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The Symmetric Quadratic Traveling Salesman Problem*

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Abstract. In the quadratic traveling salesman problem a cost is associated with any three nodes traversed in succession. This structure arises, *e. g.*, if the succession of two edges represents energetic conformations, a change of direction or a possible change of transportation means. In the symmetric case, costs do not depend on the direction of traversal. We study the polyhedral structure of a linearized integer programming formulation of the symmetric quadratic traveling salesman problem. Our constructive approach for establishing the dimension of the underlying polyhedron is rather involved but offers a generic path towards proving facetness of several classes of valid inequalities. We establish relations to facets of the boolean quadric polytope, exhibit new classes of polynomial time separable facet defining inequalities that exclude conflicting configurations of edges, and provide a generic strengthening approach for lifting valid inequalities of the usual traveling salesman problem to stronger valid inequalities for the symmetric quadratic traveling salesman problem. Applying this strengthening to subtour elimination constraints gives rise to facet defining inequalities, but finding a maximally violated inequality among these is **NP**-complete. For the simplest comb inequality with three teeth the strengthening is no longer sufficient to obtain a facet. First computational results are presented to illustrate the importance of the new inequalities.

Keywords: combinatorial optimization, quadratic 0-1 programming, angular-metric traveling salesman problem, reload cost model
MSC 2010: 90C57, 90C27, 90C09

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1 Introduction

The Traveling Salesman Problem (TSP) is one of the best studied combinatorial optimization problems with many variations and well known to be **NP**-complete [5, 16, 19]. The *Quadratic Traveling Salesman Problem* (QTSP) differs from the TSP in that the costs do not depend on two successive nodes, an *edge*, but on *three* successive nodes in the tour. As such a sequence of three nodes arises if the two corresponding edges appear in a tour we speak of a quadratic TSP. The problem was introduced by Jäger and Molitor [10, 18] in the context of solving instances motivated by an application in biology. Indeed, for the recognition of transcription factor binding sites in gene regulation, Zhao, Huang and Speed [22] proposed permuted Markov and permuted variable length Markov mixture models. These can be solved by an iterative algorithm that needs the solution of a TSP and the solution of a QTSP.

By allowing this particular quadratic cost structure, the QTSP can be used to solve instances of the Angular-Metric Traveling Salesman Problem (Angle-TSP) introduced by Aggarwal et. al. [3] which is used for the optimization of robot paths with respect to energetic aspects. Here the task is to find a tour over n points in the Euclidean space minimizing the sum of the changes in direction, *i. e.*, the costs depend on the angle of a path from a point i to a point k over a point j. It also covers the extension of this problem where the changes in direction are weighted against the length of the tour. As a further problem class we can handle TSP with reload costs [4, 11, 12, 21], *i. e.*, given an edge-colored graph find a tour minimizing the costs arising from (weighted) color changes along the tour. These problems appear for example in the planning of telecommunication networks whenever switching between two different technologies is expensive or in freight transportation networks if the costs for loading processes are high in comparison to transportation costs.

This paper investigates the polyhedral structure of the symmetric QTSP (SQTSP), *i. e.*, the QTSP where the direction of traversal of a tour is irrelevant. While formulating the problem as an integer program is straight forward, determining the dimension of the associated SQTSP polyhedron $P_{\mathbf{SQTSP}_n}$ turns out to be surprisingly difficult, see Section 2. One reason might be that the dimension grows irregularly up to $n = 6$ and reaches its canonical size only for $n \geq 7$. Our proof of the dimension of $P_{\mathbf{SQTSP}_n}$ gives an explicit construction of affinely independent tours that extend a constant initial set of (*e. g.*, 54) tours extracted by a computer algebra package from tours obtained by complete enumeration of a fixed number (*e. g.*, 5) of initial nodes. The initial enumerative part seems to cover all cases with structural irregularities so that the remaining tours can be generated following a rather natural scheme.

Due to this explicit form, the same proof technique allows to establish the property of being facet defining for several classes of valid inequalities (Section 3). In particular, we discuss facets related to the boolean quadric polytope (Section 3.1) and facets excluding conflicting edges, *i. e.*, edges that may not be selected at the same time (Section 3.2). These include an exponential family of inequalities, that can be separated in polynomial time. Section 3.3 is devoted to facets that may be interpreted as strengthenings of TSP facets prohibiting subtours. We introduce a particular strengthening technique that can be used to lift any valid inequality for TSP to a stronger valid inequality for SQTSP. This approach suffices to lift TSP subtour elimination constraints to facet defining inequalities for SQTSP. Unfortunately, more is required for comb inequalities and we present an SQTSP facet corresponding to the simplest comb with three teeth. While TSP subtour elimination constraints can be separated in polynomial time, this no longer seems to hold for their SQTSP equivalents. We prove that finding a maximally violated SQTSP subtour elimination constraint is **NP**-complete.

In order to illustrate the usefulness of the new inequalities we conclude the paper with some computational results in Section 4 comparing the basic integer programming formulation against the formulation improved by the new cutting planes for rather small random instances with general nonnegative cost structure, random Angle-TSP instances in the plane, and random TSP instances with reload costs.

2 The Model and its Associated Polyhedron

A *2-graph* G is a pair (V, E) consisting of a node set $V = \{1, \ldots, n\}$ and a set of undirected *2-edges* E to be defined as follows. A *2-edge* $\langle i, j, k\rangle \in V^{\langle 3\rangle} := \{\langle i, j, k\rangle = \langle k, j, i\rangle : i, j, k \in V, |\{i, j, k\}| = 3\}$ consists of a sequence of three distinct nodes where the reverse sequence is regarded as identical. Alternatively, it may be viewed as a path consisting of two distinct incident edges $\{i, j\}, \{j, k\} \in V^{\{2\}} := \{\{i, j\} : i, j \in V, i \neq j\}$, $i \neq k$, with the property that the direction of traversal is irrelevant. If there is no danger of confusion we simply write ij instead of $\{i, j\}$ and ijk instead of $\langle i, j, k\rangle$. We consider the complete 2-graph on V with $E := V^{\langle 3\rangle}$.

A 2-cycle C of length $k > 2$ in a 2-graph G is a set of k 2-edges $C = \{v_1v_2v_3, v_2v_3v_4, \ldots, v_{k-2}v_{k-1}v_k, v_{k-1}v_kv_1, v_kv_1v_2\}$ with pairwise distinct v_i. The 2-edges $ijk \in C$ induce a set of edges $C^{\{2\}} := \{ij \in V^{\{2\}} : ijk \in C\}$.

We consider the problem of finding a 2-cycle C in a complete 2-graph $G = (V, E)$ with $n = |V|$ nodes, called a *tour*, that minimizes the sum of given weights c_e over all 2-edges $e \in C$. Let $\mathcal{C}_n = \{C : C \text{ 2-cycle in } G, |C| = n\}$ denote the set of all tours on n nodes, then the optimization problem reads

$$\min \left\{ c(C) := \sum_{e \in C} c_e : C \in \mathcal{C}_n \right\}.$$

For a cycle C we define the incidence vector $(x^C, y^C) \in \{0, 1\}^{V^{\{2\}} \cup V^{\langle 3\rangle}}$ by

$$\forall\, e \in V^{\{2\}} : x^C_e = \begin{cases} 1 & \text{if } e \in C^{\{2\}}, \\ 0 & \text{if } e \notin C^{\{2\}}, \end{cases} \quad \text{and} \quad \forall\, e \in V^{\langle 3\rangle} : y^C_e = \begin{cases} 1 & \text{if } e \in C, \\ 0 & \text{if } e \notin C. \end{cases}$$

