



Integer Semidefinite Programming for the Quadratic Minimum Spanning Tree Problem

Joint work with Frank de Meijer, Melanie Siebenhofer, and Renata Sotirov.

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Angelika Wiegele

Alpen-Adria-Universität Klagenfurt

January 13, 2025



Goal

Compute lower bounds for the quadratic minimum spanning tree problem

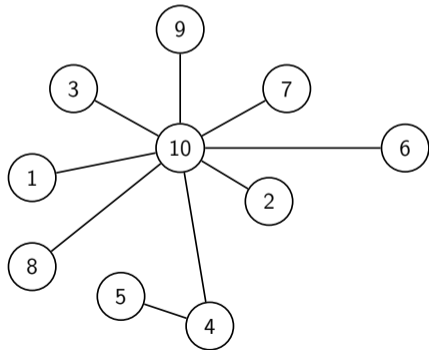
Goal

Compute lower bounds for the quadratic minimum spanning tree problem

- ▶ Quadratic minimum spanning tree problem
- ▶ Two exact integer semidefinite programming formulations
- ▶ Doubly Non-Negative Relaxation + Chvátal–Gomory cuts
- ▶ Facial reduction
- ▶ Peaceman–Rachford splitting method

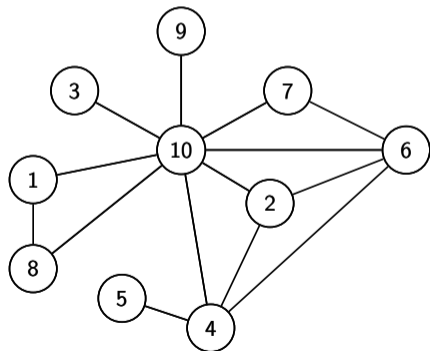
Quadratic minimum spanning tree

tree: connected acyclic graph



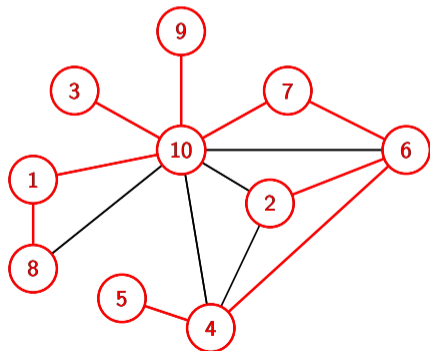
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tree: connected acyclic graph
spanning tree: subgraph, tree, spanning over all vertices



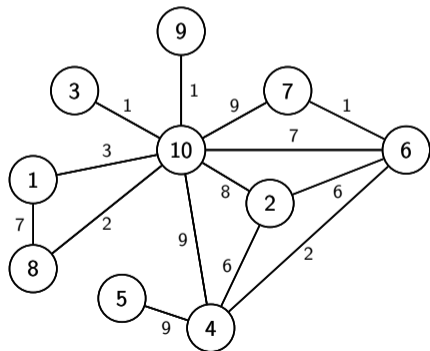
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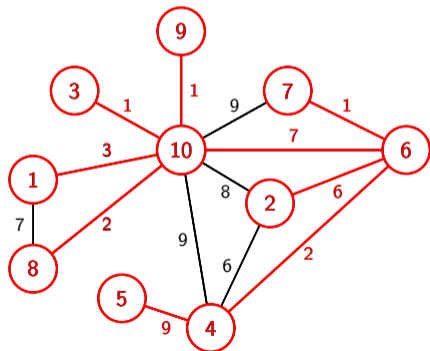
Quadratic minimum spanning tree

- tree:* connected acyclic graph
- spanning tree:* subgraph, tree, spanning over all vertices
- minimum spanning tree:* spanning tree with minimum edge weight



