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A Mixing Method based Branch-and-Bound Solver for QUBO Problems

Joint work with Valentin Durante

FWF Der Wissenschaftsfonds.

UNIVERSITÄT KLAGENFURT

Modeling - Analysis - Optimization · DOC.FUNDS DOCTORAL SCHOOL

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Quadratic Unconstrained Binary Optimization (QUBO)

Optimization Problem (QUBO)

Given $C \in \mathbb{R}^{n \times n}$*, solve*

$$\begin{aligned} \max \quad & x^\top C x \\ \textit{s.t.} \quad & x \in \{-1, 1\}^n \end{aligned} \tag{QUBO}$$

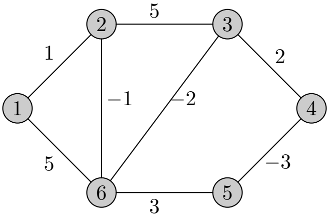
- $\mathcal{NP}$-hard problem
- LP approaches exist only for sparse C

Example:

Max-Cut Problem: $C = \frac{1}{4}L(G)$, where $L(G)$ Laplacian matrix

The (Weighted) Max-Cut Problem

Given: undirected graph $G = (V, E)$ with edge weights $w \in \mathbb{R}^E$



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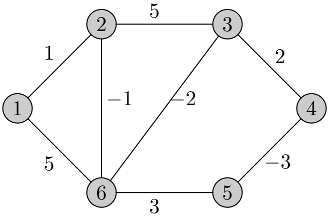

Goal: find a maximum cut in G, i.e., an optimal solution of

$$\max_{S \subseteq V} \sum_{i \in S,\ j \in V \setminus S} w_{ij} \tag{MC}$$

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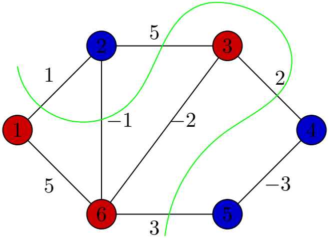

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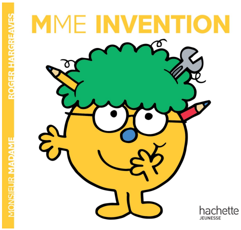
Solvers for dense C using Semidefinite Programming

BiqMac (2010)	BiqCrunch (2016)
	
MADAM (2021)	**BiqBin (2022)**
	

Semidefinite Relaxation

We introduce $X := xx^\top$:

- $x^\top Cx = \langle C, xx^\top \rangle = \langle C, X \rangle$
- $\operatorname{diag}(X) = e$
- $X \succeq 0$
- $\operatorname{rank}(X) = 1$

Equivalent formulations

$$\begin{aligned} \max \quad & x^\top Cx \\ \text{s.t.} \quad & x \in \{-1, 1\}^n \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} \max \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \operatorname{diag}(X) = e \\ & X \succeq 0 \\ & \operatorname{rank}(X) = 1 \end{aligned}$$

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Semidefinite relaxation

$$\begin{array}{rl} \max & x^\top Cx \\ \text{s.t.} & x \in \{-1,1\}^n \end{array} \quad \leq \quad \begin{array}{rl} \max & \langle C, X \rangle \\ \text{s.t.} & \operatorname{diag}(X) = e \\ & X \succeq 0 \\ & \cancel{\operatorname{rank}(X) = 1} \end{array}$$

- all mentioned solvers: additional ‘clique’ inequalities
- but competitive implementations possible without inequalities

Low-rank Factorization $X = V^\top V$

Factorization of $X \succeq 0$

$$X = V^\top V$$

for some $V = (v_1 | \dots | v_n) \in \mathbb{R}^{k \times n}$ with $k \leq n$

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Optimization Problem (SDP-vec)

$$\begin{aligned} \max \quad & \sum_{i,j=1}^n C_{ij} v_i^\top v_j \\ \text{s.t.} \quad & v_i \in \mathcal{S}^{k-1}, \; i = 1, \dots, n \end{aligned} \tag{SDP-vec}$$

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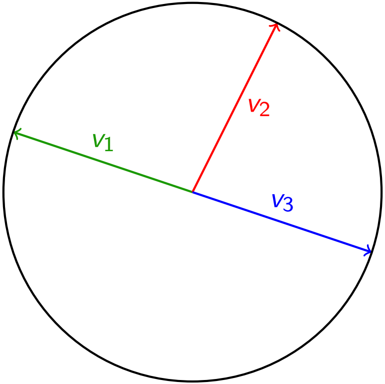
- $k > \sqrt{2n}$: (SDP) $\Leftrightarrow$ (SDP-vec) [cf. Pataki, 1998]

Geometric Interpretation

$$
\begin{aligned}
v_i^\top v_j &= \|v_i\| \cdot \|v_j\| \cdot \cos \measuredangle(v_i, v_j) \\
&= \cos \measuredangle(v_i, v_j)
\end{aligned}
$$