An integer programming formulation of all incidence vectors of 2-cycles is given by

$$\sum_{j\colon ij\in V^{\{2\}}} x_{ij} = 2, \qquad i \in V, \tag{1}$$

$$x_{ij} = \sum_{k\colon ijk\in V^{\langle 3\rangle}} y_{ijk} = \sum_{k\colon kij\in V^{\langle 3\rangle}} y_{kij}, \qquad ij \in V^{\{2\}}, \tag{2}$$

$$\sum_{\substack{ij\in V^{\{2\}}:\\ i\in S, j\in V\setminus S}} x_{ij} \geq 2, \qquad S \subset V, 2 \leq |S| \leq n-2, \tag{3}$$

$$x_{ij} \in \{0,1\}, y_{ijk} \in [0,1], \qquad ij \in V^{\{2\}}, ijk \in V^{\langle 3\rangle}. \tag{4}$$

The *degree constraints* (1) ensure that each node is visited exactly once. Equations (2) may be seen as a kind of flow conservation for each $ij \in V^{\{2\}}$, because the sum of the in-flow into ij via 2-edges $kij \in V^{\langle 3\rangle}$ has to be the same as the out-flow out of ij via 2-edges $ijk \in V^{\langle 3\rangle}$. The constraints (3) are the well known *subtour elimination constraints* [8]. That this is indeed a formulation follows from combining the well known formulation for the Symmetric Traveling Salesman Polytope [8]

$$P_{\mathbf{STSP}_n} := \operatorname{conv}\{x^C \in \{0,1\}^{V^{\{2\}}} : C \in \mathcal{C}_n\} = \operatorname{conv}\left\{x \in \{0,1\}^{V^{\{2\}}} : (1),(3)\right\}$$

with the coupling constraints (2). In fact, the model above is a linearization of the quadratic integer program

$$\min_{\left\{x\in\{0,1\}^{V^{\{2\}}}:(1),(3)\right\}} \sum_{ij,jk\in V^{\{2\}}:\, ijk\in V^{\langle 3\rangle}} c_{ijk} x_{ij} x_{jk}, \tag{5}$$

because the integrality of $y_{ijk}, ijk \in V^{\langle 3\rangle}$, follows from the integrality of the x-variables. For this, we have to check that $x_{ij}x_{jk} = y_{ijk}$ for all $ij, jk \in V^{\{2\}}$ with $ijk \in V^{\langle 3\rangle}$ and integral x. For $x_{ij} = 0$ equations (2) imply $y_{ijk} = 0$ for all $ijk \in V^{\langle 3\rangle}$, so consider the case $x_{ij} = x_{jk} = 1$. Assume $y_{ijk} < 1$, then there exists $ijl \in V^{\langle 3\rangle}, l \neq k$, with $y_{ijl} > 0$ by (2) which implies $x_{jl} = 1$ (again by (2)). This contradicts $\sum_{jm\in V^{\{2\}}} x_{jm} = 2$.

Remark 2.1 Note that the variables x_{ij} are easily eliminated by (2). *E. g.*, the degree constraints then read

$$\sum_{ijk\in V^{\langle 3\rangle}} y_{ijk} = 1 \qquad \text{for } j \in V. \tag{6}$$

However, in our experience, the classical x_{ij} variables improve readability and facilitate the presentation.

Our main object of study is the polytope arising as the convex hull of all incidence vectors of 2-cycles, the *Symmetric Quadratic Traveling Salesman Polytope*

$$P_{\mathbf{SQTSP}_n} := \operatorname{conv}\left\{(x^C, y^C) : C \in \mathcal{C}_n\right\} = \operatorname{conv}\left\{(x,y) \in \{0,1\}^{V^{\{2\}}\cup V^{\langle 3\rangle}} : (1),(2),(3)\right\}.$$

In order to determine the dimension of $P_{\mathbf{SQTSP}_n}$ we first calculate the rank of the corresponding constraint matrix.

Lemma 2.2 *The constraint matrix corresponding to equality constraints (1) and (2) has full row rank for all $n \geq 4$.*

Proof. The rows belonging to the degree constraints (1) are linearly independent, as in the STSP-case [14], because the node-edge incidence matrix of the complete graph $K_n, n \geq 3$, has full row rank. Let $A_{(i,j,1),\bullet}$ be the row of constraint $x_{ij} = \sum_{\langle i,j,k\rangle \in V^{\langle 3\rangle}} y_{\langle i,j,k\rangle}$ and $A_{(i,j,2),\bullet}$ the row of constraint $x_{ij} = \sum_{\langle k,i,j\rangle \in V^{\langle 3\rangle}} y_{\langle k,i,j\rangle}$. Our aim is to show that if $\sum_{i<j}(\alpha_{(i,j,1)}A_{(i,j,1),\bullet} + \alpha_{(i,j,2)}A_{(i,j,2),\bullet}) = 0$ we have $\alpha_{(i,j,m)} = 0$ for all $i, j \in V, i < j, m = 1, 2$. Considering, w. l. o. g., the columns belonging to $y_{\langle i,j,k\rangle}, y_{\langle i,j,l\rangle}, y_{\langle k,j,l\rangle}, i < j < k < l$, we get

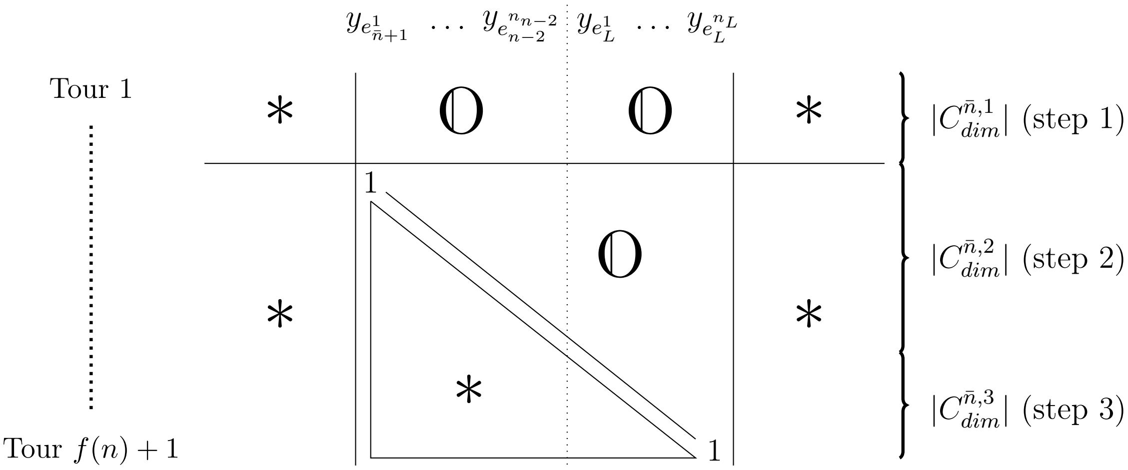
	$y_{\langle i,j,k\rangle}$	$y_{\langle i,j,l\rangle}$	$y_{\langle k,j,l\rangle}$
$(i, j, 1)$	1	1	0
$(j, k, 2)$	1	0	1
$(j, l, 2)$	0	1	1

Because all other entries of these three columns are zero and this small matrix has full row rank, $\alpha_{(i,j,1)}$ has to be zero. With the same argument we get $\alpha_{(i,j,m)} = 0$ for all $i < j, m = 1, 2$. □

This proves that the dimension of $P_{\mathbf{SQTSP}_n}$ is at most $f(n) := 3 \cdot \binom{n}{3} + \binom{n}{2} - n^2$, because there are $3\binom{n}{3} + \binom{n}{2}$ variables and n^2 equality constraints. That it is exactly $f(n)$ for $n \geq 7$ is shown next. The construction is surprisingly involved but as subsequent facet proofs build upon it, it is worth to present it in detail.

