Scalable Integer Encoding in Quadratic Unconstrained Binary Optimization

Kazuhiro Miyahara, Junya Arai, Keitaro Horikawa
NTT Software Innovation Center
Email: sic-lasolv-p-ml@hco.ntt.co.jp

(i) Introduction

- ✓ To efficiently solve combinatorial optimization problems, several companies have developed specialized computers, e.g., D-Wave's quantum annealers, Fujitsu's digital annealers, and NTT's coherent Ising machines. Since these computers employ **quadratic unconstrained binary optimization (QUBO) as the native input format**, we need QUBO formulation of problems.
- ✓ It usually uses **one-hot encoding to represent integer variables** since QUBO is defined over only binary variables. However, **one-hot encoding consumes many binary variables** per integer variable. This limits problem scale that can leverage specialized computers.
- ✓ This poster propose **scalable integer encoding 'qubyte'** and QUBO formulation of mathematical relations between qubytes. **They reduce the consumption of binary variables to logarithmic order**; hence, we can solve larger and more complex problems on QUBO computers by using qubytes.

(ii) QUBO and One-hot Integer Encoding

For given $Q \in R^{n\times n}$, QUBO problems are defined as follows:

$$\min_{x\in\{0,1\}^n} \boldsymbol{x}^T Q \boldsymbol{x}.$$

Note that an arbitrary quadratic function can be deformed into $\boldsymbol{x}^T Q \boldsymbol{x}$. If several constraints can be formulated as minimization problem of quadratic functions, sum of the functions means conjunction of the constraints.
One-hot encoding[1] α represents integer variable in $[0, N)$ by a tuple of N binary variables. We consider α represents $i-1$ iff i-th binary variable is 1 and the others are 0. In other words, one-hot encoding is valid iff only one variable is 1. We can formulate this constraint as a minimization problem of the follows:

$$\mathrm{OneHot}(\alpha) = \left(1 - \sum_{1\le i\le N} x_{\alpha,i}\right)^2.$$

The function takes the minimum value 0 iff α is valid. Assuming α and β are integers in one-hot encoding, we can also formulate mathematical constraints "equal" and "not equal" as follows:

$$\mathrm{Eq_{OH}}(\alpha,\beta) = \sum_{1\le i\le N} \left(x_{\alpha,i} - x_{\beta,i}\right)^2 \quad \text{and} \quad \mathrm{Neq_{OH}}(\alpha,\beta) = \sum_{1\le i\le N} x_{\alpha,i} x_{\beta,i}.$$

Both function takes the minimum value 0 iff α and β represents "equal" or "not equal". Note that, while the 2-base numeral system is popular in conventional computers, it is not suitable for solving combinatorial optimization problems. This is because of limitation on value ranges; considering value range $[0, N)$, N must be a power of two. Thus, it cannot always encode possible problem solutions in QUBO.

(iii) Qubyte Integer Encoding

Qubyte is based on the 2-base numeral system, but can encode integers of arbitrary value ranges. Qubyte encoding α represents integer variable in $[0, N)$ by a tuple of $\lceil \mathrm{lb}\, N \rceil$ binary variables as follows ("lb" means binary logarithm.):

$$\mathrm{I}(\alpha) = \sum_{0\le i<\lceil \mathrm{lb}\, N\rceil - 1} 2^i x_{\alpha,i} + \left(N - 2^{\lceil \mathrm{lb}\, N\rceil - 1}\right) x_{\alpha,\lceil \mathrm{lb}\, N\rceil - 1}.$$

Following polynomials are for "equal" or "not equal" constraints. (γ for $[0, 2^{\lceil \mathrm{lb}\, N\rceil + 1})$ and δ for $[0, \lceil \mathrm{lb}\, N\rceil)$ are auxiliary qubyte integers.)

$$\mathrm{Eq_{Qb}}(\alpha,\beta) = \{\mathrm{I}(\alpha) - \mathrm{I}(\beta)\}^2.$$

$$\mathrm{Neq_{Qb}}(\alpha,\beta) = \left\{\left(\mathrm{I}(\alpha) - \mathrm{I}(\beta) + 2^{\lceil \mathrm{lb}\, N\rceil}\right) - \mathrm{I}(\gamma)\right\}^2 + \left\{\sum_{0\le i<\lceil \mathrm{lb}\, N\rceil} \left(1 - x_{\gamma,i}\right) - \mathrm{I}(\delta)\right\}^2.$$

Equal to $2^{\lceil \mathrm{lb}\, N\rceil}$ iff $\mathrm{I}(\alpha) = \mathrm{I}(\beta)$.

