18 & 10 & 10 & 10 & 20 \\
10 & 10 & -29 & 10 & 20 & 20 \\
10 & 10 & 10 & -19 & 10 & 10 \\
0 & 10 & 20 & 10 & -17 & 10 \\
20 & 20 & 20 & 10 & 10 & -28
\end{bmatrix}
$$

Solving this QUBO formulation gives an optimal solution $x_1 = x_5 = 1$ (with all other variables equal to 0) to yield $y = 6$.

Remarks:

1. The QUBO approach to solving set partitioning problems has been successfully applied to large instances with thousands of variables and hundreds of constraints.

2. The special nature of the set partitioning model allows an alternative to Transformation #1 for constructing the QUBO model. Let $k_j$ denote the number of 1’s in the jth column of the constraint matrix $A$ and let $r_{ij}$ denote the number of times variables $i$ and $j$ appear
in the same constraint. Then the diagonal elements of $Q$ are given by $q_{ii} = c_i - Pk_i$ and the off–diagonal elements of $Q$ are given by $q_{ij} = q_{ji} = Pr_{ij}$. The additive constant is given by $m^*P$. These relationships make it easy to formulate the QUBO model for any set partitioning problem without having to go through the explicit algebra of Transformation # 1.

3. The set partitioning problem may be viewed as a form of clustering problem and is elaborated further in Section 6.

### 5.2 Graph Coloring

In many applications, Transformation # 1 and Transformation # 2 can be used in concert to produce an equivalent QUBO model, as demonstrated next in the context of graph coloring.

Vertex coloring problems seek to assign colors to nodes of a graph in such a way that adjacent nodes receive different colors. The K-coloring problem attempts to find such a coloring using exactly K colors. A wide range of applications, ranging from frequency assignment problems to printed circuit board design problems, can be represented by the K-coloring model.

These problems can be modeled as satisfiability problems as follows:

Let $x_{ij} = 1$ if node $i$ is assigned color $j$, and 0 otherwise.

Since each node must be colored, we have the constraints

$$\sum_{j=1}^{K} x_{ij} = 1 \quad i = 1, \ldots, n$$

where $n$ is the number of nodes in the graph. A feasible coloring, in which adjacent nodes are assigned different colors, is assured by imposing the constraints
\[ x_{ip} + x_{jp} \leq 1 \quad p = 1, \ldots, K \]

for all adjacent nodes (i,j) in the graph.

This problem, then, can be re-cast in the form of a QUBO model by using Transformation \# 1 on the node assignment constraints and using Transformation \# 2 on the adjacency constraints. This problem does not have an objective function in its original formulation, meaning our focus is on finding a feasible coloring using the K colors allowed. As a result, any positive value for the penalty P will do. (The resulting QUBO model of course has an objective function given by \( x'Qx \) where Q is determined by the foregoing re-formulation.)

**Numerical Example**

Consider the problem of finding a feasible coloring of the following graph using K= 3 colors.

Given the discussion above, we see that the goal is to find a solution to the system:

\[ x_{i1} + x_{i2} + x_{i3} = 1 \quad i = 1, 5 \]

\[ x_{ip} + x_{jp} \leq 1 \quad p = 1, 3 \]

(for all adjacent nodes i and j)
In this traditional form, the model has 15 variables and 26 constraints. As suggested above, to recast this problem into the QUBO form, we can use Transformation # 1 on the node assignment equations and Transformation # 2 on adjacency inequalities. One way to proceed here is to start with a 15-by-15 Q matrix where initially all the elements are equal to zero and then re-define appropriate elements based on the penalties obtained from Transformations # 1 and # 2. To clarify the approach, we’ll take these two sources of penalties one at a time. For ease of notation and to be consistent with earlier applications, we’ll first re-number the variables using a single subscript, from 1 to 15, as follows:

\[(x_{11}, x_{12}, x_{13}, x_{21}, x_{22}, x_{23}, x_{31}, \ldots, x_{52}, x_{53}) = (x_1, x_2, x_3, x_4, x_5, x_6, x_7, \ldots, x_{14}, x_{15})\]

As we develop our QUBO model, we’ll use the variables with a single subscript.