Theorem 2.3 *The dimension of $P_{\mathbf{SQTSP}_n}$ equals $f(n)$ for all $n \geq 7$.*

Proof. We want to show that the dimension of $P_{\mathbf{SQTSP}_n}$ equals $f(n) = 3\binom{n}{3} + \binom{n}{2} - n^2 = \frac{1}{2}n^3 - 2n^2 + \frac{1}{2}n$ for $n \geq 7$. The idea is to construct, in dependence of a fixed small parameter $\bar{n}$, a set of affinely independent tours $C^{\bar{n}}_{dim} = C^{\bar{n},1}_{dim} \dot{\cup} C^{\bar{n},2}_{dim} \dot{\cup} C^{\bar{n},3}_{dim} \subset \mathcal{C}_n$ and to prove that $|C^{\bar{n}}_{dim}| = f(n) + 1$. We use three main steps for building the following matrix structure where each row is the incidence vector of a tour. In step 1 we determine the rank of some specially structured tours $\bar{C}^{\bar{n},1}_{dim}$ and take the largest affinely independent subset $C^{\bar{n},1}_{dim} \subset \bar{C}^{\bar{n},1}_{dim}$. Next we iteratively build tours so that each tour contains at least one 2-edge that is not contained in any tour constructed before. This is achieved by ordering the tours appropriately and by using a restricted set of new 2-edges in each iteration of the step. Finally, in step 3, unused 2-edges that contain the nodes $n - 1$ or n are employed to form the remaining tours.



1. Fix a small $\bar{n} \in \mathbb{N}$, $\bar{n} \leq n-2$ (for this proof $\bar{n} = 5$ is sufficient, in later proofs we will use $\bar{n} = 6, 9$, as well) and collect in the set $\bar{C}^{\bar{n},1}_{dim}$ all tours with fixed consecutive ordering of the nodes $(\bar{n}+1)$ to n but with an arbitrary permutation of the first $\bar{n}$ nodes, $\bar{C}^{\bar{n},1}_{dim} = \{C \in \mathcal{C}_n \colon \{\langle \bar{n}+1, \bar{n}+2, \bar{n}+3\rangle, \langle \bar{n}+2, \bar{n}+3, \bar{n}+4\rangle, \ldots, \langle n-2, n-1, n\rangle\} \in C\}$. Because $\bar{n}$ is small and fixed the rank $r_{\bar{n}}$ of the incidence vectors of these tours is independent of $n \geq \bar{n}+2$ and easy to determine once and for all, *e. g.*, by some algebra package. The ranks needed in this paper are $r_5 = 54$, $r_6 = 98$ and $r_9 = 350$. Pick $r_{\bar{n}}$ tours $t \in \bar{C}^{\bar{n},1}_{dim}$ whose corresponding incidence vectors are linearly independent and collect these tours in the set $C^{\bar{n},1}_{dim}$ with $C^{\bar{n},1}_{dim} \subset \bar{C}^{\bar{n},1}_{dim} \colon |C^{\bar{n},1}_{dim}| = r_{\bar{n}}$.

2. In the second step we form $C^{\bar{n},2}_{dim} = \bigcup_{\bar{n}<k<n-1} T_k$ by iteratively constructing sets of tours $T_k = \{t^1_k, \ldots, t^{n_k}_k\}, \bar{n} < k < n-1$, so that specific coordinates of the corresponding incidence vectors, which are zero in all incidence vectors of tours $t \in C^{\bar{n},1}_{dim}$, form a lower triangular matrix, establishing the affine independence of the respective tours. We obtain this structure for each k by ordering the tours as presented next. During the following five steps each new tour $t^i_k, i = 1, \ldots, n_k$, contains a 2-edge e^i_k that fulfills

$$e^i_k \notin C \text{ for all } C \in \left(C^{\bar{n},1}_{dim} \cup \left(\bigcup_{\bar{n}<h<k} T_h \right) \cup \left(\bigcup_{1 \leq h < i} \{t^h_k\} \right) \right). \tag{7}$$

Within block k the iteration steps ($\mathsf{I}j$) below should be considered as appending new rows of incidence vectors of tours in sequence of increasing j. In this sequence the columns corresponding to underlined 2-edges of the tours $t^i_k \in T_k$ form a lower triangular matrix. The order within an iteration step ($\mathsf{I}j$) is arbitrary.

Consider a fixed k with $\bar{n} < k < n-1$. In order to simplify the presentation we only specify the relevant parts of the tours in a condensed form. In particular, the (possibly empty) fixed node sequence $(k+2)\,(k+3)\ldots(n-2)\,(n-1)$ is denoted by the symbol ϖ_k and nodes that are not listed may appear in any order within the parts denoted by "...". The decisive 2-edge e_k^i that determines the triangle structure is marked by underlining the corresponding three nodes. Each 2-edge e_k^i has one of the four types

(**Type-I1**) $\langle a,k,b\rangle, a,b \in \{1,\dots,k-1\}, a<b,$

(**Type-I2**) $\langle k,a,k+1\rangle, a \in \{2,\dots,k-1\},$

(**Type-I3**) $\langle a,b,k+1\rangle, a,b \in \{1,\dots,k-1\}, a \neq b.$

(**Type-I4**) $\langle n,a,k\rangle, \langle n,k,a\rangle, a \in \{1,\dots,k-1\}.$

The only exceptional 2-edge is $\langle k,1,k+1\rangle$, it is not used for forming the key segment of the lower triangular matrix but will be needed for patching.

The tours of $C_{dim}^{\bar{n},2}$ are built during five iteration steps:

(**I1**) $\dots \underline{a\,k\,1}\,(k+1)\,\varpi_k\, n \dots$, for $a \in \{2,\dots,k-1\}$
(the 2-edge $\langle k,1,k+1\rangle$ is not used as an e_k^i),

(**I2**) $\dots 1\,\underline{k\,a\,(k+1)}\,\varpi_k\, n \dots$, for $a \in \{2,\dots,k-1\}$,

(**I3**) $\dots \underline{a\,k\,b}\,(k+1)\,\varpi_k\, n \dots$, for $a,b \in \{2,\dots,k-1\}, a<b$,

(**I4**) $\dots k\,\underline{a\,b\,(k+1)}\,\varpi_k\, n \dots$, for $a,b \in \{1,\dots,k-1\}$, $a \neq b$,

(**I5**) $\dots (k+1)\,\varpi_k\,\underline{n\,a\,b} \dots$, for $a,b \in \{1,\dots,k\}, a\neq b, k \in \{a,b\}$.

Claim 1 The 2-edges $e_k^i, i=1,\dots,n_k$, underlined above fulfill condition (7).

Proof of Claim 1. By construction, edge $\{k,k+1\}$ is contained in all tours $t \in C_{dim}^{\bar{n},1} \cup \left(\bigcup_{\bar{n}<j<k} T_j\right)$ and edge $\{k+1,k+2\}$ is in each tour up to and including this iteration. Thus, the 2-edges of (**Type-I1**)–(**Type-I3**) have not been used before. Likewise, n and k are separated by node $k+1$ on one side and by $k-1$ nodes on the other side in each tour up to this iteration, so the 2-edges of (**Type-I4**) are unused. An underlined 2-edge e_k^i of iteration step (**I**j) is not in conflict with a further $e_k^{\hat{i}}$ of the same iteration step because at most one of these 2-edges can be present in a tour. It remains to show that a 2-edge e_k^i chosen in iteration step (**I**j) is not contained in a tour of a previous iteration step (**I**l), $l<j$.