Bind γ to $\mathrm{I}(\alpha) - \mathrm{I}(\beta) + 2^{\lceil \mathrm{lb}\, N\rceil}$; thus, $\mathrm{I}(\gamma) = 2^{\lceil \mathrm{lb}\, N\rceil}$ iff $\mathrm{I}(\alpha) = \mathrm{I}(\beta)$.

Count zeros in $x_{\gamma,i}$. It equals to $\lceil \mathrm{lb}\, N\rceil$ iff $\mathrm{I}(\gamma) = 2^{\lceil \mathrm{lb}\, N\rceil}$.

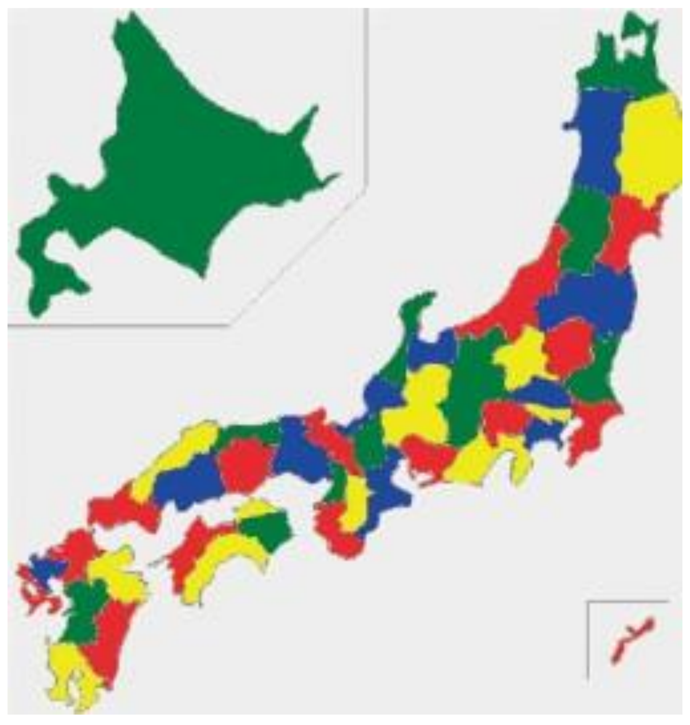
Take the minimum value 0 iff $\mathrm{I}(\delta) = \sum_{0\le i<\lceil \mathrm{lb}\, N\rceil}(1 - x_{\gamma,i})$. However, since δ is for range $[0, \lceil \mathrm{lb}\, N\rceil)$, this term takes non-zero iff $\sum_{0\le i<\lceil \mathrm{lb}\, N\rceil}(1 - x_{\gamma,i}) \ge \lceil \mathrm{lb}\, N\rceil \Leftrightarrow \mathrm{I}(\gamma) = 2^{\lceil \mathrm{lb}\, N\rceil} \Leftrightarrow \mathrm{I}(\alpha) = \mathrm{I}(\beta)$. Hence, $\mathrm{I}(a) \neq \mathrm{I}(b)$ must be held to minimize $\mathrm{Neq_{Qb}}(\alpha,\beta)$.