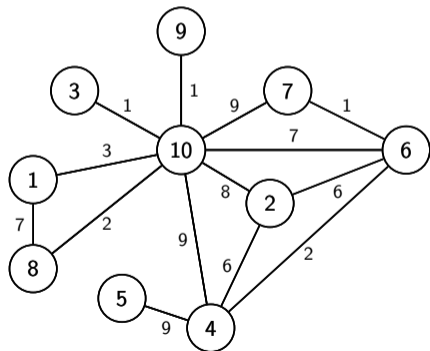
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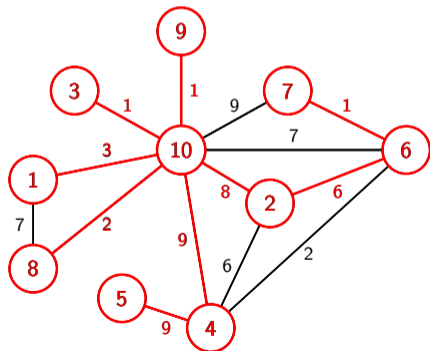
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- quadratic minimum spanning tree*: spanning tree minimizing pairwise edge costs



$$Q = \begin{pmatrix} 7 & 6 & 7 & 9 & 1 & 4 & 6 & 5 & 5 & 8 & 7 & 3 & 2 & 4 \\ 6 & 3 & 9 & 4 & 3 & 8 & 4 & 1 & 3 & 3 & 3 & 4 & 6 & 7 \\ 7 & 9 & 6 & 3 & 5 & 6 & 9 & 7 & 2 & 5 & 8 & 5 & 5 & 8 \\ 9 & 4 & 3 & 6 & 1 & 5 & 8 & 8 & 3 & 5 & 6 & 8 & 2 & 2 \\ 1 & 3 & 5 & 1 & 8 & 5 & 5 & 4 & 5 & 1 & 2 & 6 & 4 & 5 \\ 4 & 8 & 6 & 5 & 5 & 1 & 7 & 3 & 7 & 5 & 8 & 8 & 2 & 3 \\ 6 & 4 & 9 & 8 & 5 & 7 & 9 & 3 & 1 & 2 & 9 & 6 & 6 & 2 \\ 5 & 1 & 7 & 8 & 4 & 3 & 3 & 2 & 9 & 9 & 5 & 3 & 8 & 6 \\ 5 & 3 & 2 & 3 & 5 & 7 & 1 & 9 & 9 & 5 & 2 & 7 & 3 & 8 \\ 8 & 3 & 5 & 5 & 1 & 5 & 2 & 9 & 5 & 1 & 7 & 8 & 8 & 5 \\ 7 & 3 & 8 & 6 & 2 & 8 & 9 & 5 & 2 & 7 & 7 & 3 & 1 & 5 \\ 3 & 4 & 5 & 8 & 6 & 8 & 6 & 3 & 7 & 8 & 3 & 9 & 5 & 2 \\ 2 & 6 & 5 & 2 & 4 & 2 & 6 & 8 & 3 & 8 & 1 & 5 & 2 & 2 \\ 4 & 7 & 8 & 2 & 5 & 3 & 2 & 6 & 8 & 5 & 5 & 2 & 2 & 1 \end{pmatrix}$$

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QMSTP: Binary formulation

- ▶ $G = (V, E)$, $|V| = n$, $|E| = m$
- ▶ vector $x \in \{0, 1\}^m$ representing a spanning tree

$$x_e = \begin{cases} 1 & e \in E(T), \\ 0 & \text{else.} \end{cases}$$

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i characterization tree

- 1** $n - 1$ edges $\sum x_e = n - 1$
- 2** connected $\sum_{e \in \partial(S)} x_e \geq 1 \quad \forall S \subsetneq V, S \neq \emptyset$

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- ▶ cut induced by $S \subseteq V$: $\partial(S) = \{\{i, j\} \in E \mid i \in S, j \notin S\}$

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$$\min_{x \in \mathcal{T}} \sum_{e \in E} \sum_{f \in E} q_{ef} \cdot x_e \cdot x_f$$