- Tours in step (**I2**): all tours created in (**I1**) contain a 2-edge $\langle k,1,k+1\rangle$ and by (1), (2) no 2-edge $\langle k,a,k+1\rangle, a \in \{2,\dots,k-1\}$.
- Tours in step (**I3**): all tours created in (**I1**)–(**I2**) contain an edge $\{1,k\}$ which conflicts with 2-edges $\langle a,k,b\rangle, a,b \in \{2,\dots,n-1\}$, by (1), (2).
- Tours in step (**I4**): all tours created in (**I1**)–(**I3**) contain a 2-edge $\langle k,a,k+1\rangle, a \in \{1,\dots,k-1\}$ and the edge $\{k+1,k+2\}$, *i. e.*, until this step at most one node has been between k and $k+1$. It follows by (1), (2) that all variables of type (**Type-I3**) have not been used in (**I1**)–(**I3**).
- Tours in step (**I5**): in (**I1**)–(**I4**) the nodes n and k are separated by node $k+1$ on one side and by at least $n-5-|\varpi_k| = n-5-(n-k-2) = k-3$ nodes on the other side. For $k>\bar{n}\geq 5$ these are at least 3 nodes.

This completes the proof of Claim 1.

3. Because all tours constructed so far contain the edge $\{n-1,n\}$, we have

$$C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2} \subset \left\{C \in \mathcal{C}_n \colon \{n-1,n\} \in C^{\{2\}}\right\}. \tag{8}$$

It remains to build tours in which $n-1$ and n do not lie next to each other. Therefore we have three possible types for $e_L^i, i = 1,\dots,n_L$:

(**Type-L1**) $\langle a, n-1, b\rangle, a, b \in \{1,\dots,n-2\}, a < b$,

(**Type-L2**) $\langle a, n, b\rangle, a, b \in \{1,\dots,n-2\}, a < b$,

(**Type-L3**) $\langle n-1, a, n\rangle, a \in \{1,\dots,n-2\}$.

All of these 2-edges except for one are used as e_L^i during the construction.

Again the order of the tours is chosen so that the underlined 2-edge e_L^i of each tour $t_L^i, i = 1,\dots,n_L$, fulfills

$$e_L^i \notin C \text{ for all } C \in C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2} \cup \{t_L^1,\dots,t_L^{i-1}\}. \tag{9}$$

The tours of step (**L**j) are all created before the start of steps (**L**l), $l > j$, and the order within each step is arbitrary.

In the following, let $w_1, w_2, w_3 \in \{1,\dots,n-2\}$ be three arbitrary but fixed nodes with $|\{w_1,w_2,w_3\}| = 3$ (this could be the nodes 1, 2, 3; the additional freedom allows to reuse this part in later proofs).

(**L1**) $\dots \underline{a\,(n-1)\,b}\,w_1\,n\,w_2\dots$, for $a, b \in \{1,\dots,n-2\}\setminus\{w_1,w_2\}, a < b$
(the 2-edge $\langle w_1, n, w_2\rangle$ is not used as an e_L^i),

(**L2**) $\begin{cases} \dots m\,(n-1)\,o\,\underline{w_1\,n\,w_3}\dots, \\ \dots m\,(n-1)\,o\,\underline{w_2\,n\,w_3}\dots, \end{cases}$ with $m, o \in \{1,\dots,n-2\}\setminus\{w_1,w_2,w_3\}, m \neq o$,

(**L3**) $\dots \underline{a\,(n-1)\,w_1}\,w_2\,n\,w_3\dots$, for $a \in \{1,\dots,n-2\}\setminus\{w_1,w_2,w_3\}$,

(**L4**) $\dots \underline{a\,(n-1)\,w_2}\,w_1\,n\,w_3\dots$, for $a \in \{1,\dots,n-2\}\setminus\{w_1,w_2,w_3\}$,

(**L5**) $\dots \underline{a\,n\,b}\,m\,(n-1)\,o\dots$, for $a, b \in \{1,\dots,n-2\}, a < b, |\{a,b\}\cap\{w_1,w_2,w_3\}| = 1$, with $m, o \in \{1,\dots,n-2\}, \{m,o\} \not\subseteq \{w_1,w_2,w_3\}, |\{a,b,m,o\}| = 4$,

(**L6**) $\begin{cases} \dots n\,w_3\,\underline{w_1\,(n-1)\,w_2}\dots, \\ \dots n\,w_2\,\underline{w_1\,(n-1)\,w_3}\dots, \\ \dots n\,w_1\,\underline{w_2\,(n-1)\,w_3}\dots, \end{cases}$

(**L7**) $\dots \underline{a\,n\,b}\,m\,(n-1)\dots$, for $a, b \in \{1,\dots,n-2\}\setminus\{w_1,w_2,w_3\}, a < b$, with $m \in \{1,\dots,n-2\}, |\{a,b,m\}| = 3$,

(**L8**) $\dots \underline{(n-1)\,a\,n}\dots$, for $a \in \{1,\dots,n-2\}$.

Claim 2 Whenever (8) holds, then for any fixed choice $w_1, w_2, w_3 \in \{1,\dots,n-2\}$ with $|\{w_1,w_2,w_3\}| = 3$ and any feasible realization of tour $t_L^i \in C_{dim}^{\bar{n},3}$ according to (**L1**)–(**L8**) the corresponding underlined 2-edge e_L^i fulfills condition (9) for $i = 1,\dots,n_L$.

Proof of Claim 2. Note that each step (**L**j) belongs to one of the types (**Type-L1**)–(**Type-L3**). For all $C \in (C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2})$ there holds $e_L^i \notin C$ because the 2-edges of (**Type-L1**)–(**Type-L3**) are in conflict with edge $\{n-1, n\}$, which is contained in all previous tours by (8). Next, an underlined 2-edge e_L^i of step (**L**j) does not conflict with an $e_L^{\hat{\imath}}$, $i \neq \hat{\imath}$, of the same step because at most one of these 2-edges can be present in a tour by (1), (2). It remains to show (9) for the tours (**L**j) with increasing j.

- Tours in step (**L2**): all tours created in (**L1**) contain the 2-edge $\langle w_1, n, w_2\rangle$.
- Tours in step (**L3**), (**L4**): all tours created in (**L1**)–(**L2**) contain a 2-edge $\langle a, n-1, b\rangle, a, b \in \{1, \ldots, n-2\} \setminus \{w_1, w_2\}$.
- Tours in step (**L5**): all tours created in (**L1**)–(**L4**) contain a 2-edge $c \in \{\langle w_1, n, w_2\rangle, \langle w_1, n, w_3\rangle, \langle w_2, n, w_3\rangle\}$.
- Tours in step (**L6**): all tours created in (**L1**)–(**L5**) contain none of the three 2-edges $\langle w_1, n-1, w_2\rangle, \langle w_1, n-1, w_3\rangle, \langle w_2, n-1, w_3\rangle$.
- Tours in step (**L7**): all tours created in (**L1**)–(**L4**) contain a 2-edge $c \in \{\langle w_1, n, w_2\rangle, \langle w_1, n, w_3\rangle, \langle w_2, n, w_3\rangle\}$; the underlined 2-edges of (**L7**) are forbidden in (**L5**), (**L6**) because there n is adjacent to one of the nodes w_1, w_2, w_3.
- Tours in step (**L8**): in all tours created in (**L1**)–(**L7**) there are at least two nodes between nodes $n-1$ and n.

This completes the proof of Claim 2.

