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

Joint work with Valentin Durante

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Quadratic Unconstrained Binary Optimization (QUBO)

- internally solves problems of the following type:

QUBO in $\{-1, 1\}$-variables

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

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

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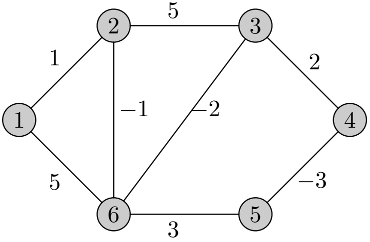
Example:

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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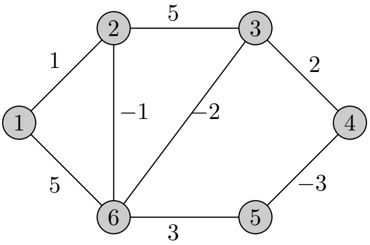

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Find a maximum cut in G, i.e., an optimal solution of

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

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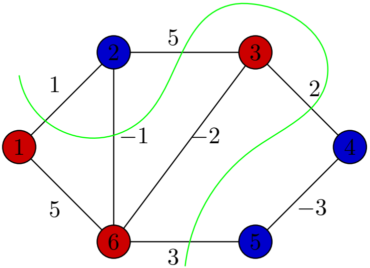

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Examples I

QUBO in $\{0,1\}$-variables

$$\max_{x \in \{0,1\}^n} \left\{ x^\top Q x + q^\top x \right\}$$

where $Q \in \mathbb{R}^{n \times n}$ and $q \in \mathbb{R}^n$.

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$$\Leftrightarrow$$

Reformulation in $\{-1,1\}$-variables

$$\max_{x \in \{-1,1\}^{n+1}} x^\top C x$$

where

$$C := \frac{1}{4} \begin{bmatrix} e^\top Q e + 2q^\top e & e^\top Q + q^\top \\ Qe + q & Q \end{bmatrix}.$$

Examples II

Linearly constrained binary quadratic problem (BQP)

$$\begin{aligned} \min \quad & x^\top Q x + q^\top x \\ \text{s.t.} \quad & Ax = b \\ & x \in \{0,1\}^n \end{aligned} \tag{BQP}$$

where $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$.

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where $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$.

For some $C \in \mathbb{R}^{(n+1)\times(n+1)}$, (BQP) is equivalent to

Reformulation (used in *BiqBin* solver)

$$\begin{aligned} \min \quad & x^\top C x \\ \text{s. t.} \quad & x \in \{-1,1\}^{n+1} \\ & x_0 = 1. \end{aligned}$$

Examples III

Maximum Stable Set Problem

$$\begin{aligned} \max \quad & e^\top x \\ \text{s.t.} \quad & x_i x_j = 0, \quad \forall ij \in E \\ & x \in \{0,1\}^n \end{aligned} \tag{MSSP}$$

Examples III

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$$\begin{aligned} \max \quad & e^\top x \\ \text{s.t.} \quad & x_i x_j = 0, \quad \forall ij \in E \\ & x \in \{0,1\}^n \end{aligned} \tag{MSSP}$$

$$\Leftrightarrow$$

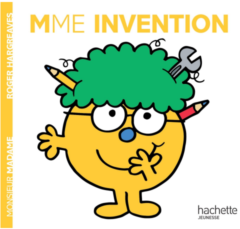
Reformulation of (MSSP)

$$\begin{aligned} \max \quad & \left\{ \frac{n}{2} + \frac{1}{2} e^\top x - n \sum_{ij \in E} (x_i + 1)(x_j + 1) \right\} \\ \text{s.t.} \quad & x \in \{-1,1\}^n \end{aligned}$$

Live demonstration!

Solvers for dense C using Semidefinite Programming

Solvers for dense C using Semidefinite Programming

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

Semidefinite Relaxation

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

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

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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

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

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

Factorization of $X \succeq 0$

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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)

$$\begin{aligned} \max \quad & \sum_{i,j=1}^n C_{ij} v_i^\top v_j \\ \text{s. t.} \quad & \|v_i\| = 1, \; i = 1, \dots, n \end{aligned} \qquad \text{(SDP-vec)}$$

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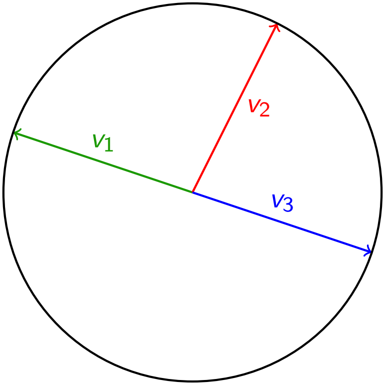
- (SDP) $\Leftrightarrow$ (SDP-vec) for $k > \sqrt{2n}$ [cf. Pataki, 1998]

