Mixed Hamming-packings for benchmarking QUBO solvers

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Outline

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Motivation

- Introducing a new QUBO problem class, that is
  - Hard to solve - in theory and in practice
  - Small sized, common
  - Models an important problem
  - Differs from already used mature QUBO benchmarks

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Preliminaries

- Ising problem
  - describes the energy of a ˜ spin glass system model

$$E(\mathbf{s}) = \sum_{(i,j)\in G} J_{i,j} s_i s_j + \sum_j h_j s_j$$
$$\mathbf{s} \in \{1,-1\}^N$$

- QUBO modeling:

$$\begin{aligned} \text{min} \quad & \mathbf{x}^\top Q \mathbf{x} \\ \text{s.t.} \quad & \mathbf{x} \in \{0,1\}^N \end{aligned}$$

- MAXCUT problem:

$$\begin{aligned} \text{min} \quad & \mathbf{s}^\top W \mathbf{s} \\ \text{s.t.} \quad & \mathbf{s} \in \{-1,1\}^N \end{aligned}$$

- All these are *equivalent*.

Hamming packings

Definition: Hamming space

$H \stackrel{\text{def}}{=} \mathbb{Z}_{k_1}\mathbb{Z}_{k_2}\ldots\mathbb{Z}_{k_n}$, with $\infty > k_1 \geqslant k_2 \geqslant \cdots \geqslant k_{n-1} \geqslant k_n \ (\geqslant 2)$

Definition: Hamming distance

$d(v,w) \stackrel{\text{def}}{=} \sum_{i=1}^{n}\left(1-\delta_{v[i],w[i]}\right)$

Definition: Hamming packing

A subset of $H (C \subseteq H)$ for a given fixed $d \in \mathbb{N}$: $\forall v \neq w \in C : d(v,w) \geqslant d$

Hamming packings

Definition: Maximal Hamming packing - cardinality

$$N(H;d) \stackrel{\text{def}}{=} \max\{|C| : C \subseteq H, \forall v \neq w \in C : d(v,w) \geqslant d\}$$

One of the key questions is the maximal Hamming packing problem. Addressing the key question: what is the densest subset of a given space that maintains a minimum pairwise distance of d?

- Any Hamming packing problem can be formulated as a packing MIP
- (wlg. upper triangular) QUBO with
  - nonpositive diagonals
  - above diagonals' nonzero elements are all positive and dominate corresponding diagonal values
  - the matrix basically is a scaled adjacency matrix

Hamming packings

Importance, applications

- Football pool systems, betting systems
- Drug screening
- Data compression
- Telecommunication protocols, ECC
- Quality assurance (SW, engineering)

Hamming packings

Binary programming model for determining $N(H;d)$

$$\begin{aligned} \max \quad & \sum_{v\in H} x_v \\ s.t. \quad & x_v + x_w \leqslant 1 \qquad \substack{\forall v,w\in H:\\ 1\leqslant d(v,w)\leqslant (d-1)} \\ & \mathbf{x} \in \{0,1\}^n \qquad . \end{aligned}$$

- The objective ensures the maximality of the chosen subset
- **This is a special maximum independent set problem**
- The constraints act as a mutex
- In corresponding QUBO model: penalize $x_v x_w$
  - A trick: DECOMPOSITION! (problem-specific, correctness?)