First, we’ll consider the node assignment equations and the penalties we get from Transformation # 1. Taking these equations in turn we have

\[P(x_1 + x_2 + x_3 - 1)^2 \text{ which becomes } P(-x_1 - x_2 - x_3 + 2x_1x_2 + 2x_1x_3 + 2x_2x_3) + P.\]

\[P(x_4 + x_5 + x_6 - 1)^2 \text{ which becomes } P(-x_4 - x_5 - x_6 + 2x_4x_5 + 2x_4x_6 + 2x_5x_6) + P.\]

\[P(x_7 + x_8 + x_9 - 1)^2 \text{ which becomes } P(-x_7 - x_8 - x_9 + 2x_7x_8 + 2x_7x_9 + 2x_8x_9) + P.\]

\[P(x_{10} + x_{11} + x_{12} - 1)^2 \text{ which becomes } P(-x_{10} - x_{11} - x_{12} + 2x_{10}x_{11} + 2x_{10}x_{12} + 2x_{11}x_{12}) + P.\]

\[P(x_{13} + x_{14} + x_{15} - 1)^2 \text{ which becomes } P(-x_{13} - x_{14} - x_{15} + 2x_{13}x_{14} + 2x_{13}x_{15} + 2x_{14}x_{15}) + P.\]

Taking P to equal 4 and inserting these penalties in the “developing” Q matrix gives the following partially completed Q matrix along with an additive constant of 5P
Note the block diagonal structure. Many problems have patterns that can be exploited in developing Q matrices needed for their QUBO representation. Looking for patterns is often a useful debugging tool.

To complete our Q matrix, it’s a simple matter of inserting the penalties representing the adjacency constraints into the above matrix. For these, we use the penalties of Transformation #2, namely $P_{x_ix_j}$, for each adjacent pair of nodes and each of the three allowed colors. We have 7 adjacent pairs of nodes and three colors, yielding a total of 21 adjacency constraints. Allowing for symmetry, we’ll insert 42 penalties into the matrix, augmenting the penalties already in place.

For example, for the constraint ensuring that nodes 1 and 2 cannot both have color #1, the penalty is $P_1x_1x_2$, implying that we insert the penalty value “2” in row 1 and column 4 of our matrix and also in column 1 and row 4. (Recall that we have re-labeled our variables such that...
the original variables $x_{1,i}$ and $x_{2,i}$ are now variables $x_i$ and $x_j$). Including the penalties for the
other adjacency constraints completes the Q matrix as shown below

\[
Q = \begin{bmatrix}
-4 & 4 & 4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\
4 & -4 & 4 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\
4 & 4 & -4 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\
2 & 0 & 0 & -4 & 4 & 4 & 2 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 \\
0 & 2 & 0 & 4 & -4 & 4 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 2 & 0 \\
0 & 0 & 2 & 4 & 4 & -4 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 2 \\
0 & 0 & 0 & 2 & 0 & 0 & -4 & 4 & 4 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 4 & -4 & 4 & 0 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2 & 4 & 4 & -4 & 0 & 0 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & -4 & 4 & 4 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 4 & -4 & 4 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 4 & 4 & -4 & 0 & 2 & 0 \\
2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & -4 & 4 & 4 \\
0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 4 & -4 & 4 & 0 \\
0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 4 & 4 & -4 & 0
\end{bmatrix}
\]

The above matrix incorporates all of the constraints of our coloring problem, yielding the equivalent QUBO model

\[
QUBO: \min \langle x, Qx \rangle
\]

Solving this model yields the feasible coloring:

\[
x_2 = x_4 = x_9 = x_{11} = x_{15} = 1 \text{ with all other variables equal to zero.}
\]

Switching back to our original variables, this solution means that nodes 1 and 4 get color #2, node 2 gets color #1, and nodes 3 and 5 get color #3.
Remark: This approach to coloring problems has proven to be very effective for a wide variety of coloring instances with hundreds of nodes.