Geometric Interpretation

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



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Coordinate Ascent

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

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

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

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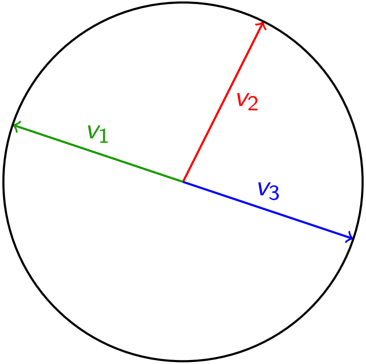
where $g = \sum_j^n c_{ij} v_j = V \cdot c_i$

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

Mixing Method (Wang el al., 2018)



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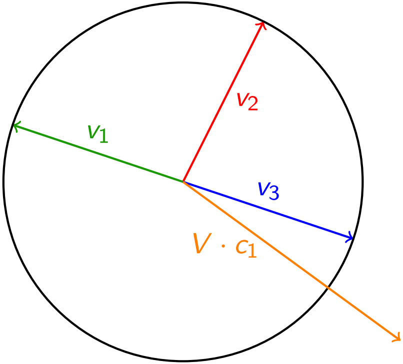

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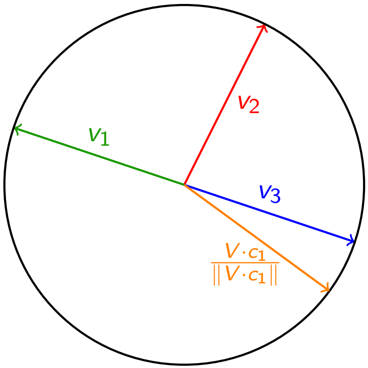

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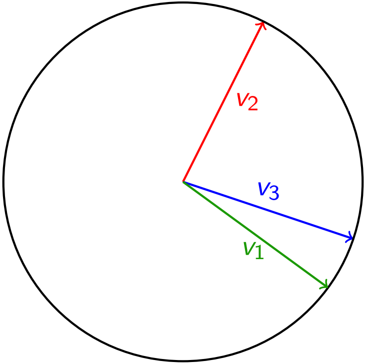

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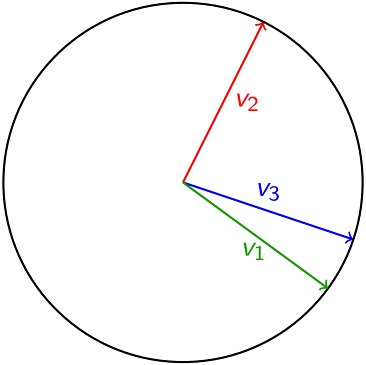

Mixing Method

- repeat for $v_1, v_2, \ldots, v_n$ again and again
- initialize $v_1, \ldots, v_n$ randomly on the unit sphere

Algorithm: Mixing Method

Algorithm 1: Mixing Method (Wang et al., 2018)

Input: $C = (c_1|\dots|c_n) \in \mathbb{R}^{n\times n}$ with $\operatorname{diag}(C) = 0$, $k \in \mathbb{N}_{\geq 1}$
Output: approximate solution $V = (v_1|\dots|v_n) \in \mathbb{R}^{k\times n}$ of (SDP-vec)

for $i \leftarrow 1$ **to** n **do**
  $v_i \leftarrow$ random vector on the unit sphere $\mathcal{S}^{k-1}$;

while *not yet converged* **do**
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- objective value is strictly increasing
- value increases by $2(\|g\| - v_i^\top g)$ for each update $g = V \cdot c_i$

Stopping criteria

δ

Let $\delta \in \mathbb{R}_+$ denote the accumulated improvement of the objective during the last execution of the **while** loop.

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Function tolerance

- stop **if** $\delta < \texttt{tol\_delta\_abs}$
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We use

- $\texttt{tol\_delta\_abs} = \texttt{tol\_delta\_rel} = \texttt{tol\_V\_abs} = 0$
- $\texttt{tol\_V\_rel} = 0.013$

Upper bounds via weak duality

Duality

$$\begin{aligned} \max \quad & \langle C, X \rangle \\ \text{s. t.} \quad & \operatorname{diag}(X) = e \\ & X \succeq 0 \end{aligned} \tag{SDP}$$

$$\begin{aligned} \min \quad & e^\top y \\ \text{s. t.} \quad & \operatorname{Diag}(y) - C \succeq 0 \\ & y \in \mathbb{R}^n \end{aligned} \tag{DSDP}$$

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Proposition [Wang et al., 2018]

Assume that $\operatorname{diag}(C) = 0$. If V^* is optimal for (SDP-vec), then the vector $y^* \in \mathbb{R}^n$ with entries $y_i^* = \|V \cdot c_i\|_2$ is optimal for (DSDP).

