

A traveling salesman problem with quadratic cost structure

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Outline

Introduction

ILP formulation

Valid inequalities

Semidefinite relaxation

Computational results

Further work

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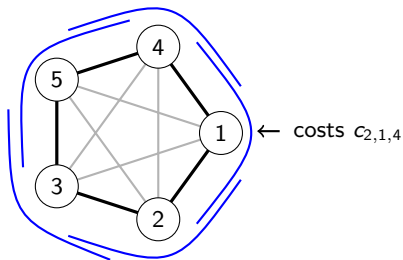
Problem description of QSTSP

Given:

- undirected complete 2-graph $G = (V, E)$, $V = \{1, \dots, n\}$,
 $V^2 := \{\{i, j\} : i, j \in V, i \neq j\}$ (write ij) – arcs
 $V^3 := \{\langle i, j, k \rangle = \langle k, j, i \rangle : i, j, k \in V, |\{i, j, k\}| = 3\}$ (write ijk) – 2-arcs
- cost function $c : V^3 \rightarrow \mathbb{R}_+$ with c_{ijk} – costs of path $i - j - k$,
 \Rightarrow quadratic cost structure

Goal: find tour $T = (i_1, \dots, i_n, i_1)$ minimizing

$$\sum_{k=1}^{n-2} c_{i_k i_{k+1} i_{k+2}} + c_{i_{n-1} i_n i_1} + c_{i_n i_1 i_2}$$



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Problem introduced by G. Jäger and P. Molitor (2008): Complexity and Algorithms for the Traveling Salesman Problem and the Assignment Problem of Second Order

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Application Biology: recognition of transcription factor binding sites in gene regulation – Leibniz Institute of Plant Genetics and Crop Plant Research (Ivo Grosse, Jens Keilwagen)

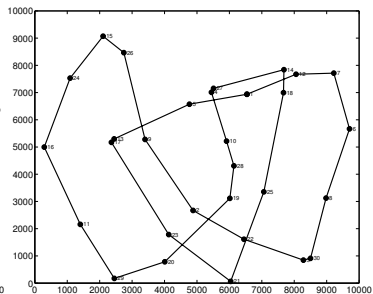
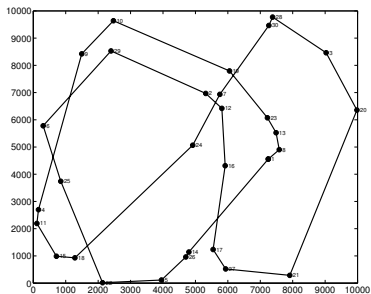
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Special case of QSTSP Angular-Metric TSP, see Aggarwal et al. (1997)
given points in the plane – find tour minimizing total direction changes
applications in robotic

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Special case of **QSTSP** Angular-Metric TSP, see Aggarwal et al. (1997)
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applications in robotic

Complexity NP-complete, even the corresponding cycle cover problem is NP-complete

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Integer Linear Program

Linearization of the following quadratic integer model

$$\min \sum_{ijk \in V^3} c_{ijk} x_{ij} x_{jk}$$

$$\text{s.t. } \sum_{ij \in V^2} x_{ij} = 2, \quad i \in V \quad (\text{degree})$$

$$\sum_{\substack{ij \in V^2 \\ i \in S, j \in V \setminus S}} x_{ij} \geq 2, \quad S \subset V, 2 \leq |S| \leq n - 2 \quad (\text{subtour})$$

$$x_{ij} \in \{0, 1\}, \quad ij \in V^2$$

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y_{ijk}

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$$x_{ij} \in \{0, 1\}, \quad ij \in V^2$$

$$x_{ij} = \sum_{ijk \in V^3} y_{ijk}, \quad ij \in V^2 \quad (\text{flow})$$

$$x_{ij} = \sum_{kij \in V^3} y_{kij}, \quad ij \in V^2 \quad (\text{flow})$$

$$y_{ijk} \in [0, 1], \quad ijk \in V^3$$

Dimension of the polytope P_{QSTSP}

variables: $3\binom{n}{3} + \binom{n}{2}$

equality constraints: $n + 2\binom{n}{2} = n^2$

Observation

The constraint matrix of the QSTSP (degree, flow) has full row rank.

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Regard the Quadratic Symmetric Cycle Cover Polytope P_{QSCCP_n} (subtours are allowed).