5.3 General 0/1 Programming

Many important problems in industry and government can be modeled as 0/1 linear programs with a mixture of constraint types. The general problem of this nature can be represented in matrix form by

\[
\begin{align*}
\text{max } & cx \\
\text{st } & Ax = b \\
& x \text{ binary}
\end{align*}
\]

where slack variables are introduced as needed to convert inequality constraints into equalities. Given a problem in this form, Transformation # 1 can be used to re-cast the problem into the QUBO form

\[
\begin{align*}
\text{max } & x_0 = x^TQx \\
\text{st } & x \text{ binary}
\end{align*}
\]

As discussed earlier, problems with inequality constraints can be handled by introducing slack variables, via a binary expansion, to create the system of constraints \( Ax = b \). The maximization objective is again handled by multiplying through by -1 and then minimizing.

Numerical Example

Consider the general 0/1 problem
\[
\begin{align*}
\text{max} & \quad 6x_1 + 4x_2 + 8x_3 + 5x_4 + 5x_5 \\
\text{st} & \\
2x_1 + 2x_2 + 4x_3 + 3x_4 + 2x_5 & \leq 7 \\
1x_1 + 2x_2 + 2x_3 + 1x_4 + 2x_5 & = 4 \\
3x_1 + 3x_2 + 2x_3 + 4x_4 + 4x_5 & \geq 5 \\
x & \in \{0, 1\}
\end{align*}
\]

Since Transformation # 1 requires all constraints to be equations rather than inequalities, we convert the 1st and 3rd constraints to equations by including slack variables via a binary expansion. To do this, we first estimate upper bounds on the slack activities as a basis for determining how many binary variables will be required to represent the slack variables in the binary expansions. Typically, the upper bounds are determined simply by examining the constraints and estimating a reasonable value for how large the slack activity could be. For the problem at hand, we can refer to the slack variables for constraints 1 and 3 as \( s_1 \) and \( s_3 \) with upper bounds 3 and 6 respectively. Our binary expansions are:

\[
\begin{align*}
0 \leq s_1 & \leq 3 \quad \Rightarrow \quad s_1 = x_6 + 2x_7 \\
0 \leq s_3 & \leq 6 \quad \Rightarrow \quad s_3 = x_8 + 2x_9 + 4x_{10}
\end{align*}
\]

Where \( x_6, x_7, x_8, x_9, \) and \( x_{10} \) are new binary variables. Note that these new variables will have objective function coefficients equal to zero. Including these slack variables gives the system \( Ax = b \) with \( A \) given by:

\[
A = \begin{bmatrix}
2 & 2 & 4 & 3 & 2 & 1 & 2 & 0 & 0 & 0 \\
1 & 2 & 2 & 1 & 2 & 0 & 0 & 0 & 0 & 0 \\
3 & 3 & 2 & 4 & 4 & 0 & 0 & -1 & -2 & -4
\end{bmatrix}
\]
We can now use Transformation # 1 to reformulate our problem as a QUBO instance. Changing to minimization and adding the penalties to the objective function gives

\[
\begin{align*}
\min \ y &= -6x_1 - 4x_2 - 8x_3 - 5x_4 - 5x_5 \\
&\quad + P(2x_1 + 2x_2 + 4x_3 + 3x_4 + 2x_5 + 1x_6 + 2x_7 - 7)^2 \\
&\quad + P(1x_1 + 2x_2 + 2x_3 + 1x_4 + 2x_5 - 4)^2 \\
&\quad + P(3x_1 + 3x_2 + 2x_3 + 4x_4 + 4x_5 - 1x_8 - 2x_9 - 4x_{10} - 5)^2
\end{align*}
\]

