January 26, 2023

An Exact Solver for QUBO Problems using the Mixing Method

Joint work with Valentin Durante

FWF Der Wissenschaftsfonds.

UNIVERSITÄT KLAGENFURT

Modeling - Analysis - Optimization DOC.FUNDS DOCTORAL SCHOOL

Quadratic Unconstrained Binary Optimization (QUBO)

- goal: branch-and-bound solver for

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

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

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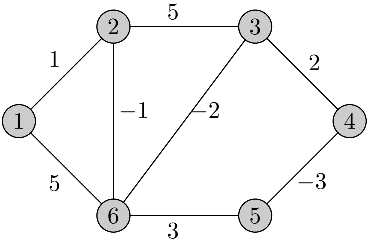
Example

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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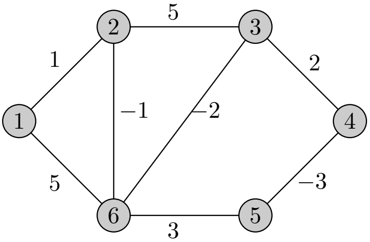

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Find a maximum cut in G, i.e., an optimal solution of

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

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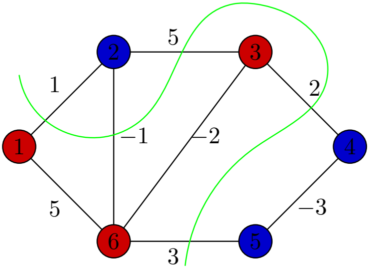

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(QUBO) is quite general...

- minimization $\leftrightarrow$ maximization
- linear quadratic objective $x^\top Qx + q^\top x$
- variables in $\{0,1\}^n \leftrightarrow \{-1,1\}^n$
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Linearly constrained binary quadratic problems

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

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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- Any BQP instance in n variables can be reformulated as a QUBO instance in $n+1$ variables!

Example: Exact Penalty Function

- undirected, simple graph $G = (V, E)$ with $|V| = n$

Maximum Stable Set Problem

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

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Reformulation of (MSSP)

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

Semidefinite Relaxation of (QUBO)

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

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

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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 (SDP)

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All solvers in the literature use additional 'clique' inequalities:

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

(QUBO) Solvers using Semidefinite Programming

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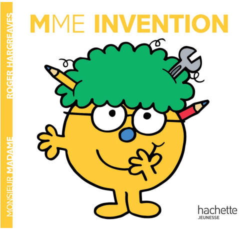	

Low-rank Factorization

Factorization of $X \succeq 0$

$$X = V^\top V \succeq 0$$

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]

Coordinate Ascent Method

Optimization Problem (SDP-vec)

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Coordinate Ascent

We fix all but one column 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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- closed-form solution: $v_i = \frac{g}{\|g\|}$ for $g \neq 0$

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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Theorem (Wang et al., 2018)

The Mixing Method converges linearly to the global optimum under a non-degeneracy assumption.

Example with $n = 4$ and $k = 2$

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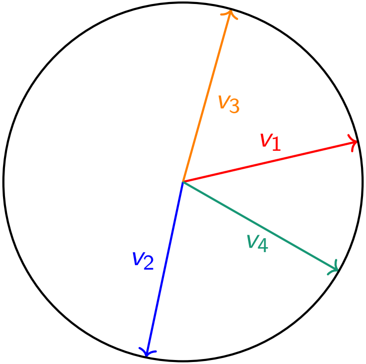

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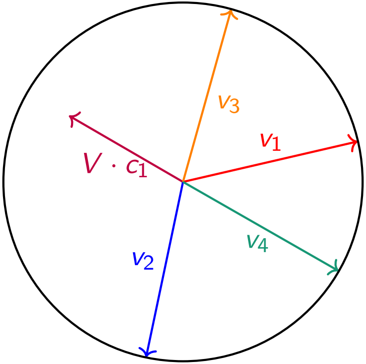

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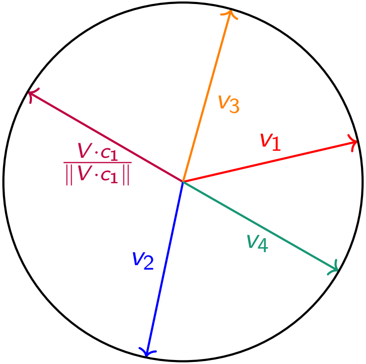