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i QMSTP is NP-hard

Mixed-Integer Programming Problem

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⇒ linearize objective

$$x_e \cdot x_f = y_{ef}, Y \in \mathcal{S}^m$$

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- ⇨ linearize objective
- ⇨ couple x and Y

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Mixed-Integer Programming Problem [Arjang Assad and Weixuan Xu (1995)]

$$\min \langle Q, Y \rangle$$

$$\text{s.t. } \text{diag}(Y) = x, Ye_m = (n-1)x$$

$$0 \leq Y \leq 1, Y \in \mathcal{S}^m, x \in \mathcal{T}$$

Connectivity constraint

▶ $\sum_{e \in \partial(S)} x_e \geq 1 \quad \forall S \subsetneq V, S \neq \emptyset \quad \dots \quad \text{cut-set constraints}$

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➡ $2^{n-1} - 1$ constraints ☹

i Laplacian matrix L of a graph $G = (V, E)$ is a matrix of dimension $n \times n$ with

$$(L)_{i,j} = \begin{cases} -1 & \{i,j\} \in E, \\ d(i) & i = j, \\ 0 & \text{else.} \end{cases}$$

Connectivity constraint

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- ❶ algebraic connectivity of trees

$$2\left(1 - \cos\left(\frac{\pi}{n}\right)\right) \leq \lambda_2(L) \leq 1$$

algebraic connectivity of a path: $2\left(1 - \cos\left(\frac{\pi}{n}\right)\right)$

algebraic connectivity of a star: 1

Theorem (de Meijer, Siebenhofer, Sotirov, W., 2024⁺)

Let G be a graph with $n \geq 3$ vertices and $n - 1$ edges and let $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq \frac{\beta}{n}$ and $0 < \beta \leq 2\left(1 - \cos\left(\frac{\pi}{n}\right)\right)$. Then

$$G \text{ is a tree} \iff L + \alpha J_n - \beta I_n \succeq 0.$$

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➔ linear matrix inequality ☺

Integer Semidefinite Programming formulation (1)

From $x \in \{0, 1\}^m$ to Laplacian matrix L ?

⇒ adjacency matrix from x

$$\mathcal{A}(x)_{ij} = \begin{cases} x_{\{i,j\}} & \{i,j\} \in E \\ 0 & \text{else} \end{cases}$$

Integer Semidefinite Programming formulation (1)

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$$\text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x)$$

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$$L + \alpha J_n - \beta I_n \succeq 0 \iff \text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x) + \alpha J_n - \beta I_n \succeq 0$$

Integer Semidefinite Programming formulation (1)

ISDP (1)

$$\min \langle Q, Y \rangle$$

$$\text{s.t. } e_m^\top x = (n - 1)$$

$$\text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x) + \alpha J_n - \beta I_n \succeq 0$$

$$Ye_m = (n - 1)x$$

$$0 \leq Y \leq 1, Y \in \mathcal{S}^m, x \in \{0, 1\}^m$$

Integer Semidefinite Programming formulation (2)

Lemma (Laurent & Poljak (1995), Helmberg (2000))

Let $x \in \{0, 1\}^m$, $Y \in \mathcal{S}^m$ with $\text{diag}(Y) = x$ and $Y - xx^\top \succeq 0$, then $Y = xx^\top$.

Integer Semidefinite Programming formulation (2)

