

QUBO to Ising Hamiltonian Model Transformation

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

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

Now we expand its component:

$$\mu''^T b = \sum_i u''_i b_i, \quad (2)$$

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

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

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

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

$$= \underbrace{\frac{1}{2} \sum_i u''_i}_{\text{constant}} + \underbrace{\frac{1}{2} \sum_i u''_i s_i}_{\text{linear}} \quad (6)$$

Substitute $b_i b_j$

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

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

$$= -\underbrace{\frac{q}{4} \sum_{i,j} \Sigma''_{ij}}_{\text{constant}} - \underbrace{\frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_i}_{\text{linear}} - \underbrace{\frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_j}_{\text{linear}} - \underbrace{\frac{q}{4} \sum_{i,j} \Sigma''_{ij} s_i s_j}_{\text{quadratic}} \quad (9)$$

Since Σ'' is symmetric, we have:

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

Penalty term:

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

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

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

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

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

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):

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

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

$$(17)$$

The Ising objective function from the paper is written as:

$$\min_s L(s) : \min_s \left(\sum_i h_i s_i + \sum_{i,j} J_{i,j} s_i s_j + \lambda \left(\sum_i \pi_i s_i - \beta \right)^2 \right), \quad (18)$$

s.t. $s_{i,j} \in \{-1, 1\} \quad \forall i, j$

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

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

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

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