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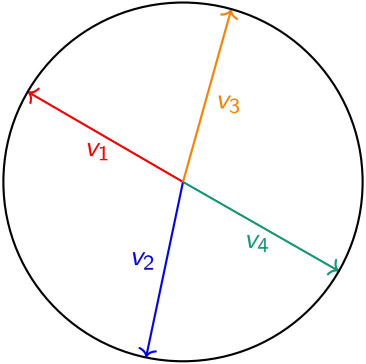

$$\langle C, V^\top V \rangle = 0.0701836938398076$$

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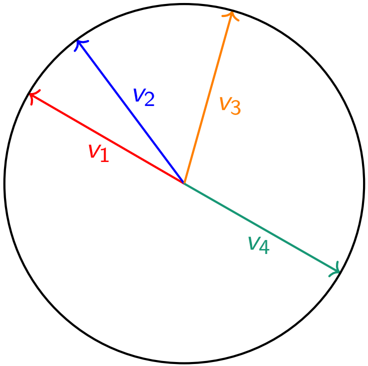

$$\langle C, V^\top V \rangle = 2.1042821481042009$$

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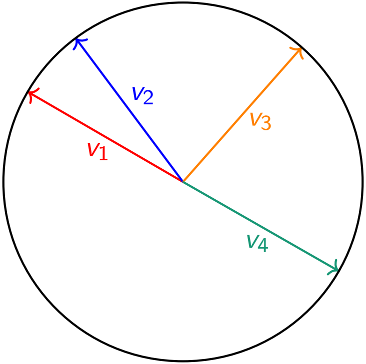

$$\langle C, V^\top V \rangle = 2.1248497956082537$$

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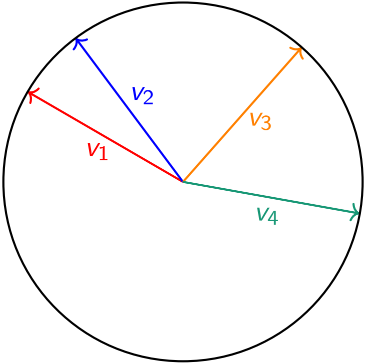

$$\langle C, V^\top V\rangle = 2.2584781813631301$$

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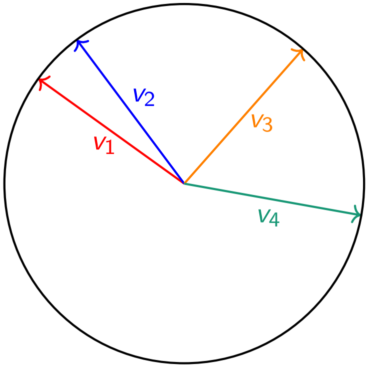

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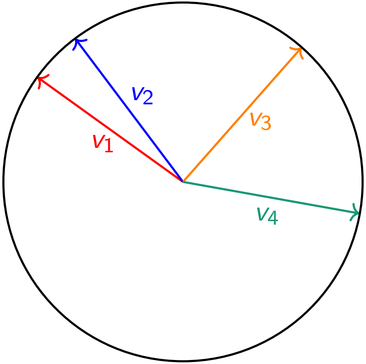

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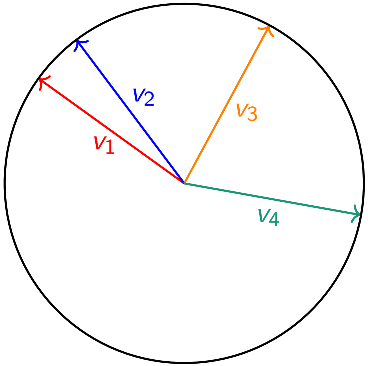

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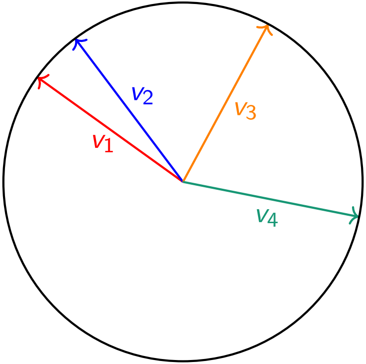

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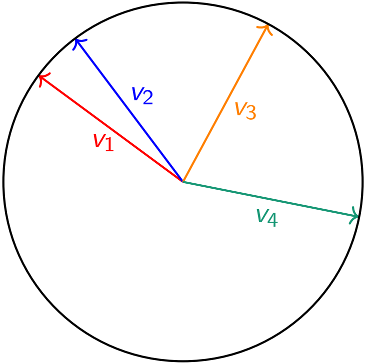

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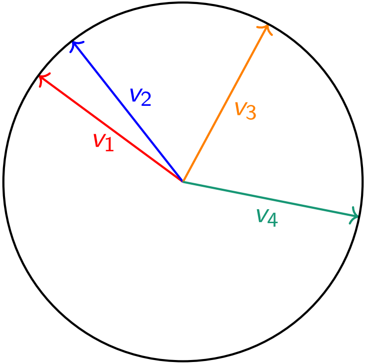