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$$\text{s.t. } e_m^\top x = (n - 1)$$

$$\text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x) + \alpha J_n - \beta I_n \succeq 0$$

$$\text{diag}(Y) = x$$

$$\begin{pmatrix} Y & x \\ x^\top & 1 \end{pmatrix} \succeq 0$$

$$Y \in \mathcal{S}^m, x \in \{0, 1\}^m$$

Chvátal–Gomory cuts

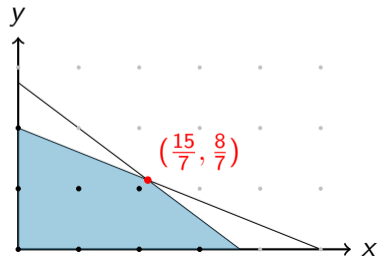
... in integer programming

$$\max x + 2y$$

$$\text{s.t. } 3x + 4y \leq 11$$

$$2x + 5y \leq 10$$

$$x, y \in \mathbb{Z}_{\geq 0}$$



Chvátal–Gomory cuts

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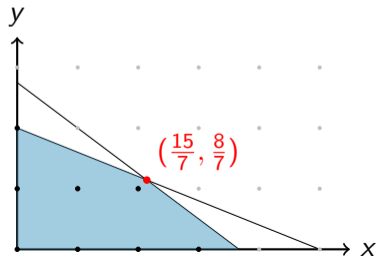
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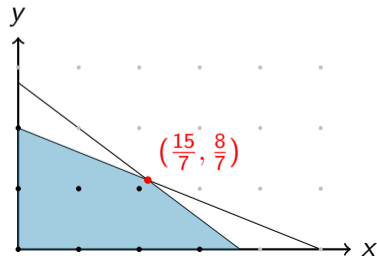
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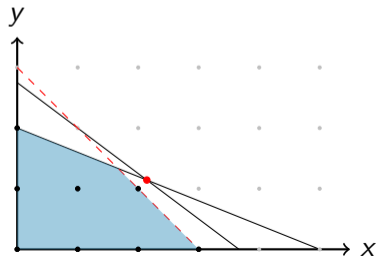
$$x + y \leq 3$$

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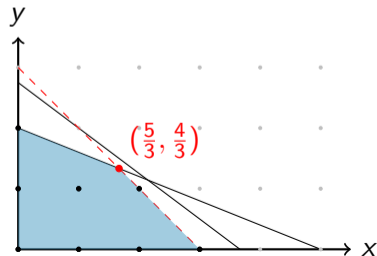
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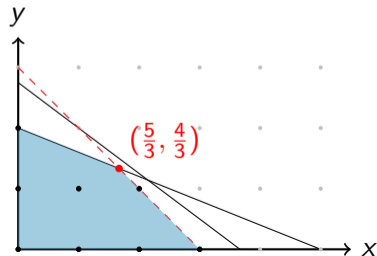
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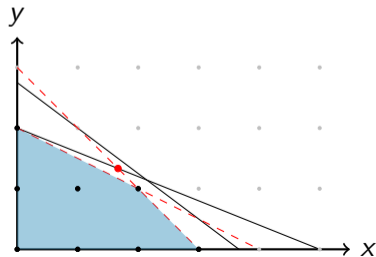
$$x + y \leq 3$$

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$$x + 2y \leq \left\lfloor \frac{13}{3} \right\rfloor$$



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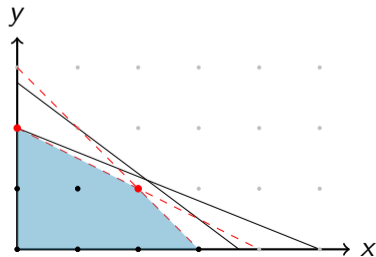
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Chvátal–Gomory cuts

... in integer semidefinite programming

$$\mathbf{i} \quad A, B \succeq 0 \Rightarrow \langle A, B \rangle \geq 0$$

Chvátal–Gomory cuts

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i $A, B \succeq 0 \Rightarrow \langle A, B \rangle \geq 0$

- X ... feasible adjacency for ISDP formulations (1) and (2)
- let $S \subsetneq V$, $S \neq \emptyset$, and $\mathbb{1}_S$ its indicator vector

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➤ $\langle \mathbb{1}_S \mathbb{1}_S^\top, \text{Diag}(X e_n) - X + \alpha J_n - \beta I_n \rangle \geq 0$