Taking \( P = 10 \) and re-writing this in the QUBO format gives

\[
\min \ y = x'Qx
\]

with an additive constant of 900 and a Q matrix

\[
Q = \begin{bmatrix}
-526 & 150 & 160 & 190 & 180 & 20 & 40 & -30 & -60 & -120 \\
150 & -574 & 180 & 200 & 200 & 20 & 40 & -30 & -60 & -120 \\
160 & 180 & -688 & 220 & 200 & 40 & 80 & -20 & -40 & -80 \\
190 & 200 & 220 & -645 & 240 & 30 & 60 & -40 & -80 & -160 \\
180 & 200 & 200 & 240 & -605 & 20 & 40 & -40 & -80 & -160 \\
20 & 20 & 40 & 30 & 20 & -130 & 20 & 0 & 0 & 0 \\
40 & 40 & 80 & 60 & 40 & 20 & -240 & 0 & 0 & 0 \\
-30 & -30 & -20 & -40 & -40 & 0 & 0 & 110 & 20 & 40 \\
-60 & -60 & -40 & -80 & -80 & 0 & 0 & 20 & 240 & 80 \\
-120 & -120 & -80 & -160 & -160 & 0 & 0 & 40 & 80 & 560 \\
\end{bmatrix}
\]

Solving \( \min \ y = x'Qx \) gives the non-zero values

\[
x_1 = x_4 = x_5 = x_9 = x_{10} = 1
\]

for which \( y = -916 \). Note that the third constraint is loose. Adjusting for the additive constant, and recalling that we started with a maximization problem, gives an objective function value of
16. Alternatively, we could have simply evaluated the original objective function at the solution 
\[ x_1 = x_4 = x_5 = 1 \] to get the objective function value of 16.

**Remarks**: Any problem in linear constraints and bounded integer variables can be converted through a binary expansion into \( \min y = x'Qx \) as illustrated here. In such applications, however, the elements of the Q matrix can, depending on the data, get unacceptably large and may require suitable scaling to mitigate this problem.

5.4 Quadratic Assignment

The Quadratic Assignment Problem (QAP) is a renowned problem in combinatorial optimization with applications in a wide variety of settings. It is also one of the more challenging models to solve. The problem setting is as follows: We are given \( n \) facilities and \( n \) locations along with a flow matrix \( (f_{ij}) \) denoting the flow of material between facilities \( i \) and \( j \).

A distance matrix \( (d_{ij}) \) specifies the distance between sites \( i \) and \( j \). The optimization problem is to find an assignment of facilities to locations to minimize the weighted flow across the system. Cost information can be explicitly introduced to yield a cost minimization model, as is common in some applications.

The decision variables are \( x_{ij} = 1 \) if facility \( i \) is assigned to location \( j \); otherwise, \( x_{ij} = 0 \). Then the classic QAP model can be stated as:

Minimize \[ \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} f_{ij}d_{kl}x_{ik}x_{jl} \]

Subject to \[ \sum_{i=1}^{n} x_{ij} = 1 \quad j = 1,n \]

\[ \sum_{j=1}^{n} x_{ij} = 1 \quad i = 1,n \]

\[ x_{ij} \in \{0,1\}, \quad i, j = 1,n \]
All QAP problems have $n^2$ variables, which often yields large models in practical settings.

This model has the general form presented at the beginning of this section and consequently Transformation # 1 can be used to convert any QAP problem into a QUBO instance.

**Numerical Example**

Consider a small example with $n = 3$ facilities and 3 locations with flow and distance matrices respectively given as follows:

\[
\begin{bmatrix}
0 & 5 & 2 \\
5 & 0 & 3 \\
2 & 3 & 0
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
0 & 8 & 15 \\
8 & 0 & 13 \\
15 & 13 & 0
\end{bmatrix}
\]

It is convenient to re-label the variables using only a single subscript as we did previously in the graph coloring problem, thus replacing

\[(x_{11}, x_{12}, x_{13}, x_{21}, x_{22}, x_{23}, x_{31}, x_{32}, x_{33}) \text{ by } (x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9)\]