Coordinate Ascent Method

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Coordinate Ascent

We fix all but one vector v_i. (SDP-vec) reduces to

$$\begin{aligned} \max \quad & g^\top v_i = \|g\| \cdot \|v_i\| \cdot \cos \measuredangle(g, v_i) \\ \text{s.t.} \quad & \|v_i\| = 1, \ v_i \in \mathbb{R}^k \end{aligned}$$

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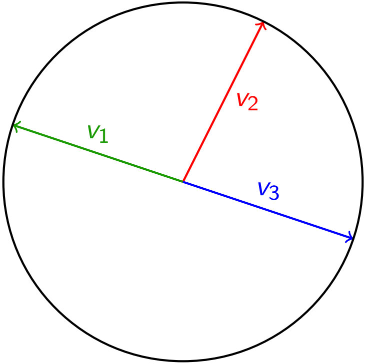
where $g = \sum_j^n c_{ij} v_j = V \cdot c_i$

- closed-form solution: $v_i = \frac{g}{\|g\|}$ for $g \neq 0$

Mixing Method (Wang el al., 2018)



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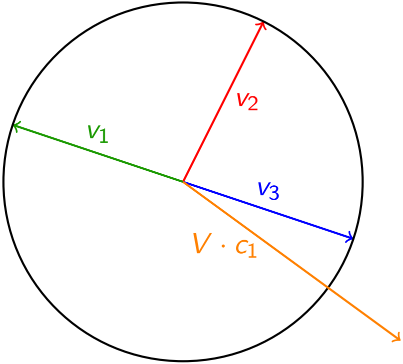

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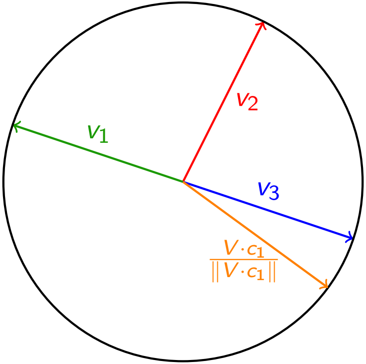

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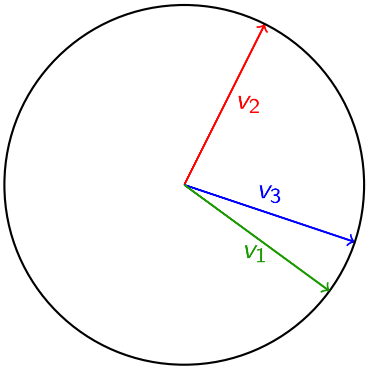

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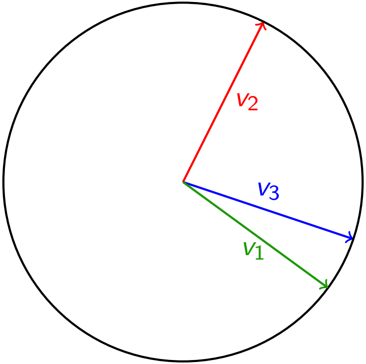
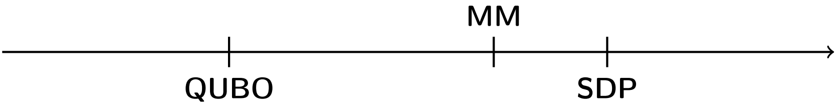


Mixing Method

- repeat for $v_1, v_2, \ldots, v_n$ again and again
- initialize V randomly on the unit sphere
- converges to optimal solution with linear rate

Exact Approach for QUBO



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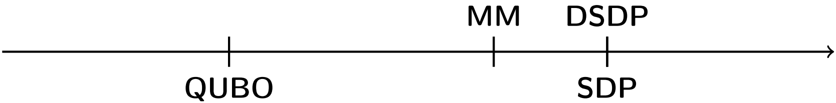

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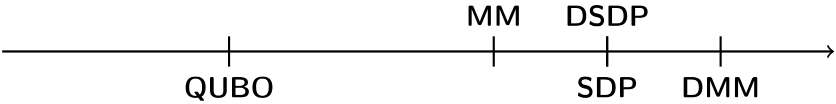

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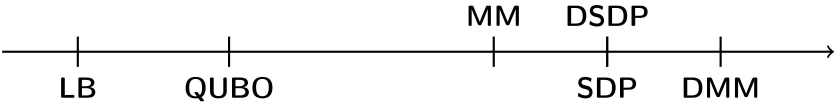

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- heuristics provide lower bound: LB $\leq$ QUBO

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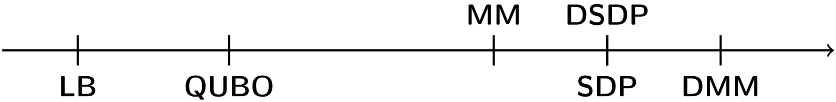

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Branch-and-Bound

If DMM $>$ LB, partition QUBO into two smaller subproblems and proceed recursively.

Results and Future Work

- C implementation using Intel MKL
- tested on many instances with $n \leq 100$

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