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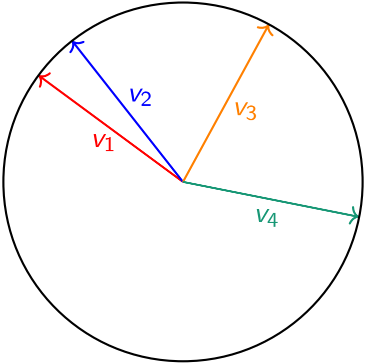

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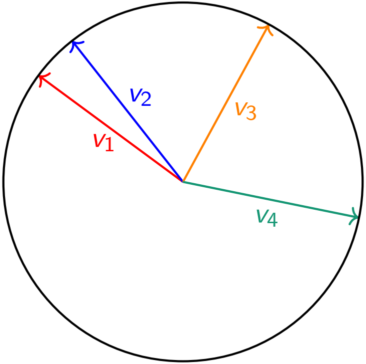

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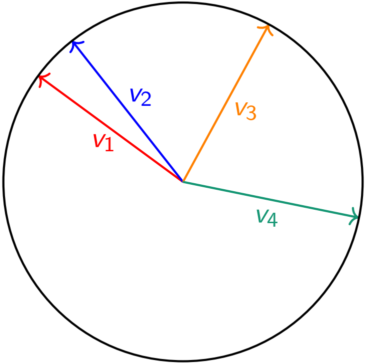

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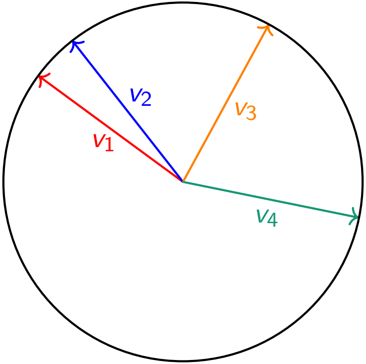

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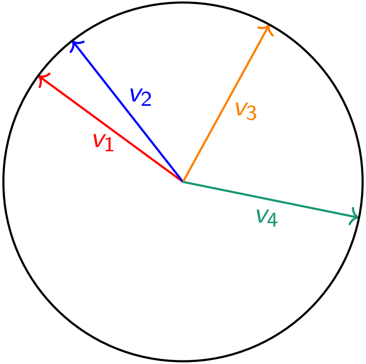

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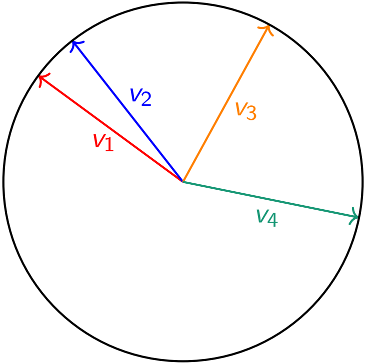

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- parameter-free and easy to implement
- objective value is strictly increasing
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How do we get an upper bound?

Upper Bounds via Weak Duality

Duality

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

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

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Proposition [Wang et al., 2018]

If V and $X = V^\top V$ are optimal for (SDP-vec) and (SDP), 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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- approximate but non-feasible dual variables: $\tilde{y}_i = \|\tilde{V} \cdot c_i\|_2$
- feasible dual variables: $y = \tilde{y} - \lambda_{\min}\left(\operatorname{Diag}(\tilde{y}) - C\right) e$

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

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- slightly better bounds
- more expensive

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: $x \in \{-1, 1\}^n$

$h \leftarrow$ 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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- local search to improve the solution (one-opt and two-opt)
- detect reasonable candidates for local search
- use a 'good'/biased hyperplane

Branch-and-Bound Algorithm

Branching:

- branching on products $X_{ij} \in \{-1, 1\}$
- branch on (i, j) where sum of dual variables is large
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Features:

- early branching
- variable fixing

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 $X_{23} = x_2 \cdot x_3 = 1$:

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

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- SDP approaches in literature only use X for branching decision
  - often: branching on most fractional variable
  - some solvers branch in first row/column only

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1. Find $i = \text{argmax}_k \{y_k\}$.
2. Find $j = \text{argmax}_k \{(y_i + y_k) \cdot f(X_{ik}) \colon |X_{ik}| \leq 0.875\}$.

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

Feature: Early Branching

Assumption

Finding an optimal solution with heuristics is easy.

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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.

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

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

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

□

Variable Fixing

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

'Free' dual bound if we would branch

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

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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)!

Preliminary Results

- C implementation using Intel MKL
- tested on instances from the *BiqMac Library* with $n \leq 100$

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- 100–1000 times more subproblems than other approaches
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Current goal: including *triangle inequalities*

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Lagrangian Relaxation

(SDP) with triangle inequalities $\langle A_i, X \rangle \leq b_i,\ i = 1, \ldots, m$:

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