Lemma

The dimension of P_{QSCCP_n} equals $3\binom{n}{3} + \binom{n}{2} - n^2$ for $n \geq 7$.

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Conjecture

The dimension of P_{QSTSP_n} equals $3\binom{n}{3} + \binom{n}{2} - n^2$ for $n \geq 7$.

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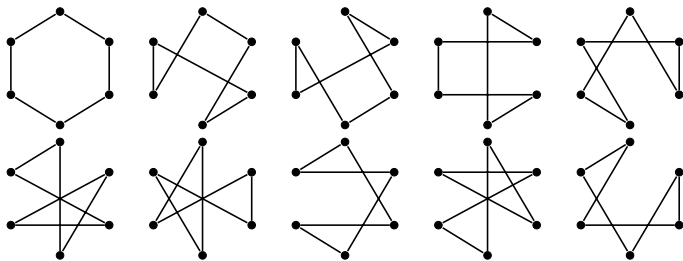
The dimension of P_{QSTSP_n} equals $3\binom{n}{3} + \binom{n}{2} - n^2$ for $n \geq 7$.

For the STSP: Grötschel and Padberg used an arc-disjoint Hamiltonian cycle decomposition of the complete graph G_n .

Dimension of the polytope P_{QSTSP}

Question

Is there a 2-arc-disjoint Hamiltonian cycle decomposition of the complete 2-graph G_n , $n \geq 3$?



Related to an open question (Bailey, Stevens) concerning the decomposition of complete uniform hypergraphs into arc-disjoint Hamiltonian cycles.

Dimension of the polytope P_{QATSP} resp. P_{QACCP_n}

$$\sum_{(j,i) \in V^2} x_{(j,i)} = \sum_{(i,j) \in V^2} x_{(i,j)} = 1, \quad i \in V,$$

$$x_{(i,j)} = \sum_{(i,j,k) \in V^3} y_{(i,j,k)} = \sum_{(k,i,j) \in V^3} y_{(k,i,j)}, \quad (i,j) \in V^2,$$

$$\sum_{\substack{(i,j) \in V^2: \\ i \in S, j \in V \setminus S}} x_{(i,j)} \geq 1, \quad S \subset V, 1 \leq |S| \leq n-1,$$

$$x_{(i,j)} \in \{0, 1\}, y_{(i,j,k)} \in [0, 1], \quad (i,j) \in V^2, (i,j,k) \in V^3$$

$$V^2 = \{(i,j) : i, j \in V, i \neq j\}, V^3 = \{(i,j,k) : i, j, k \in V, |\{i,j,k\}| = 3\}$$

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Lemma

The dimension of P_{QACCP_n} equals $\underbrace{n(n-1)^2}_{\# \text{ variables}} - \underbrace{(2n^2 - 1 - n)}_{\text{rank of constr. matrix}}$ for $n \geq 7$.

Conjecture

The dimension of P_{QATSP_n} equals $n(n-1)^2 - (2n^2 - 1 - n)$ for $n \geq 7$.

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Valid inequalities

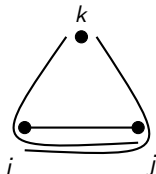
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Valid inequalities

- forbid certain triangles



$$y_{kij} + y_{ijk} \leq x_{ij}$$

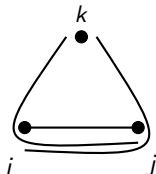
$$x_{ij} + x_{ik} + x_{jk} \leq 2 \mid \cdot x_{ij}$$

lift the constraint

strengthen triangle inequalities of *Boolean Quadratic Polytope* (Padberg, 1989)

Valid inequalities

- forbid certain triangles

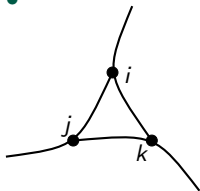


$$y_{kij} + y_{ijk} \leq x_{ij}$$

$$x_{ij} + x_{ik} + x_{jk} \leq 2 \mid \cdot x_{ij} \quad \text{lift the constraint}$$

strengthen triangle inequalities of *Boolean Quadratic Polytope* (Padberg, 1989)

-



Equivalent to:

$$x_{ij} + x_{ik} + x_{jk} - y_{ijk} - y_{ikj} - y_{jik} \leq 1$$

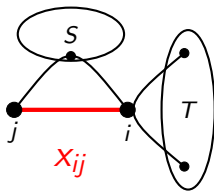
see triangle inequalities of Boolean Quadratic Polytope

conflicting arcs inequalities

At most one of the following variables can be 1:

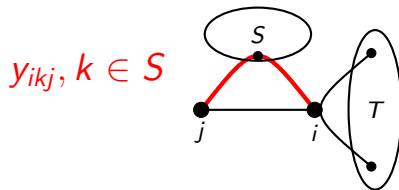
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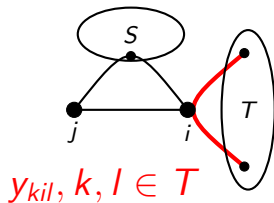
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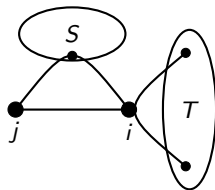
At most one of the following variables can be 1:



conflicting arcs inequalities

$$x_{ij} + \sum_{\substack{ikj \in V^3 \\ k \in S}} y_{ikj} + \sum_{\substack{lim \in V^3 \\ l, m \in T}} y_{lim} \leq 1$$

for all $i, j \in V, i \neq j$, and $S, T \subset V \setminus \{i, j\}, S \cap T = \emptyset$



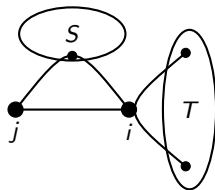
Lemma

The conflicting arcs inequalities can be separated in polynomial time.

conflicting arcs inequalities

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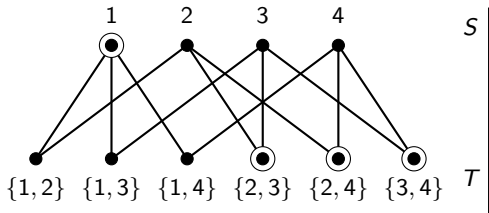
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Lemma

The conflicting arcs inequalities can be separated in polynomial time.

Proof: Transformation to *Maximal Weight Independent Set Problem* in bipartite graphs.

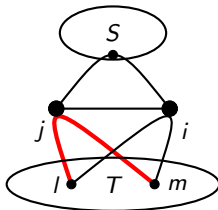


$$n = 6, i = 5, j = 6 : \\ S = \{1\}, T = \{2, 3, 4\}$$

strengthened conflicting arcs constraints

Case $|T| = 2$

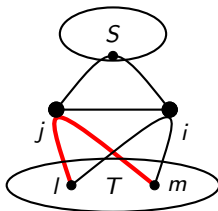
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strengthened conflicting arcs constraints

Case $|T| = 2$

At most one of the following variables can be 1:



$$x_{ij} + \sum_{\substack{ikj \in V^3: \\ k \in S}} y_{ikj} + y_{lim} + y_{ljm} \leq 1$$

for all $i, j \in V, i \neq j$, and $S, T \subset V \setminus \{i, j\}, S \cap T = \emptyset, T = \{l, m\}$

Subtour elimination constraints

$$\sum_{\substack{ij \in V^2: \\ i \in S, j \in V \setminus S}} x_{ij} \geq 2, \quad \text{for all } S \subset V, 2 \leq |S| \leq n - 2$$

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Using only y -variables

$$\sum_{\substack{ijk \in V^3: \\ i \in S, j, k \in V \setminus S}} y_{ijk} + 2 \cdot \sum_{\substack{ijk \in V^3: \\ i, k \in S, j \in V \setminus S}} y_{ijk} \geq 2, \quad \text{for all } S \subset V, 2 \leq |S| \leq n-2$$

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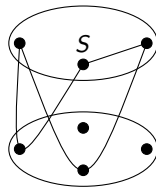
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$$\forall S \subset V, 2 \leq |S| < \frac{n}{2}: \quad (1)$$

$$\sum_{\substack{ijk \in V^3: \\ i \in S, j, k \in V \setminus S}} y_{i,j,k} \geq 2,$$



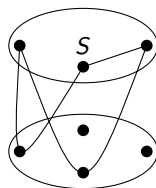
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$$\forall S \subset V, 2 \leq |S| < \frac{n}{2}: \\ \sum_{\substack{ijk \in V^3: \\ i \in S, j, k \in V \setminus S}} y_{i,j,k} \geq 2, \quad (1)$$



Lemma

The separation problem for inequalities (1) is **NP-complete**.