Given the flow and distance matrices our QAP model becomes:

\[
\begin{align*}
\min x_0 &= 80x_1x_5 + 150x_1x_6 + 32x_1x_8 + 60x_1x_9 + 80x_2x_4 + 130x_2x_6 + 60x_2x_7 + 52x_2x_9 \\
&\quad + 150x_3x_4 + 130x_3x_5 + 60x_3x_7 + 52x_3x_8 + 48x_4x_8 + 90x_4x_9 + 78x_5x_9 + 78x_6x_8 \\
\end{align*}
\]

subject to

\[
\begin{align*}
x_1 + x_2 + x_3 &= 1 \\
x_4 + x_5 + x_6 &= 1 \\
x_7 + x_8 + x_9 &= 1 \\
x_1 + x_4 + x_7 &= 1 \\
x_2 + x_5 + x_8 &= 1 \\
x_3 + x_6 + x_9 &= 1 
\end{align*}
\]

Converting the constraints into quadratic penalty terms and adding them to the objective function gives the unconstrained quadratic model
min \ y = 80x_1x_5 + 150x_1x_6 + 32x_1x_8 + 60x_1x_9 + 80x_2x_4 + 130x_2x_6 + 60x_2x_7 + 52x_2x_9 \\
+ 150x_3x_4 + 130x_3x_5 + 60x_3x_7 + 52x_3x_8 + 48x_4x_8 + 90x_4x_9 + 78x_5x_9 + 78x_6x_8 \\
+ P(x_1 + x_2 + x_3 - 1)^2 + P(x_4 + x_5 + x_6 - 1)^2 + P(x_7 + x_8 + x_9 - 1)^2 \\
+ P(x_1 + x_4 + x_7 - 1)^2 + P(x_2 + x_5 + x_8 - 1)^2 + P(x_3 + x_6 + x_9 - 1)^2

Choosing a penalty value of \( P = 200 \), this becomes the standard QUBO problem

QUBO: \[ \min \ y = x'Qx \]

with an additive constant of 1200 and the following 9-by-9 \( Q \) matrix:

\[
\begin{bmatrix}
-400 & 200 & 200 & 200 & 40 & 75 & 200 & 16 & 30 \\
200 & -400 & 200 & 40 & 200 & 65 & 16 & 200 & 26 \\
200 & 200 & -400 & 75 & 65 & 200 & 30 & 26 & 200 \\
200 & 40 & 75 & -400 & 200 & 200 & 200 & 24 & 45 \\
40 & 200 & 65 & 200 & -400 & 200 & 200 & 24 & 39 \\
75 & 65 & 200 & 200 & 200 & -400 & 45 & 39 & 200 \\
200 & 16 & 30 & 200 & 24 & 45 & -400 & 200 & 200 \\
16 & 200 & 26 & 24 & 200 & 39 & 200 & -400 & 200 \\
30 & 26 & 200 & 45 & 39 & 200 & 200 & 200 & -400
\end{bmatrix}
\]

Solving QUBO gives \( y = -982 \) at \( x_1 = x_5 = x_9 = 1 \) and all other variables = 0. Adjusting for the additive constant, we get the original objective function value of \( 1200 - 982 = 218 \).

**Remark:** A QUBO approach to solving QAP problems, as illustrated above, has been successfully applied to problems with more than 30 facilities and locations.
5.5 Quadratic Knapsack

Knapsack problems, like the other problems presented earlier in this section, play a prominent role in the field of combinatorial optimization, having widespread application in such areas as project selection and capital budgeting. In such settings, a set of attractive potential projects is identified and the goal is to identify a subset of maximum value (or profit) that satisfies the budget limitations. The classic linear knapsack problem applies when the value of a project depends only on the individual projects under consideration. The quadratic version of this problem arises when there is an interaction between pairs of projects affecting the value obtained.

For the general case with n projects, the Quadratic Knapsack Problem (QKP) is commonly modeled as

$$\max \sum_{i=1}^{n-1} \sum_{j=i}^{n} v_{ij} x_i x_j$$

subject to the budget constraint

$$\sum_{j=1}^{n} a_j x_j \leq b$$

where $x_j = 1$ if project j is chosen: else, $x_j = 0$. The parameters $v_{ij}$, $a_j$ and $b$ represent, respectively, the value associated with choosing projects i and j, the resource requirement of project j, and the total resource budget. Generalizations involving multiple knapsack constraints are found in a variety of application settings.