Claim 3: For $\bar{n} = 5, 6, 9$ we have $|C_{dim}^{\bar{n}}| = f(n) + 1$.
Proof of Claim 3. We determine $|C_{dim}^{\bar{n}}| = |C_{dim}^{\bar{n},1} \dot\cup C_{dim}^{\bar{n},2} \dot\cup C_{dim}^{\bar{n},3}| = |C_{dim}^{\bar{n},1}| + |C_{dim}^{\bar{n},2}| + |C_{dim}^{\bar{n},3}|$ with

- $|C_{dim}^{\bar{n},1}| = r_{\bar{n}}$,
- $|C_{dim}^{\bar{n},2}| = \sum\limits_{k=\bar{n}+1}^{n-2} |T_k| = \sum\limits_{k=\bar{n}+1}^{n-2} \Big(\underbrace{2(k-2)}_{(\mathbf{I1})+(\mathbf{I2})} + \underbrace{\binom{k-2}{2}}_{(\mathbf{I3})} + \underbrace{(k-1)(k-2)}_{(\mathbf{I4})} + \underbrace{2(k-1)}_{(\mathbf{I5})} \Big)$

$= \sum\limits_{k=\bar{n}+1}^{n-2} \left(\frac{3}{2}k^2 - \frac{3}{2}k - 1\right) = \frac{1}{2}n^3 - 3n^2 + \frac{9}{2}n - 1 - \frac{1}{2}\bar{n}^3 + \frac{3}{2}\bar{n}$,

- $|C_{dim}^{\bar{n},3}| = \underbrace{\binom{n-4}{2}}_{(\mathbf{L1})} + \underbrace{2}_{(\mathbf{L2})} + \underbrace{2(n-5)}_{(\mathbf{L3})+(\mathbf{L4})} + \underbrace{3(n-5)}_{(\mathbf{L5})} + \underbrace{3}_{(\mathbf{L6})} + \underbrace{\binom{n-5}{2}}_{(\mathbf{L7})} + \underbrace{(n-2)}_{(\mathbf{L8})}$

$= n^2 - 4n + 3$

We get $|C_{dim}^{\bar{n}}| = \frac{1}{2}n^3 - 2n^2 + \frac{1}{2}n + 2 + r_{\bar{n}} - \frac{1}{2}\bar{n}^3 + \frac{3}{2}\bar{n}$ affinely independent tours for $\bar{n} \geq 5$, *i. e.*, for $\bar{n} \geq 5$ and $n \geq \bar{n} + 2$ the described constructions are possible. Choosing $\bar{n} = 5, 6, 9$ Claim 3 and Theorem 2.3 follow because in each case the constant term evaluates to 1. Indeed, for $r_5 = 54$ we get $2 + r_5 - \frac{1}{2} \cdot 5^3 + \frac{3}{2} \cdot 5 = 2 + 54 - \frac{125}{2} + \frac{15}{2} = 1$, $r_6 = 98$ yields $2 + 98 - 108 + 9 = 1$ and for $r_9 = 350$ we obtain $2 + 350 - \frac{729}{2} + \frac{27}{2} = 1$.□

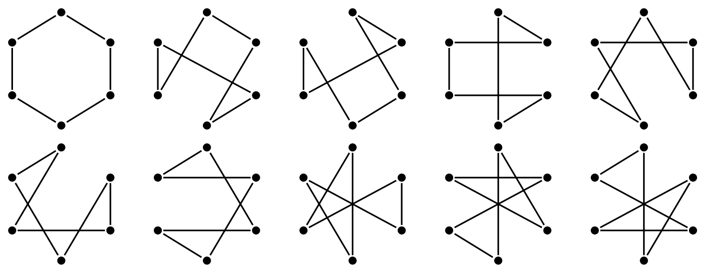


Figure 1: 2-edge disjoint Hamiltonian cycle decomposition of the complete 2-graph with $n = 6$

For small values of n the dimensions of $P_{\mathbf{SQTSP}_n}$ are 0 for $n = 3$, 2 for $n = 4$, 10 for $n = 5$ and 34 for $n = 6$. These values were calculated by means of a linear algebra package.

As pointed out before, the proof is quite involved, but unfortunately, we did not succeed in our attempts to adapt the idea used for proving the dimension of the $\mathbf{STSP}_n$-polytope, v. [14]. On the one hand it is not clear if there exists a decomposition of the complete 2-graph on n nodes into $\binom{n-1}{2}$ Hamiltonian cycles which are disjoint regarding all $ijk \in V^{\langle 3\rangle}$. Such a decomposition is shown in Figure 1 for $n = 6$. This statement is related to a part of a conjecture by Bailey and Stevens [6], page 2 with $k = 3$, on the decomposition of complete uniform hypergraphs into hyperedge-disjoint Hamiltonian cycles. On the other hand, if we had this decomposition for n nodes, we could include the new node $n + 1$ at each position of that smaller tours as done for the $\mathbf{STSP}_n$ but then the number of constructed cycles would be too small.

Remark 2.4 The Symmetric Quadratic Cycle Cover Problem $\mathbf{SQCC}_n$ asks for a set of cycles of length at least three covering all nodes of an undirected 2-graph $\tilde{G} = (\tilde{V}, \tilde{E}), |\tilde{V}| = n$. In comparison to $\mathbf{SQTSP}_n$, the subtour inequalities (3) are not needed. $\mathbf{SQCC}_n$ is $\mathbf{NP}$-complete because the $\mathbf{NP}$-complete problems of determining a minimum angle cycle cover [3] and a minimum reload cost cycle cover [11] can be reduced to it. Its corresponding polytope is

$$P_{\mathbf{SQCC}_n} := \text{conv}\left\{(x, y) \in \mathbb{R}^{V^{\{2\}} \cup V^{\langle 3\rangle}} : (x, y) \text{ fulfills } (1), (2), (4)\right\}.$$

Lemma 2.2 and Theorem 2.3 also prove that the dimension of $P_{\mathbf{SQCC}_n}$ equals $f(n)$. By similar arguments, all inequalities that are valid for $P_{\mathbf{SQCC}_n}$ and facets of $P_{\mathbf{SQTSP}_n}$ are facets of $P_{\mathbf{SQCC}_n}$, too.

3 Valid inequalities and facets of $P_{\mathbf{SQTSP}_n}$

In this section we present valid inequalities and facets of $P_{\mathbf{SQTSP}_n}$. We start with inequalities that are related to the *Boolean Quadric Polytope* (BQP) [20]. After that we present the exponential family of *conflicting edges inequalities* which can be separated in polynomial time. Because $P_{\mathbf{STSP}_n}$ is a projection of $P_{\mathbf{SQTSP}_n}$, valid inequalities for $P_{\mathbf{STSP}_n}$ remain valid for $P_{\mathbf{SQTSP}_n}$ but typically they can be strengthened. For facets corresponding to such a strengthening of the subtour elimination constraints of the $\mathbf{STSP}_n$ the problem of finding a maximally violated constraint is **NP**-complete. It is also possible to find facets corresponding to strengthened comb-inequalities [7, 13, 14, 15].

3.1 Inequalities related to the Boolean Quadric Polytope

In Section 2 we argued that $P_{\mathbf{SQTSP}_n}$ arises as a linearization of the quadratic zero-one problem (5). Therefore it is natural to consider inequalities that are known to be valid for the BQP. The simplest ones are the sign constraints.

Corollary 3.1 *For $n \geq 4$ the inequalities*

$$y_{ijk} \geq 0$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $ijk \in V^{\langle 3 \rangle}$.

Proof. For $4 \leq n \leq 6$ we verified the statement by determining the rank of the incidence vectors of all tours not containing, w. l. o. g., 2-edge $\langle 1, 2, 3 \rangle$ by means of a computer algebra package. For $n \geq 7$ the result follows directly from the proof of Theorem 2.3. Indeed, consider the 2-edge $\langle n-1, n-2, n \rangle$ (w. l. o. g.) and observe that it is only used in step (**L8**) in the tour created last. Therefore the $f(n)$ other tours are affinely independent and do not contain $\langle n-1, n-2, n \rangle$. □

The next important class are the *triangle inequalities* of BQP [20]. In our notation the relevant inequalities read $-x_{ij} + y_{ijk} + y_{kij} - y_{ikj} \leq 0$ for all $ij \in V^{\{2\}}, k \in V \setminus \{i, j\}$, but this can be strengthened as follows.