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$$\begin{aligned} \langle \mathbb{1}_S \mathbb{1}_S^\top - \mathbb{1}_S e_n^\top, X \rangle &\leq \left[\langle \mathbb{1}_S \mathbb{1}_S^\top, \alpha J_n - \beta I_n \rangle \right] \\ &= \sum_{i \in S} \sum_{j \notin S} X_{ij} \leq \lfloor |S|(|S|\alpha - \beta) \rfloor \end{aligned}$$

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$$- \sum_{i \in S} \sum_{j \notin S} x_{ij} \leq \lfloor |S|(|S|\alpha - \beta) \rfloor$$

$$\sum_{e \in \partial(S)} x_e \geq 1 \quad \dots \text{ cut-set constraint}$$

Chvátal–Gomory cuts

Proposition (de Meijer, Siebenhofer, Sotirov, W., 2024⁺)

Let $S \subsetneq V$, $S \neq \emptyset$. Then the cut-set constraint

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is a Chvátal–Gomory cut with respect to the integer semidefinite programming formulations (1) and (2).

Proposition (de Meijer, Siebenhofer, Sotirov, W., 2024⁺)

Let $S \subsetneq V$, $S \neq \emptyset$. Then the constraints

$$\sum_{e \in \partial(S)} y_{ef} \geq x_f \quad \forall f \in E$$

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Positive Semidefinite Matrices

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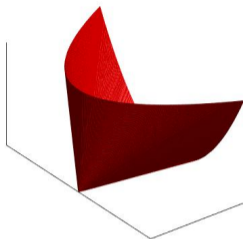
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Example of a positive semidefinite matrix: $X = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$

Positive Semidefinite Matrices

Let $n = 2$ and $X = \begin{pmatrix} x & y \\ y & z \end{pmatrix}$.

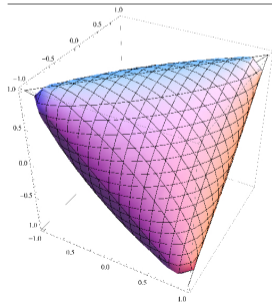
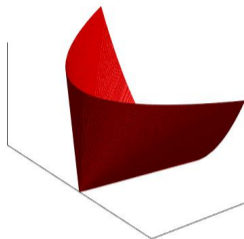
$$X \succeq 0 \iff \begin{cases} x \geq 0, \\ z \geq 0, \\ xz - y^2 \geq 0. \end{cases}$$



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Elliptope $\mathcal{E}_3 = \{X \in \mathcal{S}^3:$
 $X_{ii} = 1, i \in \{1, 2, 3\},$
 $X \succeq 0\}$

$$X \in \mathcal{E}_3 \implies X = \begin{pmatrix} 1 & x & y \\ x & 1 & z \\ y & z & 1 \end{pmatrix}$$

Semidefinite Programming

Linear Program

$$(LP) \begin{cases} \min & c^T x \\ \text{s.t.} & Ax = b \\ & x \geq 0, x \in \mathbb{R}^n \end{cases}$$

Semidefinite Program

$$(SDP) \begin{cases} \min & \langle C, X \rangle \\ \text{s.t.} & \mathcal{A}X = b \\ & X \succeq 0, X \in \mathcal{S}^n \end{cases}$$

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- ▶ Strong duality does not hold in general!
- ▶ Slater conditions guarantees strong duality,
- ▶ solvable in polynomial time.