Numerical Example

Consider the QKP model with four projects:

$$\max 2x_1 + 5x_2 + 2x_3 + 4x_4 + 8x_1 x_2 + 6x_1 x_3 + 10x_1 x_4 + 2x_2 x_3 + 6x_2 x_4 + 4x_3 x_4$$

subject to the knapsack constraint:

$$8x_1 + 6x_2 + 5x_3 + 3x_4 \leq 16$$
We re-cast this into the form of a QUBO model by first converting the constraint into an equation and then using the ideas embedded in Transformation # 1. Introducing a slack variable in the form of the binary expansion $1x_5 + 2x_6$, we get the equality constraint

$$8x_1 + 6x_2 + 5x_3 + 3x_4 + 1x_5 + 2x_6 = 16$$

which we can convert to penalties to produce our QUBO model as follows.

Changing to minimization and including the penalty term in the objective function gives the unconstrained quadratic model:

$$\min y = -2x_1 - 5x_2 - 2x_3 - 4x_4 - 8x_1x_2 - 6x_1x_3$$
$$-10x_1x_4 - 2x_2x_3 - 6x_2x_4 - 4x_3x_4$$
$$+ P(8x_1 + 6x_2 + 5x_3 + 3x_4 + 1x_5 + 2x_6 - 16)^2$$

Choosing a penalty $P = 10$, and cleaning up the algebra gives the QUBO model

$$\text{QUBO: } \min y = x^TQx$$

with an additive constant of 2560 and the Q matrix

$$
\begin{bmatrix}
1922 & 476 & 397 & 235 & 80 & 160 \\
476 & -1565 & 299 & 177 & 60 & 120 \\
397 & 299 & -1352 & 148 & 50 & 100 \\
235 & 177 & 148 & -874 & 30 & 60 \\
80 & 60 & 50 & 30 & -310 & 20 \\
160 & 120 & 100 & 60 & 20 & -600 \\
\end{bmatrix}
$$

Solving QUBO gives $y = -2588$ at $x = (1, 0, 1, 1, 0, 0)$. Adjusting for the additive constant and switching back to “maximization” gives the value 28 for the original objective function.

**Remark:** The QUBO approach to QKP has proven to be successful on problems with several hundred variables and as many as five knapsack constraints.
Section 6: Connections to Quantum Computing and Machine Learning

Quantum Computing QUBO Developments: As noted in Section 1, one of the most significant applications of QUBO emerges from the observation that it is equivalent to the famous Ising problem in physics. In common with the earlier demonstration that many NP-hard problems such as graph and number partitioning, covering and set packing, satisfiability, matching, spanning tree as well as others can converted into the QUBO form, Lucas (2014) more recently has observed that such problems can be converted into the Ising form. Ising problems replace $x \in \{0, 1\}^n$ by $x \in \{-1, 1\}^n$ and can be put in the QUBO form by defining $x_j = (x_j + 1)/2$ and then redefining $x_j$ to be $x_j'$. Efforts to solve Ising problems are often carried out with annealing approaches, motivated by the perspective in physics of applying annealing methods to find a lowest energy state.

More effective methods for QUBO problems, and hence for Ising problems, are obtained using modern metaheuristics. Among the best metaheuristic methods for QUBO are those based on tabu search and path relinking as described in Glover (1996, 1997), Glover and Laguna (1997) and adapted to QUBO in Wang et al. (2012, 2013).

A bonus from this development has been to create a link between QUBO problems and quantum computing. A new type of quantum computer based on quantum annealing with an integrated physical network structure of qubits known as a Chimera graph has incorporated ideas from Wang et al. (2012) in its software and has been implemented on the D-Wave System. The ability to obtain a quantum speedup effect for this system applied to QUBO problems has been demonstrated in Boixo et al. (2014).