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After stopping the Mixing Method with approximate $\tilde{V}$:

- approximate but non-feasible dual variables: $\tilde{y}_i = \|\tilde{V} \cdot c_i\|_2$

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After stopping the Mixing Method with approximate $\tilde{V}$:

- approximate but non-feasible dual variables: $\tilde{y}_i = \|\tilde{V} \cdot c_i\|_2$
- feasible dual variables: $y = \tilde{y} - \lambda_{\min}(\operatorname{Diag}(\tilde{y}) - C)\, e$

Other possibility

We use the dual bound

$$e^\top \tilde{y} - n\lambda_{\min}\left(\mathrm{Diag}(\tilde{y}) - C\right).$$

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Better upper bound [Jansson et al., 2007]

Let $\tilde{y} \in \mathbb{R}^n$ and $\bar{x}$ such that $\lambda_{\max}(X) \leq \bar{x}$ for some optimal X of (SDP). Then

$$e^\top \tilde{y} - \sum_{\lambda_k(\mathrm{Diag}(\tilde{y}) - C) < 0} \lambda_k \bar{x}$$

is an upper bound on (SDP).

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We use the dual bound

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$$e^\top \tilde{y} - \sum_{\lambda_k(\mathrm{Diag}(\tilde{y})-C)<0} \lambda_k \bar{x}$$

is an upper bound on (SDP).

- slightly better bounds
- but: computing $\bar{x}$ requires another eigenvalue computation

Branch-and-Bound

Branching:

- we branch on products X_{ij} (like in *BiqMac*)
- branching on $X_{n-1,n}$ results in $C' \in \mathbb{R}^{(n-1)\times(n-1)}$ with entries

$$c'_{ij} = \begin{cases} c_{ij} & 1 \leq i,j \leq n-1 \\ c_{i,n-1} \pm c_{in} & 1 \leq i < n-1,\ j = n-1 \\ c_{n-1,j} \pm c_{n,j} & i = n-1,\ 1 \leq j < n-1 \\ c_{n-1,n-1} \pm 2c_{n-1,n} + c_{n,n} & i = j = n-1 \end{cases}$$

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- best-first search (largest upper bound)

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- we branch on products X_{ij} (like in *BiqMac*)
- branching on $X_{n-1,n}$ results in $C' \in \mathbb{R}^{(n-1)\times(n-1)}$ with entries

$$c'_{ij} = \begin{cases} c_{ij} & 1 \leq i, j \leq n-1 \\ c_{i,n-1} \pm c_{in} & 1 \leq i < n-1,\ j = n-1 \\ c_{n-1,j} \pm c_{n,j} & i = n-1,\ 1 \leq j < n-1 \\ c_{n-1,n-1} \pm 2c_{n-1,n} + c_{n,n} & i = j = n-1 \end{cases}$$

- best-first search (largest upper bound)

Bounding:

- primal (lower) bounds via heuristics
- dual (upper) bounds like discussed before

Branching Example

$$C = \begin{pmatrix} 2 & -1 & 3 & -2 \\ -1 & -1 & 1 & 2 \\ 3 & 1 & 1 & -1 \\ -2 & 2 & -1 & 1 \end{pmatrix}$$

Branching on $(2,3)$ with $X_{23} = x_2 \cdot x_3 = 1$:

$$\begin{pmatrix} 2 & -1+3 & 3 & -2 \\ -1+3 & -1+1+2\cdot 1 & 1 & 2-1 \\ 3 & 1 & 1 & -1 \\ -2 & 2-1 & -1 & 1 \end{pmatrix} \xrightarrow[\text{row/column 3}]{\text{remove}} C' = \begin{pmatrix} 2 & 2 & -2 \\ 2 & 2 & 1 \\ -2 & 1 & 1 \end{pmatrix}$$

Branching on $(2,3)$ with $X_{23} = x_2 \cdot x_3 = -1$:

$$\begin{pmatrix} 2 & -1-3 & 3 & -2 \\ -1-3 & -1+1-2\cdot 1 & 1 & 2+1 \\ 3 & 1 & 1 & -1 \\ -2 & 2+1 & -1 & 1 \end{pmatrix} \xrightarrow[\text{row/column 3}]{\text{remove}} C' = \begin{pmatrix} 2 & -4 & -2 \\ -4 & -2 & 3 \\ -2 & 3 & 1 \end{pmatrix}$$

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  - often: branching on most fractional variable
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1. Find $i = \operatorname{argmax}_k \{y_k\}$.
2. Find $j = \operatorname{argmax}_k \{(y_i + y_k) \cdot f(X_{ik}) \colon |X_{ik}| \leq 0.875\}$.