Integer Semidefinite Programming formulation (1) and (2)

$$\min \langle Q, Y \rangle$$

$$\text{s.t. } e_m^\top x = (n-1)$$

$$\text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x) + \alpha J_n - \beta I_n \succeq 0$$

$$Ye_m = (n-1)x$$

$$0 \leq Y \leq 1, Y \in \mathcal{S}^m, x \in \{0, 1\}^m$$

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$$\begin{pmatrix} Y & x \\ x^\top & 1 \end{pmatrix} \succeq 0, Y \in \mathcal{S}^m, x \in \{0, 1\}^m$$

Doubly Non-Negative (DNN) Relaxation with CG-cuts

... derived from the integer SDP formulations (1) and (2)

$$\begin{aligned} \min \quad & \langle Q, Y \rangle \\ \text{s.t.} \quad & e_m^\top x = (n-1) \\ & \text{Diag}(\mathcal{A}(x)e_n) - \mathcal{A}(x) + \alpha J_n - \beta I_n \succeq 0 \\ & Ye_m = (n-1)x \\ & \text{diag}(Y) = x \\ & \begin{pmatrix} Y & x \\ x^\top & 1 \end{pmatrix} \succeq 0, \quad Y \geq 0 \end{aligned}$$

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Facial Reduction

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\leftrightarrow

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$\tilde{Y} v = 0$ for every feasible \tilde{Y}

→ apply facial reduction

Facial Reduction

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$$\text{s.t. } \tilde{Y} \begin{pmatrix} e_m \\ -(n-1) \end{pmatrix} = 0$$

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- ▶ positive semidefiniteness constraint on R
- ▶ linear constraints on $\tilde{Y} = WRW^T$
- ➔ split variables into 2 parts

$$\begin{aligned} \min \quad & \langle \tilde{Q}, WRW^T \rangle \\ \text{s.t.} \quad & \text{diag}(WRW^T) = WRW_{:,m+1}^T \\ & WRW_{m+1,m+1}^T = 1 \\ & WRW^T \succeq 0 \\ & R \succeq 0 \end{aligned}$$

The Peaceman–Rachford splitting method (PRSM)

$$\mathcal{Y} = \left\{ \tilde{Y} \in \mathcal{S}^{m+1} : \tilde{Y} = \begin{pmatrix} Y & x \\ x^\top & 1 \end{pmatrix}, \text{diag}(Y) = x, 0 \leq \tilde{Y} \leq 1, \text{tr}(\tilde{Y}) = n \right\}$$
$$\mathcal{R} = \{R \in \mathcal{S}^m : R \succeq 0, \text{tr}(R) = n\}$$

Doubly Non-Negative Relaxation

$$\begin{aligned} \min \quad & \langle \tilde{Q}, \tilde{Y} \rangle \\ \text{s.t.} \quad & \tilde{Y} = WRW^\top \\ & \tilde{Y} \in \mathcal{Y}, R \in \mathcal{R} \end{aligned}$$

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Augmented Lagrangian \mathcal{L}_μ

$$\mathcal{L}_\mu(\tilde{Y}, R; S) = \langle \tilde{Q}, \tilde{Y} \rangle + \langle S, \tilde{Y} - WRW^\top \rangle + \frac{\mu}{2} \|\tilde{Y} - WRW^\top\|^2$$

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Algorithm: PRSM for the DNN relaxation of QMST

Initialize (R^0, \tilde{Y}^0, S^0) , μ and γ_1, γ_2 , set $k = 0$;

repeat

$$R^{k+1} =;$$

$$S^{\frac{k+1}{2}} =;$$

$$\tilde{Y}^{k+1} =;$$

$$S^{k+1} =;$$

until convergence;

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$$S^{k+1} = S^{\frac{k+1}{2}} + \gamma_2 \mu (\tilde{Y}^{k+1} - WR^{k+1}W^\top);$$

until convergence;

The Peaceman–Rachford splitting method (PRSM)

$$\mathcal{L}_\mu(\tilde{Y}, R; S) = \langle \tilde{Q}, \tilde{Y} \rangle + \langle S, \tilde{Y} - WRW^\top \rangle + \frac{\mu}{2} \|\tilde{Y} - WRW^\top\|^2$$
$$\mathcal{R} = \{R \in \mathcal{S}^m : R \succeq 0, \text{tr}(R) = n\}$$

$$\begin{aligned} R^{k+1} &= \arg \min_{R \in \mathcal{R}} \mathcal{L}_\mu(\tilde{Y}^k, R, S^k) \\ &= \arg \min_{R \in \mathcal{R}} \langle S^k, -WRW^\top \rangle + \frac{\beta}{2} \|\tilde{Y}^k - WRW^\top\|_F^2 \\ &= \mathcal{P}_{\mathcal{R}}(W^\top(\tilde{Y}^k + \frac{1}{\mu}S^k)W) \end{aligned}$$