Additional advances incorporating methodology from Wang et al. (2012, 2013) are provided in the D-Wave open source software system Qbsolv (2017) and in the supplementary QMASM system by Pakin (2018). Recent QUBO quantum computing applications in the literature include those for Graph Partitioning Problems (Mniszewski et al., 2016) and Maximum Clique Problems (Chapuis et al., 2018). In another recent development, QUBO models are being studied using the IBM neuromorphic computer at Lawrence Livermore National Laboratory, as reported in Alom et al. (2017).

There has been some controversy about the relative merits of different quantum computing frameworks. One of the most active debates concerns the promise of quantum gate systems, also known as quantum circuit systems, versus the promise of adiabatic or quantum annealing systems. Now an important new discovery by Yu et al. (2018) shows that these two systems offer effectively the same potential for achieving the gains inherent in quantum computing processes, with a mathematical demonstration that the quantum circuit algorithm can be transformed into quantum adiabatic algorithm with the exact same time complexity. This has valuable implications for the relevance of QUBO models in the D-Wave adiabatic system, disclosing that analogous advances associated with QUBO models may ultimately be realized through quantum adiabatic systems.

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1 This adds a constant to (1), which is irrelevant for optimization.
circuit systems. The study of the QUBO/Ising model in neuromorphic computing suggests the growing recognition of the universality and significance of this model.

One of the major initiatives currently underway is to unite quantum computing and classical computing in order to exploit specific advantages unique to each. Here, too, QUBO models are actively entering the picture. A new classical computing system, called Alpha-QUBO (2018), is under development for the purpose of integrating classical and quantum computing to provide more effective solutions to QUBO and QUBO-related problems.

**Unsupervised Machine Learning with QUBO:** -- One of the most salient forms of unsupervised machine learning is the type represented by clustering. As remarked earlier, the QUBO set partitioning model provides a very natural form of clustering, and hence offers a useful model for unsupervised machine learning. Surprisingly, to date, very little exploration of this model has been undertaken in the machine learning context. An exception is the recent use of clustering to facilitate the solution of QUBO models in Samorani et al. (2018).

**Supervised Machine Learning with QUBO:** -- By an interesting contrast with unsupervised learning, two different types of QUBO proposals have been made for supervised machine learning. Viewed from the physics perspective, Schneidman, Berry, Segev and Bialek (2006) argue that the Ising model is useful for any model of neural function, because a statistical model for neural activity should be chosen using the principle of maximum entropy. Pudenz and Lidar (2013) more explicitly show how a QUBO based quantum computing model can be used in unsupervised machine learning. A still more recent application of QUBO to unsupervised machine learning is proposed in Glover et al. (2018), which can be employed either together with quantum computing or independently.

**Machine Learning to Improve QUBO Solution Processes:** -- Devising rules and strategies to learn the implications of specific model instances has had a long history. Today it permeates the field of mixed integer programming, for example, to identify relationships such as values or bounds that can be assigned to variables, or inequalities that can constrain feasible spaces more tightly. Cast under the name of pre-processing, such approaches have not traditionally be viewed through the lens of machine learning, but it is evident that they qualify as a viable and important example of the field.

Efforts to apply this type of machine learning to QUBO problems have proceeded more slowly. A landmark paper in this regard is the work of Boros et al. (2008), which uses roof duality and a max-flow algorithm to provide useful inferences. More recently, sets of logical tests were developed to learn relationships among variables in QUBO applications in Glover et al. (2017), which were successful in setting many variables a priori, leading to significantly smaller problems. In about half of the problems in the test bed the learning approach achieved a 45% reduction in size and exactly solved 10 problems. The rules also identified many significant implied relationships between pairs of variables resulting in many simple logical inequalities.
A different type of learning approach proposed many years ago in Glover (1977) that uses clustering in association with population-based metaheuristics was recently updated and implemented with a path relinking algorithm for QUBO problems in Samorani et al. (2018). Instead of using pre-processing to learn solution implications, this approach generates and exploits clusters as the solution algorithm progresses and has proved particularly effective for solving larger QUBO instances.

Other types of machine learning approaches also merit a closer look in the future for applications with QUBO. Among these is the Programming by Optimization approach of Hoos (2012) and the Integrative Population Analysis approach of Glover et al. (1998).