Adding contact graph-based cut planes

Binary programming model for determining $N(H;d)$

$$\begin{aligned} \max \quad & \sum_{v \in H} x_v \\ s.t. \quad & x_v + x_w \leqslant 1 \qquad \forall v,w \in H: 1 \leqslant d(v,w) \leqslant (d-1) \\ & \mathbf{x} \in \{0,1\}^n \\ & \sum_{d(v,w)=d} x_w \geqslant x_v \quad \forall v \in H. \end{aligned}$$

Additional constraints for the $N(H,d)$ MILP model. Naszvadi et al., Mathematics 13 2633 (2025)

QUBO-specific model tweaks

QUBO-specific model tweaks

QUBO model to determine $N(H; d)$

$$- \min_{\mathbf{x} \in \{0,1\}^n} \quad \mathbf{x}^\top Q \mathbf{x} \quad .$$

- Normalizing - penalty weights can be 2 or even 1!
- Decomposition: pruning one ball at least (further CG-based)
- On quantum devices, because every subpacking is feasible, providing equidistant corresponding energy levels in the Hamiltonian

Benchmarks vs solvers

Platforms used for testing Hamming packing optimization models:

- SCIP: scipopt.org , used for solving reference exact ILP models
- Gurobi: gurobi.com , QUBO exact solutions
- MQLib: github.com/MQLib/MQLib , comprehensive collection of QUBO heuristics
- Simulated Bifurcation Engine: physics-motivated heuristics implementations by quantumz.io
- D-Wave: dwavequantum.com , NISQ hardware quantum annealer

Exact solvers' benchmark

MILP

- SCIP, used as the reference solver, found feasible primal solutions for all instances.
- Extended models with CG-based constraints and ad-hoc pruning were applied.
- All instances were solved within a 1-hour time limit.

Exact QUBO solver

- Tough problem class; instability and cycling are common.
- Finding best dual bounds is hard.

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MQLib statistics and algorithm setup

MQLib: tested with all 133 QUBO models - duplication due to the decompositions

MQLib algorithms evaluated

ALKHAMIS1998	BEASLEY1998SA	BEASLEY1998TS	GLOVER1998a
GLOVER2010	HASAN2000GA	HASAN2000TS	KATAYAMA2000
KATAYAMA2001	LODI1999	LU2010	MERZ1999CROSS
MERZ1999GLS	MERZ1999MUTATE	MERZ2002GREEDY	MERZ2002GREEDYKOPT
MERZ2002KOPT	MERZ2002ONEOPT	MERZ2004	PALUBECKIS2004bMST1
PALUBECKIS2004bMST2	PALUBECKIS2004bMST3	PALUBECKIS2004bMST4	PALUBECKIS2004bMST5
PALUBECKIS2004bSTS	PALUBECKIS2006	PARDALOS2008	

MQLib algorithms evaluated (27 total).

Instances with most algorithm failures - MQLib

Instance	n	Optimum	Alg. failing
82222222_3_0_qubo.csv	939	-63	12/27
7666_3_0_qubo.csv	1325	-35	11/27
433322_3_0_qubo.csv	371	-26	10/27
443322_3_0_qubo.csv	505	-35	9/27
543322_3_0_qubo.csv	639	-35	9/27
6665_3_0_qubo.csv	925	-29	9/27
4432222_4_0_qubo.csv	542	-12	8/27
73333_3_0_qubo.csv	480	-26	8/27
6322222_3_0_qubo.csv	508	-31	7/27
633322_3_0_qubo.csv	569	-35	7/27

Instances with the highest number of MQLib algorithms failing to reach the exact optimum.

SBM sub-optimal instances

Instance	Optimum	SBM best	Gap
43332_3_0_qubo.csv	-13	-11	2
44332_3_0_qubo.csv	-17	-15	2
6322222_3_0_qubo.csv	-31	-29	2
443332_4_0_qubo.csv	-13	-12	1
522222_3_0_qubo.csv	-10	-9	1
433322_3_0_qubo.csv	-26	-25	1
6522222_4_0_qubo.csv	-10	-9	1

The only instances where SBM does not reach the exact optimum.

- SBM discrete version 4096 samples, 4000 steps, $dt = 0.05$.
- Total time: ≈ 0.2 s.

D-Wave embedding results

D-Wave was partially successful in embedding. The solved models were $N_{7,2}(1,5;d=3)$ and $N_3(5;d=3)$, yielding optimal or near-optimal results.