Obviously, $\mathrm{Eq_{Qb}}$ takes the minimum value 0 iff $\mathrm{I}(\alpha) = \mathrm{I}(\beta)$. $\mathrm{Neq_{Qb}}$ is minimized iff green box and orange box takes 0. Green box minimized iff γ represents offset difference of α and β. Orange box minimized iff δ represents the number of zeros in the offset difference except the head bit. Note that orange box can takes minimum value zero iff $\mathrm{I}(\alpha) \neq \mathrm{I}(\beta)$, because $\mathrm{I}(\delta) < \lceil \mathrm{lb}\, N\rceil$. With these polynomials α and β consumes logarithmic order binary variables. $\mathrm{Eq_{Qb}}(\alpha,\beta)$ doesn't consume additional binary variables. $\mathrm{Neq_{Qb}}(\alpha,\beta)$ consumes additional variables for γ ($\lceil \mathrm{lb}\, N\rceil + 1$ variables) and δ ($\lceil \mathrm{lb}\lceil \mathrm{lb}\, N\rceil\rceil$ variables).

(iv) Evaluation

Graph coloring problem

We compared consumptions of binary variables between one-hot encoding and qubyte encoding using the graph coloring problem. Specifically, we consider the problem to find coloring of the Japanese map that every adjacent prefecture has different colors.
The number of colors K is scaled from 1 to 300. A color for prefecture p is represented by an integer $\alpha_p \in [0, K)$ with one-hot or qubyte encoding.
We consider the Japanese map as graph $G = (V, E)$. Set V contains the prefectures, and set E contains pairs of the adjacent prefectures.



One-hot Encoding

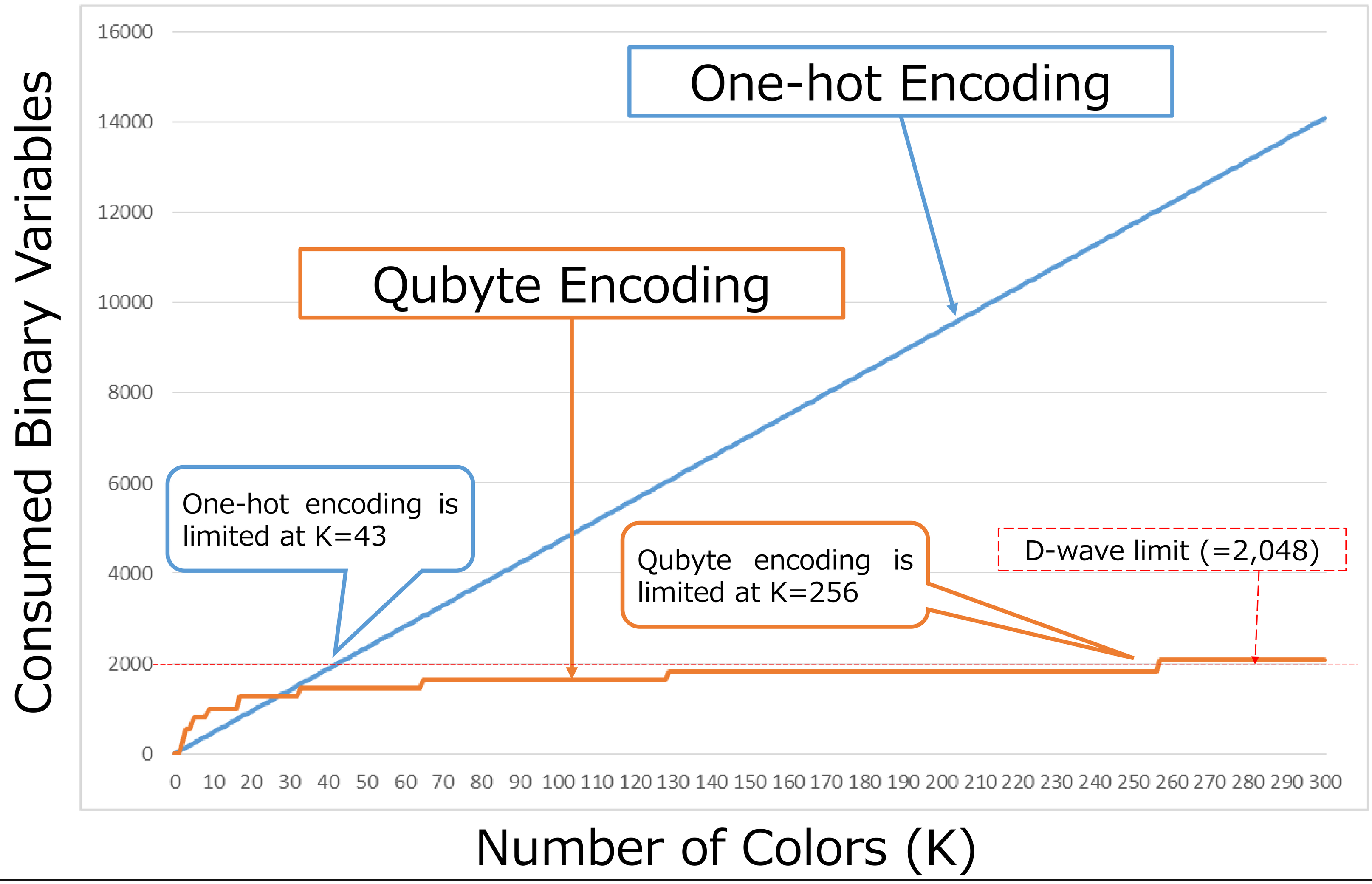
$$\sum_{p\in V} \mathrm{OneHot}(\alpha_p) + \sum_{(p,q)\in E} \mathrm{Neq_{OH}}(\alpha_p, \alpha_q).$$