Section 7: Concluding Remarks
In the preceding sections we have undertaken to illustrate the basics of re-casting problems into the QUBO framework, to enable a given binary optimization problem to be solved by a specialized QUBO solver. In the comments below we highlight additional ideas relevant to QUBO modeling and its applications in classical and quantum computing.

1. The uses of logical analysis to identify relationships between variables in the work of Glover et al. (2017) can be implemented in the setting of quantum computing to combat the difficulties of applying current quantum computing methods to scale effectively for solving large problems. Approximation methods based on such analysis can be used for decomposing and partitioning large QUBO problems to solve large problems and provide strategies relevant to a broad range of quantum computing applications.

2. The National Academies of Sciences, Engineering and Medicine have released a consensus study report on progress and prospects in quantum computing (2018) that disclose the relevance of marrying quantum and classical computing, which accords with the objectives of the Alpha-QUBO system (2018). As stated in the National Academies report, “formulating an R&D program with the aim of developing commercial applications for near-term quantum computing is critical to the health of the field. Such a program would include … identification of algorithms for which hybrid classical-quantum techniques using modest-size quantum subsystems can provide significant speedup.” Studies devoted to the use of Alpha-QUBO in conjunction with quantum computing initiatives at Los Alamos National Laboratory are investigating the possibilities for achieving such speedup.

3. In both classical and quantum settings, the transformation to QUBO can sometimes be aided considerably by first employing a change of variables. This is particularly useful in settings where the original model is an edge-based graph model, as in clique partitioning where the standard models can have millions of variables due to the number of edges in the graph. A useful alternative is to introduce node-based variables, by replacing each edge variable with the product of two node variables. Such a change converts a linear model into a quadratic model with many fewer variables, since a graph normally has a
much smaller number of nodes than edges. The resulting quadratic model, then, can be
converted to a QUBO model by the methods illustrated earlier.

4. Problems with higher order polynomials arise in certain applications and can be re-cast
into a QUBO framework by employing a reduction technique. For example, consider a
problem with a cubic term $x_1 x_2 x_3$ in binary variables. Replace the product $x_1 x_2$ by a
binary variable, $y_1$ and add a penalty to the objective function of the form

$$P(x_1 x_2 - 2x_1 y_1 - 2x_2 y_1 + 3y_1).$$

By this process, when the optimization drives the penalty
term to 0, which happens only when $y_1 = x_1 x_2$, we have reduced the cubic term to an
equivalent quadratic term $(y_1 x_3)$. This procedure can be used recursively to convert
higher order polynomials to quadratic models of the QUBO form.

5. The general procedure of Transformation # 1 has similarities to the Lagrange Multiplier
approach of classical optimization. The key difference is that our scalar penalties ($P$) are
not “dual” variables to be determined by the optimization. Rather, they are parameters
set a priori to encourage the search process to avoid candidate solutions that are
infeasible. Moreover, the Lagrange Multiplier approach is not assured to yield a solution
that satisfies the problem constraints except in the special case of convex optimization, in
contrast to the situation with the QUBO model. To determine good values for Lagrange
multipliers (which in general only yield a lower bound instead of an optimum value for
the problem objective) recourse must be made to an additional type of optimization called
subgradient optimization, which QUBO models do not depend on.

6. Solving QUBO models: QUBO models belong to a class of problems known to be NP-
hard. The practical meaning of this is that using exact solvers (like CPLEX or Gurobi) to
find “optimal” solutions will most likely be unsuccessful except for very small problem
instances. Realistic sized problems can run for days and even weeks when using exact
methods without producing high quality solutions. As discussed in Section 6, to
overcome this computational difficulty, QUBO models are typically solved by using
modern Metaheuristic methods (such as Tabu Search and Path Relinking), which are
designed to find high quality but not necessarily optimal solutions in a modest amount of
computer time, and which are actively being adapted for creating QUBO solution
approaches in quantum computing. Continuing progress in the design and
implementation of such methods will have an impact across a wide range of practical
applications of optimization and machine learning.
Bibliography:


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