Theorem 3.2 *For $n \geq 5$ the inequalities*

$$y_{ijk} + y_{kij} \leq x_{ij} \tag{10}$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $ij \in V^{\{2\}}$ and all $k \in V \setminus \{i, j\}$.

Proof. The inequality is valid, because with y_{ijk} or y_{kij} also x_{ij} must be one while the sequences $\langle i, j, k \rangle$ and $\langle k, i, j \rangle$ cannot appear in any tour of length at least four at the same time. We set, w. l. o. g., $i = n-2, j = n, k = n-1$. A tour satisfying (10) with equality, $y_{\langle n-2,n,n-1 \rangle} + y_{\langle n-1,n-2,n \rangle} = x_{\{n-2,n\}}$, either does not contain the edge $\{n-2, n\}$ or contains with this edge one of the edges $\{n-1, n-2\}, \{n, n-1\}$. For $n = 5, 6$ we verified the statement by means of a computer algebra package and for $n \geq 7$ the construction of the $f(n)$ affinely independent tours is similar to the construction in the proof of Theorem 2.3. We only point out the differences.

Among all tours $t \in C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2}$ only those generated for $k = n-2$ in (**I5**) may contain the edge $\{n-2, n\}$ because otherwise n lies between node $n-1$ and a node $c \in \{1, \ldots, n-3\}$. If $k = n-2$ in (**I5**), all tours with $b = k = n-2$ do not contain the edge $\{n-2, n\}$, and whenever $a = n-2$ the tour also contains the 2-edge $\langle n-1, n, n-2 \rangle$.

So consider steps (**L1**)–(**L8**).

- (**L1**)–(**L4**): By choosing $w_1, w_2, w_3 \in \{1, \dots, n-3\}$ node n is not adjacent to $n-2$.
- (**L5**): We split this into two parts. First we restrict a, b to lie in $\{1, \dots, n-3\}$ so that n and $n-2$ are separated. Second we replace the remaining tours by different tours $\dots \underline{a\, n\, (n-2)}\, (n-1) \dots,\ a \in \{w_1, w_2, w_3\}$. These tours contain the 2-edge $\langle n, n-2, n-1\rangle$, so the corresponding e_L^i drops out of (**L8**).
- (**L6**): We slightly adapt this step in order to prevent the case n adjacent to $n-2$,

$$\begin{aligned}
&\dots m\, n\, w_3\, \underline{w_1\, (n-1)\, w_2} \dots, \text{ with } m \in \{1, \dots, n-3\} \setminus \{w_1, w_2, w_3\},\\
&\dots m\, n\, w_2\, \underline{w_1\, (n-1)\, w_3} \dots, \text{ with } m \in \{1, \dots, n-3\} \setminus \{w_1, w_2, w_3\},\\
&\dots m\, n\, w_1\, \underline{w_2\, (n-1)\, w_3} \dots, \text{ with } m \in \{1, \dots, n-3\} \setminus \{w_1, w_2, w_3\}.
\end{aligned}$$

- (**L7**): Again we split the construction into two parts. First we restrict a, b to lie in $\{1, \dots, n-3\} \setminus \{w_1, w_2, w_3\}$ and build the tours as described before. Second we create new tours $\dots \underline{a\, n\, (n-2)}\, (n-1) \dots,\ a \in \{1, \dots, n-3\} \setminus \{w_1, w_2, w_3\}$.
- (**L8**): As pointed out in step (**L5**), we restrict a to $\{1, \dots, n-3\}$ and form $\dots \underline{(n-1)\, a\, n} \dots$

This construction works out for $\bar{n} = 5$ and all $n \geq 7$. All in all this generates exactly one tour less than in the proof of Theorem 2.3 and so the inequality is facet defining for $P_{\mathbf{SQTSP}_n}, n \geq 5$. □

Inequalities (10) can also be interpreted as a special kind of subtour elimination constraint forbidding cycles of length three. This relation is not surprising, because, alternatively, the constraint can be derived by multiplying (and thereby lifting) $x_{ij}+x_{jk}+x_{ki} \leq 2$ by x_{ij} and using the definition of the y-variables. Further inequalities known to be valid for BQP are the *cycle-inequalities* [20]. Some of these can be visualized in our context, see Figure 2. For $\{i, j, k\} \subset V, |\{i, j, k\}| = 3$, we get $\sum_{ijl \in V^{\langle 3\rangle}, l \neq k} y_{ijl} + \sum_{jkl \in V^{\langle 3\rangle}, l \neq i} y_{jkl} + \sum_{kil \in V^{\langle 3\rangle}, l \neq j} y_{kil} \leq 1$ because 2-edge positions in the shape of a T are not allowed. By substituting (2) this simplifies to $x_{ij} + x_{ik} + x_{jk} - y_{ijk} - y_{ikj} - y_{jik} \leq 1$, which is again a triangle inequality (and a special cycle-inequality).

Theorem 3.3 *For $n \geq 6$ the inequalities*

$$x_{ij} + x_{ik} + x_{jk} - y_{ijk} - y_{ikj} - y_{jik} \leq 1 \tag{11}$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $i, j, k \in V, |\{i, j, k\}| = 3$.

Proof. Validity holds, because not all three x-variables can be one and if two are one, so is exactly one of the y-variables. We set, w. l. o. g., $i = 1, j = n-1, k = n$. Equality holds, $x_{\{1,n-1\}} + x_{\{1,n\}} + x_{\{n-1,n\}} - y_{\langle 1,n-1,n\rangle} - y_{\langle 1,n,n-1\rangle} - y_{\langle n-1,1,n\rangle} = 1$, if and only if exactly one or two of the three edges $\{1, n-1\}, \{1, n\}, \{n-1, n\}$ are contained in the tour. For $n = 6$ we verified the statement by means of a computer algebra package and for $n \geq 7$ the construction of the $f(n)$ affinely independent tours is similar to the construction in the proof of Theorem 2.3. Therefore we use the same notation and only mention the differences.

All tours $t \in C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2}$ contain the edge $\{n-1, n\}$. So it remains to look at steps (**L1**)–(**L8**). For this we set $w_1 = 1$ and $w_2, w_3 \in \{2, \ldots, n-2\}, w_2 \neq w_3$.

- (**L1**): Using the same construction, the nodes $w_1 = 1$ and n are adjacent.
- (**L2**): We only build the tour $\ldots m\,(n-1)\,o\,\underline{w_1\,n\,w_3}\ldots$ with $m, o \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}, m \neq o$, *i. e.*, the 2-edge $\langle w_2, n, w_3 \rangle$ is not used as an e_L^i here.
- (**L3**): The edge $\{w_1, n-1\}$ is contained in the tour.
- (**L4**), (**L6**): In the standard construction one of the edges $\{w_1, n-1\}, \{w_1, n\}$ is contained in the tours.
- (**L5**): We distinguish two cases. Either $w_1 \notin \{a, b\}$ then we set $m = w_1$, which implies an edge $\{w_1, n-1\}$, or $w_1 \in \{a, b\}$, which implies an edge $\{w_1, n\}$.
- (**L7**): We build tours $\ldots \underline{a\,n\,b}\,w_1\,(n{-}1)\ldots,\ a, b \in \{1, \ldots, n{-}2\} \setminus \{w_1, w_2, w_3\}, a < b$ which contain an edge $\{w_1, n-1\}$.
- (**L8**): If $a = w_1$ the tour contains both edges $\{w_1, n-1\}, \{w_1, n\}$. In all other cases we can position node w_1 next to node n.