Qubyte Encoding

$$\sum_{(p,q)\in E} \mathrm{Neq_{Qb}}(\alpha_p, \alpha_q).$$

Result

As shown in the plot below, qubyte encoding scales significantly better for problem complexity compared with one-hot encoding. For example, D-Wave 2000Q, which offers 2,048 variables, fails to solve the graph coloring for K > 43 in one-hot encoding. Qubyte encoding extends that limitation to K = 256 by reducing the variable consumption from linear order to logarithmic order.



(v) Future Directions

QUBO computers have limitation on a value range of the elements in matrix Q. For example, D-Wave 2000Q allows only 4- or 5-bit values for Q[3]. However, qubyte encoding tends to require a larger range than one-hot encoding. We are going to study how to minimize the value range.
Additionaly, we will evaluate the constraint of "less than" as follows (γ for $[0, 2^{\lceil \mathrm{lb}\, N\rceil})$ is auxiliary qubyte integer.):

$$\mathrm{LessThan_{Qb}}(\alpha,\beta) = \left\{\left(\mathrm{I}(\alpha) - \mathrm{I}(\beta) + 2^{\lceil \mathrm{lb}\, N\rceil}\right) - \mathrm{I}(\gamma)\right\}^2.$$

Less than $2^{\lceil \mathrm{lb}\, N\rceil}$ iff $\mathrm{I}(\alpha) < \mathrm{I}(\beta)$

Take the minimum value 0 iff $\mathrm{I}(\gamma) = \mathrm{I}(\alpha) - \mathrm{I}(\beta) + 2^{\lceil \mathrm{lb}\, N\rceil}$ and $0 \le \mathrm{I}(\alpha) - \mathrm{I}(\beta) + 2^{\lceil \mathrm{lb}\, N\rceil} < 2^{\lceil \mathrm{lb}\, N\rceil}$ since γ is for $[0, 2^{\lceil \mathrm{lb}\, N\rceil})$; therefore, $\mathrm{I}(\alpha) < \mathrm{I}(\beta)$ must be held to minimize $\mathrm{LessThan_{Qb}}(\alpha,\beta)$.

(vi) References

[1]: Kumar, V., Bass, G., Tomlin, C., & Dulny, J. (2018). Quantum annealing for combinatorial clustering. Quantum Information Processing, 17(2), 39.
[2]: Karimi, S., & Ronagh, P. (2019). Practical integer-to-binary mapping for quantum annealers. Quantum Information Processing, 18(4), 94.
[3]: https://support.dwavesys.com/hc/en-us/community/posts/360029507594-What-is-the-resolution-of-the-control-parameters-in-D-Wave-devices-

ISC High Performance 2020, June 21-25, Frankfurt, Germany