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i $M = U\text{Diag}(\lambda)U^\top$... eigenvalue decomposition of M , then

$$\mathcal{P}_{\mathcal{R}}(M) = U\text{Diag}(\mathcal{P}_{\Delta_n}(\lambda))U^\top$$

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→ projecting the eigenvalues onto the n -simplex Δ_n .

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$$\mathcal{Y} = \left\{ \tilde{Y} \in \mathcal{S}^{m+1} : \tilde{Y} = \begin{pmatrix} Y & x \\ x^\top & 1 \end{pmatrix}, \text{diag}(Y) = x, 0 \leq \tilde{Y} \leq 1, \text{tr}(\tilde{Y}) = n \right\}$$

$$\begin{aligned} \tilde{Y}^{k+1} &= \arg \min_{\tilde{Y} \in \mathcal{Y}} \mathcal{L}_\mu(\tilde{Y}, R^{k+1}, S^{\frac{k+1}{2}}) \\ &= \arg \min_{\tilde{Y} \in \mathcal{Y}} \langle \tilde{Q}, \tilde{Y} \rangle + \langle S^{\frac{k+1}{2}}, \tilde{Y} \rangle + \frac{\beta}{2} \|\tilde{Y} - WR^{k+1}W^\top\|_F \\ &= \mathcal{P}_{\mathcal{Y}} \left(WR^{k+1}W^\top - \frac{1}{\mu} (\tilde{Q} + S^{\frac{k+1}{2}}) \right) \end{aligned}$$

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i $\mathcal{P}_{\mathcal{Y}} \left(\begin{pmatrix} Z & z \\ z^\top & \omega \end{pmatrix} \right) = \mathcal{P}_{[0,1]} \left(\begin{pmatrix} Z - \text{Diag}(\text{diag}(Z)) + v & v \\ v^\top & 1 \end{pmatrix} \right), v = \mathcal{P}_{\bar{\Delta}(n-1)} \left(\frac{1}{3} \text{diag}(Z) + \frac{2}{3} z \right)$

Algorithm to compute lower bounds on the QMST

Further ingredients:

- ▶ iteratively add violated cuts
- ▶ projection onto $\mathcal{P}_{\mathcal{Y}_c}$, i.e., the set $\mathcal{Y} + \text{cuts}$, using [Dijkstra's projection algorithm](#)
- ▶ approximate solution of the DNN ➡ post processing

Algorithm to compute lower bounds on the QMST

Input: graph $G = (V, E)$, cost matrix \tilde{Q}

Output: lower bound LB

initialize $\tilde{Y}^0, S^0, \beta, \gamma_1, \gamma_2$, set $\mathcal{C} = \emptyset$;

compute W , e.g., apply QR decomposition to $((n-1)I_m \quad e_m)^\top$;

$k = 0$;

while no stopping criteria met **do**

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$$R^{k+1} = \mathcal{P}_{\mathcal{R}}(W^\top(\tilde{Y}^k + \frac{1}{\beta}S^k)W);$$

$$S^{\frac{k+1}{2}} = S^k + \gamma_1\beta(\tilde{Y}^k - WR^{k+1}W^\top);$$

$$\tilde{Y}^{k+1} = \mathcal{P}_{\mathcal{Y}_{\mathcal{C}}}(WR^{k+1}W^\top - \frac{1}{\beta}(\tilde{Q} + S^{\frac{k+1}{2}}));$$