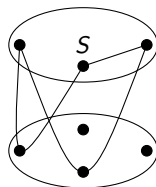
Subtour elimination constraints

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Case $|S| \geq \frac{n}{2}$:

$$\sum_{\substack{ij \in V^2: \\ i \in S, j \in V \setminus S}} x_{ij} - 2 \sum_{\substack{ikj \in V^3: \\ i, j \in S, k \in T}} y_{i,k,j} \geq 2, \quad \text{for all } S, T \subset V, S \cap T = \emptyset, |S| + |T| = n-1$$

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Semidefinite relaxation

semidefinite relaxation bases on QIP:

$$\begin{aligned} \min \quad & \sum_{ijk \in V^3} c_{i,j,k} \cdot x_{ij} x_{jk} \\ \text{s.t. } \quad & x \in \mathbf{TSP}(n) \quad (\text{TSP-polytope}) \end{aligned}$$

with $x = (x_{12}, x_{13}, \dots, x_{n-1,n})^T$

Construction of rank-one matrix: $X = \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T$

Notation: $x_{ij,kl} \hat{=} x_{ij} \cdot x_{kl}$

Semidefinite relaxation

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$$x_{ij} = \sum_{k \in V \setminus \{i,j\}} x_{ki,ij}, \quad ij \in V^2$$

$$X_{1,1} = 1$$

$$X_{1,i} = X_{i,i}, \forall i = 2, \dots, n+1 \quad (x_{ij} = x_{ij,ij})$$

$$0 \leq X \leq E$$

$$\text{rank}(X) = 1$$

$$X \succeq 0$$

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strengthening: presented cuts, inequalities of the Boolean Quadratic Polytope

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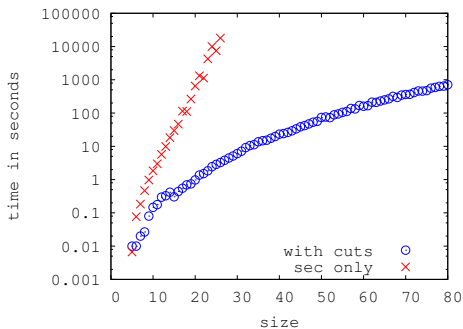
Semidefinite relaxation

Computational results

Further work

Computational results – real-world instances

- 3 instances $5 \leq n \leq 80$
- # variables for $n = 80$: ~ 500000
- all instances solved in < 13 minutes with the presented cuts
- only SEC: running times much higher



Computational results – random instances

10 instances

uni random asymmetric: c_{ijk} uniformly at random in $\{0, 1, \dots, 10000\}$

random angular: points $i \in V$ uniformly at random in $\{0, 1, \dots, 10000\}^2$,

$$c_{ijk} = \left\lfloor \frac{18000}{\pi} \arccos \left(\left(\frac{\mathbf{v}_j - \mathbf{v}_i}{\|\mathbf{v}_j - \mathbf{v}_i\|} \right)^T \left(\frac{\mathbf{v}_k - \mathbf{v}_j}{\|\mathbf{v}_k - \mathbf{v}_j\|} \right) \right) \right\rfloor$$

uni random symmetric: c_{ijk} uniformly at random in $\{0, 1, \dots, 10000\}$

Computational results – random instances

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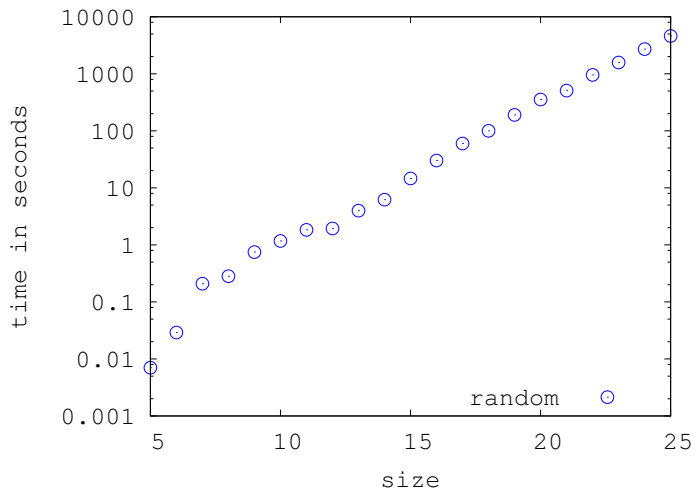
$$c_{ijk} = \left\lfloor \frac{18000}{\pi} \arccos \left(\left(\frac{\mathbf{v}_j - \mathbf{v}_i}{\|\mathbf{v}_j - \mathbf{v}_i\|} \right)^T \left(\frac{\mathbf{v}_k - \mathbf{v}_j}{\|\mathbf{v}_k - \mathbf{v}_j\|} \right) \right) \right\rfloor$$