- where $f\colon \{-1, 1\} \to [0, 1]$ decreasing in $|X_{ik}|$

Feature: Early branching

Assumption

Finding an optimal solution with heuristics is easy.

Observation

The Mixing Method produces primal feasible iterates for (SDP).

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Early branching

Immediately branch if we have done at least 4 iterations of the **while** loop and we know that the optimal value of (SDP) will be larger than the best known lower bound found by heuristics.

Feature: Variable fixing

Given: Dual feasible solution $\mathrm{Diag}(y) - C \succeq 0$ for $C \in \mathbb{R}^{n \times n}$.

Notation

- $C_{/j}$ denotes matrix C without row j and column j.
- $y_{/j}$ denotes vector y without entry j.

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Branching on $(1, j)$ would yield cost matrix $\tilde{C} \in \mathbb{R}^{(n-1)\times(n-1)}$ with $C_{/j} - \tilde{C} = \begin{pmatrix} 0 & \delta^\top \\ \delta & 0 \end{pmatrix}$ for some $\delta \in \mathbb{R}^{n-2}$.

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Lemma

$$\tilde{y} := y_{/j} + \begin{pmatrix} \|\delta\|_1 \\ |\delta_1| \\ \vdots \\ |\delta_{n-2}| \end{pmatrix}$$ is dual feasible, i.e., $\mathrm{Diag}(\tilde{y}) - \tilde{C} \succeq 0$.

Proof.

$$\operatorname{Diag}(\tilde{y}) - \tilde{C} = \operatorname{Diag}\left(y_{/j} + \begin{pmatrix} \|\delta\|_1 \\ |\delta_1| \\ \vdots \\ |\delta_{n-2}| \end{pmatrix} \right) - \left(C_{/j} - \begin{pmatrix} 0 & \delta^\top \\ \delta & 0 \end{pmatrix} \right)$$

$$= \operatorname{Diag}\left(y_{/j}\right) + \operatorname{Diag}\left(\begin{pmatrix} \|\delta\|_1 \\ |\delta_1| \\ \vdots \\ |\delta_{n-2}| \end{pmatrix} \right) - C_{/j} + \begin{pmatrix} 0 & \delta^\top \\ \delta & 0 \end{pmatrix}$$

$$= \underbrace{\operatorname{Diag}\left(y_{/j}\right) - C_{/j}}_{\succeq 0} + \underbrace{\operatorname{Diag}\left(\begin{pmatrix} \|\delta\|_1 \\ |\delta_1| \\ \vdots \\ |\delta_{n-2}| \end{pmatrix} \right) + \begin{pmatrix} 0 & \delta^\top \\ \delta & 0 \end{pmatrix}}_{\succeq 0} \succeq 0$$

□

Variable fixing

- bound at current node: $e^\top y$

'Free' dual bound if we would branch

Dual bound after branching on (i, j): $e^\top \tilde{y} + 2\|\delta\|_1 \pm 2c_{ij}$.

- difference of bounds: $-y_j + 2\sum_{k\neq i,j} |c_{jk}| \pm 2c_{ij}$

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- check all $\mathcal{O}(n^2)$ candidates in $\mathcal{O}(n^2)$ time
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Issue

Conflict with early branching (no dual feasible solution)!

Primal heuristic

Algorithm 2: Goemans-Williamson hyperplane rounding

Input: $V = (v_1, \dots, v_n) \in \mathbb{R}^{k \times n}$ (such that $V^\top V = X$)
Output: $x \in \{-1, 1\}^n$ (feasible solution for QUBO/Max-Cut)

$h \leftarrow$ random vector on the unit sphere $\mathcal{S}^{k-1}$;
for $i \leftarrow 1$ **to** n **do**

$$x_i \leftarrow \begin{cases} +1, & \text{if } h^\top v_i \geq 0 \\ -1, & \text{otherwise} \end{cases}$$

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- 'good' hyperplane idea