Instance	Adv 4.1	Adv 6.4	Adv2 1.11	Adv2 2.1	Adv2 4.3
722222	OK (45 s)	OK (82 s)	OK (56 s)	OK (73 s)	FAIL (150 s)
33333	OK (156 s)	OK (293 s)	FAIL (431 s)	FAIL (379 s)	FAIL (62 s)
443322	FAIL (1012 s)	FAIL (1008 s)	FAIL (1006 s)	FAIL (1008 s)	FAIL (516 s)

Embedding results. Time in seconds spent by the embedding algorithm.

- chain-breaks were common
- unsolvable setups due to the many failed embeddings

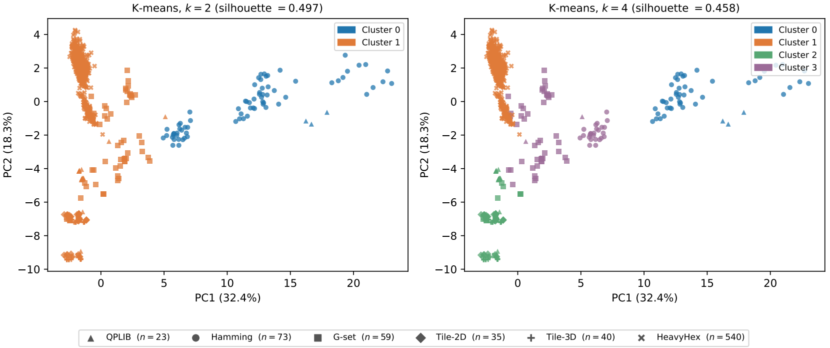
Classification

- 58 graph-theoretic features of the MAX-CUT graph of the problem
- defined in Appendix B of Dunning et al., INFORMS J. Comput. 30 608 (2018).
- Benchmark families to compare:

Family	Count	Description
Hamming QUBOs	73	Mixed Hamming packing problems; dense, all-positive coupling weights.
G-set	59	Classic Max-Cut benchmarks; sparse, mixed weights, up to $n = 5000$.
QPLIB	23	Unconstrained binary QP instances (type QBN) from QPLIB 2018; 120–3000 variables.
Tile-planting 2D	35	2D Ising spin-glass via tile-planting; square-lattice topology, mixed weights.
Tile-planting 3D	40	3D tile-planting; cubic-lattice, mixed weights, $L \in \{6, 8, 10, 12\}$.
IBM Heavy-Hex	540	QUBO reformulations of heavy-hex IBM quantum hardware instances; three penalty strengths.
Total	**770**	

Classification

Cluster analysis on solution metrics (MQLib-based)



Classifying candidate problem class metrics compared to existing ones

PCA projection, K-means cluster assignment. PC1 separates the Hamming/dense group from the sparse families

Hamming-QUBO characteristics

Prediction	Status	Evidence
D-Wave: long chains and chain breaks	**Confirmed**	Chain overhead 16.7–$23\times$; chains up to 43; largest instance fails embedding
Discrete local search: flat-landscape traps	**Partially confirmed**	Best-of-27 reaches 100 % optimal; weakest 3 algorithms 13–46 %; hardest instance defeats 12/27
Continuous methods unaffected by flat landscape	**Confirmed**	SBM optimal on 95 % of instances in < 2.3 s
Small max. indep. set $\Rightarrow$ coordinated moves needed	**Partially confirmed**	Per-algorithm success rate 13–100 %; QPU gap grows with n

Conclusion

Comparing solvers

- MQLib beats MILP primal solutions (time to find)
- MQLib and MILP primal solutions show positive correlation in time to find the best primal solution
- MILP dual bound lookup outperforms exact QUBO/Max-Cut solvers
- SBM was fastest up to medium-sized problems

Model classification

- New benchmark model class with unique properties

An online repository is about to be released containing the detailed statistics above

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