uni random symmetric: c_{ijk} uniformly at random in $\{0, 1, \dots, 10000\}$

Computer: Intel Core i7 CPU 920, 2.67 GHz, 12 GB RAM

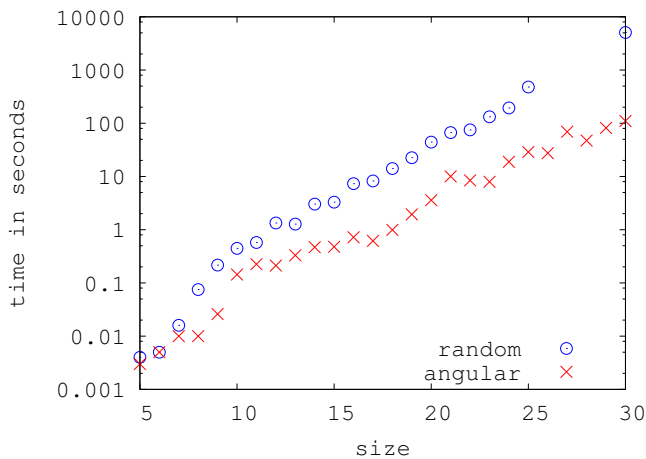
- **(MIP):** use SCIP, LP with CPLEX 12.1,
- **(SDP):** use Matlab and SDPT3

Computational results – asymmetric random instances



Computational results – symmetric instances

random and random angular instances



But: for random instances better not to separate additional inequalities

Computational results – symmetric random instances

Comparison of the value of the gaps $[(opt - relax)/relax] \cdot 100\%$ at the root node

IP root relaxation of IP

SDP1 SDP relaxation, all inequalities only on the y -support

SDP2 additional $x_{ij,kl} \geq 0$ for all matrix entries

SDP3 additional triangle inequalities on whole matrix

Computational results – symmetric random instances

Comparison of the value of the gaps $[(opt - relax)/relax] \cdot 100\%$ at the root node

IP root relaxation of IP

SDP1 SDP relaxation, all inequalities only on the y -support

SDP2 additional $x_{ij,kl} \geq 0$ for all matrix entries

SDP3 additional triangle inequalities on whole matrix

n	IP	SDP1	SDP2	SDP3
5	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00
8	1.74	0.43	0.30	0.00
9	2.73	1.09	0.69	0.02
10	10.35	4.79	2.99	0.76
11	13.58	8.30	5.21	2.63
12	18.60	11.77	8.38	5.32
13	19.05	10.93	6.79	4.17
14	23.18	14.55	9.94	7.48
15	23.61	13.31	8.50	6.45

Computational results – symmetric random instances

Comparison of the value of the gaps $[(opt - relax)/relax] \cdot 100\%$ at the root node

IP root relaxation of IP

SDP1 SDP relaxation, all inequalities only on the y -support

SDP2 additional $x_{ij,kl} \geq 0$ for all matrix entries

SDP3 additional triangle inequalities on whole matrix

n	IP	SDP1	SDP2	SDP3
5	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00
8	1.74	0.43	0.30	0.00
9	2.73	1.09	0.69	0.02
10	10.35	4.79	2.99	0.76
11	13.58	8.30	5.21	2.63
12	18.60	11.77	8.38	5.32
13	19.05	10.93	6.79	4.17
14	23.18	14.55	9.94	7.48
15	23.61	13.31	8.50	6.45

n	IP
16	35.21
17	31.69
18	36.53
19	40.11
20	44.80
21	47.36
22	41.65
23	46.44
24	42.75
25	51.03
30	60.14

Outline

Introduction

ILP formulation

Valid inequalities

Semidefinite relaxation

Computational results

Further work

Further work

- further polyhedral studies, includes dimension of the corresponding polytopes
- separation heuristics for extended SEC
- use SDP-bounds for Branch-and-Cut
- use spectral bundle method for SDP
 - Which support extension is useful?
 - Which (in-)equalities should be used?
- extend neighborhood

Thank you for your attention. Questions?



The Cluster of Excellence "Energy-Efficient Product and Process Innovation in Production Engineering" (eniPROD®) is funded by the European Union (European Regional Development Fund) and the Free State of Saxony.