This construction works for $\bar{n} = 5$ and all $n \geq 7$ and creates exactly one tour less than in the proof of Theorem 2.3. Thus, the inequality defines a facet of $P_{\mathbf{SQTSP}_n}, n \geq 6$. $\square$

Generalizing the idea of conflicting T-structures along a cycle $I_k = \{i_1, \ldots, i_k\} \subset V$ of odd length $|I_k| = k$ leads to

$$\sum_{l=1}^{k-2} \sum_{\substack{i_l i_{l+1} m \in V^{\langle 3 \rangle} \\ m \neq i_{l+2}}} y_{i_l i_{l+1} m} + \sum_{\substack{i_{k-1} i_k m \in V^{\langle 3 \rangle} \\ m \neq i_1}} y_{i_{k-1} i_k m} + \sum_{\substack{i_k i_1 m \in V^{\langle 3 \rangle} \\ m \neq i_2}} y_{i_k i_1 m} \leq \left\lfloor \frac{k}{2} \right\rfloor .$$

Via (2) these correspond to the following cycle-inequalities.

Observation 3.4 *For $n \geq 3$ the inequalities*

$$\sum_{ij \in C^{\{2\}}} x_{ij} - \sum_{ijk \in C} y_{ijk} \leq \left\lfloor \tfrac{|C|}{2} \right\rfloor \tag{12}$$

are valid for $P_{\mathbf{SQTSP}_n}$ for all 2-cycles $C \subset V^{\langle 3 \rangle}, |C| \geq 3$.

Proof. For any two consecutive x-variables that have value one, the corresponding y-variable also has value one. $\square$

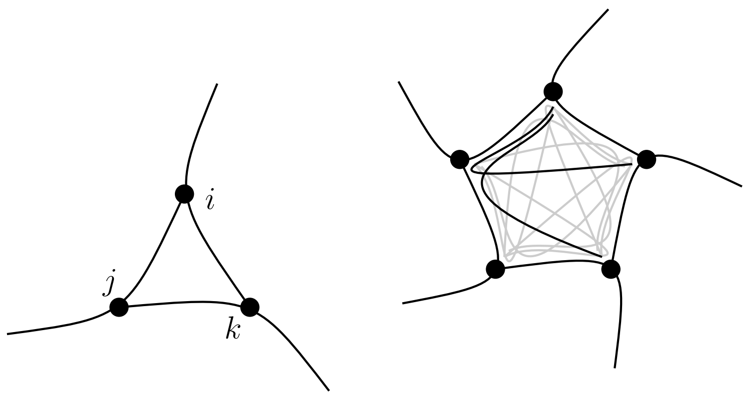


Figure 2: Visualization of certain cycle-inequalities

Remark 3.5 For $|C| = 5$ and $n \geq 5$, inequality (12) defines a facet of $P_{\mathbf{SQTSP}_n}$; a proof of this is given in the appendix. For $|C| \geq 6$, however, inequality (12) can be strengthened and is thus not facet defining. Indeed, for a 2-cycle $C = \{i_1i_2i_3, i_2i_3i_4, \dots, i_{|C|}i_1i_2\}, |C| \geq 6$, adding the variable $y_{\langle i_1,i_4,i_{|C|}\rangle}$ to the left hand side of the inequality preserves validity for $P_{\mathbf{SQTSP}_n}$, because the presence of $\langle i_1, i_4, i_{|C|}\rangle$ in a tour excludes the use of edges $\{i_1, i_{|C|}\}$, $\{i_3, i_4\}$, $\{i_4, i_5\}$ so that the remaining edges of $C^{\{2\}}$ can be grouped into two paths, one corresponding to $x_{\{i_1,i_2\}} + x_{\{i_2,i_3\}} - y_{\langle i_1,i_2,i_3\rangle} \leq 1$ and one to $\sum_{k=5}^{|C|-1} x_{\{i_k,i_{k+1}\}} - \sum_{k=6}^{|C|-1} y_{\langle i_{k-1},i_k,i_{k+1}\rangle} \leq \left\lceil \frac{|C|-5}{2} \right\rceil$. Hence, whenever $\langle i_1, i_4, i_{|C|}\rangle$ is in the tour, the strengthened left hand side sums to at most $1+1+\left\lceil \frac{|C|-5}{2} \right\rceil = \left\lceil \frac{|C|-1}{2} \right\rceil = \left\lfloor \frac{|C|}{2} \right\rfloor$.

The inequality remains valid if all edges and 2-edges of the induced subgraph are employed.

Observation 3.6 *For $n \geq 3$ the inequalities*

$$\sum_{ij \in S^{\{2\}}} x_{ij} - \sum_{ijk \in S^{\langle 3\rangle}} y_{ijk} \leq \left\lfloor \frac{|S|}{2} \right\rfloor \tag{13}$$

are valid for $P_{\mathbf{SQTSP}_n}$ for all $S \subset V$.

Proof. Whenever two x-variables indexed by incident edges within $S^{\{2\}}$ have value one, the corresponding y-variable is also one. Intersecting a tour with $S^{\{2\}}$ decomposes the tour into at most $\left\lfloor \frac{|S|}{2} \right\rfloor$ paths of at least one edge and only such path segments contribute one unit to the left hand side. □

In fact, inequalities (13) define facets for all odd $m \geq 3$ with $S \subset V, m = |S|$ for $n \geq \frac{3}{2}(m+1)$. We defer the proof of this to the appendix.

3.2 Conflicting edges inequalities

The conflicting edges inequalities presented next forbid subtours and T-structures. In the simplest case a subtour is implied if there is more than one path of length less or equal to two between two nodes $i, j \in V, i \neq j$, *i. e.*, an edge $\{i, j\} \in V^{\{2\}}$ or a 2-edge $\langle i, k, j\rangle \in V^{\langle 3\rangle}$.

Theorem 3.7 *For $n \geq 6$ the inequalities*

$$x_{ij} + \sum_{ikj \in V^{\langle 3\rangle}} y_{ikj} \leq 1 \tag{14}$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $ij \in V^{\{2\}}$.

Proof. For $n = 6, 7$ we verified the statement by means of a linear algebra package and for $n \geq 8$ the proof is similar to the proof of Theorem 2.3 but this time we need to adapt the $\bar{n}$-permutation-block used for $\bar{C}^{\bar{n},1}_{dim}$ as well as the iterative steps of $C^{\bar{n},2}_{dim}$. For the tours of $C^{\bar{n},3}_{dim}$ we only have to show that the desired structure can be achieved.

We set, w. l. o. g., $i = 1, j = 2$. In a tour satisfying $x_{12} + \sum_{1k2 \in V^{\langle 3\rangle}} y_{1k2} = 1$ either nodes 1 and 2 are adjacent or there is exactly one node between them. Thus, $\bar{C}^{\bar{n},1}_{dim}$ is formed for the choice of $\bar{n}$ by all tours of the form

$$\begin{cases} \ldots\, 1\, 2\, \ldots\, (\bar{n}+1)\, \varpi_{\bar{n}}\, n\, \ldots & \text{or} \\ \ldots\, 1\, h\, 2\, \ldots\, (\bar{n}+1)\, \varpi_{\bar{n}}\, n\, \ldots & \text{with } h \in \{3, \ldots, \bar{n}\}. \end{cases} \tag{15}$$

In comparison to taking all tours $\ldots\, (\bar{n}+1)\, \varpi_{\bar{n}}\, n\, \ldots$ as in the proof of Theorem 2.3 this reduces the rank by two in the case $\bar{n} = 5$ and by one for $\bar{n} = 6$. Thus, for $\bar{n} = 6$ the same approach still works if no more e^i_k are lost in the remainder of the proof. Therefore, we choose $\bar{n} = 6$, collect $r_6 - 1$ linearly independent tours of $\bar{C}^{\bar{n},1}_{dim}$ in the set $\tilde{C}^{\bar{n},1}_{dim}$ and proceed in constructing $\tilde{C}^{\bar{n}}_{dim} = \tilde{C}^{\bar{n},1}_{dim} \dot\cup \tilde{C}^{\bar{n},2}_{dim} \dot\cup \tilde{C}^{\bar{n},3}_{dim}$.

