QUBO formulation for sparse estimation

LASSO Problem Statement

The LASSO optimization problem is defined as:

$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \tag{1}$$

where:

- $y \in R^n$: Response vector
- $X \in R^{n \times p}$: Measurement matrix
- $\beta \in R^p$: Sparse coefficient vector
- $\lambda > 0$: Regularization parameter

QUBO Formulation for ℓ_1-Norm

For a scalar m, the ℓ_1-norm $|m|$ is expressed using auxiliary variables $z_1, z_2 \geq 0$:

$$|m| = \min_{z_1, z_2} \left[z_1 + z_2 + M(-m - z_1 + z_2)^2 \right] \tag{2}$$

where $M \gg 1$ enforces the constraint $z_2 = m + z_1$.

For the vector $\beta \in R^p$, introduce pairs of auxiliary variables (z_{1i}, z_{2i}) for each β_i, such that $z_{1i}, z_{2i} \geq 0$ to model $|\beta_i| = z_{1i} + z_{2i}$:

$$\|\beta\|_1 = \sum_{i=1}^{p} |\beta_i| \to \sum_{i=1}^{p} \left(z_{1i} + z_{2i} + M(-\beta_i - z_{1i} + z_{2i})^2 \right)$$

where $M \gg 1$ enforces $z_{2i} = \beta_i + z_{1i}$.

Reduction to DQM

Represent each β_i using B binary variables $b_{ik} \in \{0, 1\}$ (e.g., fixed-point precision with B bits):

$$\beta_i \approx \sum_{k=1}^{B} b_{ik} \cdot 2^{-k} \tag{3}$$

Full QUBO Model for LASSO

Combine the least-squares term and ℓ_1 penalty:

$$\text{Minimize:} \quad \underbrace{\sum_{j=1}^{n} \left(y_j - \sum_{i=1}^{p} X_{ji} \sum_{k=1}^{B} b_{ik} \cdot 2^{-k} \right)^2}_{\text{Least-squares term}} \\ + \lambda \underbrace{\sum_{i=1}^{p} \left(z_{1i} + z_{2i} + M \left(-\sum_{k=1}^{B} b_{ik} \cdot 2^{-k} - z_{1i} + z_{2i} \right)^2 \right)}_{\ell_1 \text{ penalty term}} \tag{4}$$

Graph Representation of QUBO Structure

The QUBO matrix can be visualized as a graph where:

- **Nodes**: Binary variables $\{b_{ik}\}$ and auxiliary variables $\{z_{1i}, z_{2i}\}$
- **Edges**: Quadratic interactions between variables:
  - Between b_{ik} and b_{jl} from the least-squares term
  - Between b_{ik} and z_{1i}/z_{2i} from the ℓ_1 penalty
  - Between z_{1i} and z_{2i} via the constraint term

By integrating the ℓ_1-norm QUBO formulation into LASSO, you can leverage quantum annealing for sparse regression tasks.

References

[1] Tomohiro Yokota, Makiko Konoshima, Hirotaka Tamura, Jun Ohkubo "Derivation of QUBO formulations for sparse estimation", `https://arxiv.org/pdf/2001.03715v2`