$$S^{k+1} = S^{\frac{k+1}{2}} + \gamma_2\beta(\tilde{Y}^{k+1} - WR^{k+1}W^\top);$$

$$k = k + 1;$$

 compute a lower bound LB from S^k ;

 separate violated cuts and add the most violated ones to \mathcal{C} ;

 cluster the cuts in \mathcal{C} ;

return LB

	This study				Guimarães et al.	
	DNN		DNN + CUTS		LAGN	
	gap (%)	time (s)	gap (%)	time (s)	gap (%)	time (s)
$n = 10$	4.64	0.08	2.03	9.31	3.78	0.41
$n = 15$	5.54	0.41	4.24	18.77	5.25	4.81
$n = 20$	5.91	1.02	5.32	27.30	6.43	30.64
$n = 25$	7.52	2.32	6.83	35.80	8.72	122.87
$n = 30$	8.66	5.85	8.37	54.10	11.86	358.20
$n = 35$	9.87	7.62	9.68	58.70	15.96	897.69
$n = 40$	11.46	14.34	11.32	68.10	23.53	1597.73
$n = 45$	11.88	27.13	11.78	84.40	27.34	3195.97
$n = 50$	13.08	45.58	13.03	103.22	31.45	6030.00
$d = 33\%$	4.98	1.97	4.02	23.31	4.84	145.89
$d = 67\%$	8.99	7.02	8.17	44.53	14.28	1124.67
$d = 100\%$	12.22	25.79	12.01	85.39	25.65	2808.88

Table: Comparison of averaged results for CP instances.

[1] Dilson A. Guimarães, Alexandre S. da Cunha, and Dilson L. Pereira (2020)

Instance			DNN			DNN + CUTS			
n	m	UB	LB	gap	time (s)	LB	gap	time (s)	iterations
6	15	541.20	421.57	22.10	0.01	499.51	7.70	3.80	279.8
7	21	783.70	568.79	27.42	0.03	743.62	5.11	27.81	526.2
8	28	1020.10	706.73	30.72	0.04	956.62	6.22	55.29	548.3
9	36	1356.00	1113.97	17.85	0.05	1313.50	3.13	74.30	695.3
10	45	1427.10	1044.20	26.83	0.07	1362.01	4.56	118.12	643.2
11	55	1545.10	1122.77	27.33	0.12	1431.81	7.33	223.74	873.6
12	66	1901.60	1420.73	25.29	0.13	1815.21	4.54	432.63	993.1
13	78	2175.30	1684.29	22.57	0.18	2051.16	5.71	430.93	943.8
14	91	2527.90	1911.59	24.38	0.46	2367.42	6.35	720.47	1107.6
15	105	2588.80	2173.45	16.04	0.52	2426.66	6.26	468.08	810.8
16	120	2980.10	2360.16	20.80	1.07	2765.42	7.20	834.69	1214.3
17	136	3372.20	2327.66	30.98	1.00	3165.01	6.14	1933.56	1678.0
18	153	3569.00	2645.32	25.88	1.06	3281.36	8.06	1947.79	1403.7
30	435	8056.70	6114.86	24.10	17.30	7174.26	10.95	10045.11	1244.4
50	1225	15788.80	13030.28	17.47	406.93	13333.52	15.55	10923.68	800.5

Table: Averaged results for OPesym instances.

Summary

- ▶ Quadratic minimum spanning tree problem
- ▶ Exact integer semidefinite programming formulations
- ▶ Relaxation + Chvátal–Gomory cuts
- ▶ Facial reduction
- ▶ Peaceman–Rachford splitting method
- ▶ Code available at Melanie Siebenhofer's github repository <https://github.com/melaniesi/QMST.jl>, paper at <https://arxiv.org/abs/2410.04997>.

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Thank you!

Frank de Meijer (Delft), Melanie Siebenhofer (Klagenfurt), Renata Sotirov (Tilburg)