QUBO to Ising Hamiltonian Model Transformation

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Starting from the equation (13) from the paper, we have the following QUBO problem:

$$\max_b L(b) = \max_b \left(\mu''^T b - q b^T \Sigma'' b \underbrace{-\lambda(P''^T b - 1)^2}_{penalty} \right) \tag{1}$$

Now we expand its component:

$$\mu''^T b = \sum_i u''_i b_i, \tag{2}$$

$$-q b^T \Sigma'' b = -q \sum_{i,j} \Sigma''_{ij} b_i b_j, \tag{3}$$

$$-\lambda(P''^T b - 1)^2 = -\lambda \left(\sum_i P''_i b_i - 1 \right)^2 . \tag{4}$$

We have the transformation of $b_i = \frac{1+s_i}{2}; b_j = \frac{1+s_j}{2}$

$$\sum_i u''_i b_i = \sum_i u''_i \frac{1+s_i}{2} \tag{5}$$

$$= \underbrace{\frac{1}{2} \sum_i u''_i} + \underbrace{\frac{1}{2} \sum_i u''_i s_i}, \tag{6}$$

Substitute $b_i b_j$

$$b_i b_j = \frac{1+s_i}{2} \cdot \frac{1+s_j}{2} = \frac{(1+s_i)(1+s_j)}{4} = \frac{1}{4}(1 + s_i + s_j + s_i s_j) \tag{7}$$

$$-q \sum_{i,j} \Sigma''_{ij} b_i b_j = -q \sum_{i,j} \Sigma''_{ij} \frac{1}{4}(1 + s_i + s_j + s_i s_j) \tag{8}$$

$$= \underbrace{-\frac{q}{4} \sum_{i,j} \Sigma''_{ij}} \underbrace{-\frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_i - \frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_j} \underbrace{-\frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_i s_j} \tag{9}$$

Since Σ'' is symmetric, we have:

$$-\frac{q}{4}\sum_{i,j}\Sigma''_{ij}s_i - \frac{q}{4}\sum_{i,j}\Sigma''_{ij}s_j = -\frac{q}{2}\sum_{i}\left(\sum_{j}\Sigma''_{ij}\right)s_i \tag{10}$$

Penalty term:

$$-\lambda\left(\sum_i P''_i b_i - 1\right)^2 = -\lambda\left(\sum_i P''_i \frac{1+s_i}{2} - 1\right)^2 \tag{11}$$

$$= -\lambda\left(\frac{1}{2}\sum_i P''_i(1+s_i) - 1\right)^2 \tag{12}$$

$$= -\lambda\left(\frac{1}{2}\sum_i P''_i + \frac{1}{2}\sum_i P''_i s_i - 1\right)^2 \tag{13}$$

According to equation (15) from the paper, we have the penalty term in the as:

$$+\lambda\left(\sum_i \pi_i s_i - \beta\right)^2 \tag{14}$$

Let $\pi_i = \frac{1}{2}P''_i$ and $\beta = 1 - \frac{1}{2}\sum_i P''_i$, equation (13) can be written as (flip the sign to convert maximization to minimization):

$$+\lambda\left(\sum_i \pi_i s_i - \beta\right)^2 \tag{15}$$

$$\Rightarrow \lambda\left(\left(\sum_i \pi_i s_i\right)^2 - 2\left(\sum_i \pi_i s_i\right)\beta + \beta^2\right) \tag{16}$$

$$\tag{17}$$

The Ising objective function from the paper is written as:

$$\min_s L(s) : \min_s \left(\sum_i h_i s_i + \sum_{i,j} J_{i,j}s_i s_j + \lambda\left(\sum_i \pi_i s_i - \beta\right)^2\right), \tag{18}$$
$$\text{s.t} \quad s_{i,j} \in \{-1, 1\} \quad \forall i, j$$

From equations (6), (9) , (10), we can derive h , J, and other constant as:

$$h_i = \frac{1}{2}\mu''_i - \frac{q}{2}\sum_j \Sigma''_{ij} \tag{19}$$

$$J_{i,j} = -\frac{q}{4}\Sigma''_{i,j} \tag{20}$$

$$\text{Constant} = \frac{1}{2}\sum_i u''_i - \frac{q}{4}\sum_{i,j}\Sigma''_{ij} \tag{21}$$