The set $\tilde{C}^{\bar{n},2}_{dim} = \bigcup_{\bar{n}<k<n-1} \tilde{T}_k, \tilde{T}_k = \{\tilde{t}^1_k, \ldots, \tilde{t}^{n_k}_n\}$, is built iteratively, similarly to $C^{\bar{n},2}_{dim}$. Again the aim is to construct tours during steps $\bar{n} < k < n-1$ whose incidence vectors are roots of (14) and form a lower triangular matrix on variables $\tilde{e}^i_k, i = 1, \ldots, n_k$.

The adapted iterative steps for $\bar{n} < k < n - 1$ are:

(i1) $\ldots\, \underline{a\, k\, 3}\, (k+1)\, \varpi_k\, n\, 1\, 2 \ldots$, for $a \in \{4, \ldots, k-1\}$
(2-edge $\langle k, 3, k+1\rangle$ is not used as $\tilde{e}^i_k$),

(i2) $\ldots\, 3\, \underline{k\, a\, (k+1)}\, \varpi_k\, n\, 1\, 2 \ldots$, for $a \in \{4, \ldots, k-1\}$,

(i3) $\ldots\, \underline{a\, k\, b}\, (k+1)\, \varpi_k\, n\, 1\, 2 \ldots$, for $a, b \in \{4, \ldots, k-1\}, a < b$,

(i4) $\ldots\, k\, \underline{a\, b\, (k+1)}\, \varpi_k\, n\, 1\, 2 \ldots$, for $a, b \in \{3, \ldots, k-1\}, a \neq b$,

(i5) $\begin{cases} \ldots\, (k+1)\, \varpi_k\, n\, 2\, \underline{1\, k\, a} \ldots, \\ \ldots\, (k+1)\, \varpi_k\, n\, 1\, \underline{2\, k\, a} \ldots, \end{cases}$ for $a \in \{3, \ldots, k-1\}$,

$$(\mathbf{i6})\quad \begin{cases} \dots k\,1\,\underline{2\,a\,(k+1)}\,\varpi_k\,n\dots, \\ \dots k\,2\,\underline{1\,a\,(k+1)}\,\varpi_k\,n\dots, \\ \dots k\,1\,\underline{a\,2\,(k+1)}\,\varpi_k\,n\dots, \\ \dots k\,2\,\underline{a\,1\,(k+1)}\,\varpi_k\,n\dots, \end{cases} \text{for } a \in \{3,\dots,k-1\},$$

$$(\mathbf{i7})\quad \begin{cases} \dots k\,\underline{1\,2\,(k+1)}\,\varpi_k\,n\dots, \\ \dots k\,\underline{2\,1\,(k+1)}\,\varpi_k\,n\dots, \end{cases}$$

$$(\mathbf{i8})\quad \dots \underline{1\,k\,2}\,3\,(k+1)\varpi_k\,n\dots,$$

$$(\mathbf{i9})\quad \begin{cases} \dots 2\,\underline{k\,1\,(k+1)}\,\varpi_k\,n\dots, \\ \dots 1\,\underline{k\,2\,(k+1)}\,\varpi_k\,n\dots, \end{cases}$$

$$(\mathbf{i10})\quad \dots 1\,2\,(k+1)\,\varpi_k\,\underline{n\,a\,b}\dots, \text{ for } a,b \in \{3,\dots,k\}, a \neq b, \{a,b\} \cap \{k\} \neq \emptyset,$$

$$(\mathbf{i11})\quad \begin{cases} \dots (k+1)\,\varpi_k\,\underline{n\,k\,1}\,2\dots, \\ \dots (k+1)\,\varpi_k\,\underline{n\,k\,2}\,1\dots, \\ \dots (k+1)\,\varpi_k\,\underline{n\,1\,k}\,2\dots, \\ \dots (k+1)\,\varpi_k\,\underline{n\,2\,k}\,1\dots. \end{cases}$$

In each tour either node 1 is next to node 2 or there is exactly one node between them.
Claim 1: $|C^{\bar{n},2}_{dim}| = |\tilde{C}^{\bar{n},2}_{dim}|$.
Proof of Claim 1.

$$\begin{aligned} |\tilde{T}_k| &= \underbrace{(k-4)}_{(\mathbf{i1})} + \underbrace{(k-4)}_{(\mathbf{i2})} + \underbrace{\binom{k-4}{2}}_{(\mathbf{i3})} + \underbrace{(k-3)(k-4)}_{(\mathbf{i4})} + \underbrace{2(k-3)}_{(\mathbf{i5})} \\ &\quad + \underbrace{4(k-3)}_{(\mathbf{i6})} + \underbrace{2}_{(\mathbf{i7})} + \underbrace{1}_{(\mathbf{i8})} + \underbrace{2}_{(\mathbf{i9})} + \underbrace{2(k-3)}_{(\mathbf{i10})} + \underbrace{4}_{(\mathbf{i11})} \\ &= \tfrac{3}{2}k^2 - \tfrac{3}{2}k - 1 = |T_k|, \end{aligned}$$

hence $|C^{\bar{n},2}_{dim}| = |\tilde{C}^{\bar{n},2}_{dim}|$ and the claim is proved.
Claim 2: Each $\tilde{e}^i_k$ fulfills

$$\tilde{e}^i_k \notin C \text{ for all } C \in \left(\tilde{C}^{\bar{n},1}_{dim} \cup \left(\bigcup_{\bar{n}<h<k} \tilde{T}_h \right) \cup \left(\bigcup_{1\leq h<i} \{\tilde{t}^h_k\} \right) \right).$$

Proof of Claim 2. Consider a fixed k with $\bar{n} < k < n-1$. In all previous tours $t \in \tilde{C}^{\bar{n},1}_{dim} \cup \left(\bigcup_{\bar{n}<h<k} \tilde{T}_h \right)$ node k is adjacent to node $k+1$ while node n is a neighbor of node $n-1$ and the next two nodes on the other side of n are out of $\{1,\dots,k-1\}$, so the underlined 2-edges have not appeared before. By construction, 2-edges $\tilde{e}^i_k$ and $\tilde{e}^{\hat{\imath}}_k$, $i \neq \hat{\imath}$, being built in the same step $(\mathbf{i}j)$ cannot be contained in the same tour. It remains to show that a 2-edge $\tilde{e}^i_k$ chosen in iteration step $(\mathbf{i}j)$ is not contained in a tour of a previous iteration step $(\mathbf{i}l)$, $l < j$.

- Tours in step (**i2**): all tours created in (**i1**) contain the 2-edge $\langle k, 3, k+1\rangle$.
- Tours in step (**i3**): all tours created in (**i1**)–(**i2**) contain the edge $\{3, k\}$.
- Tours in step (**i4**): in all tours created in (**i1**)–(**i3**) there is exactly one node between node k and node $k+1$.
- Tours in step (**i5**): in all tours created in (**i1**)–(**i3**) the edges $\{1, k\}, \{2, k\}$ are forbidden. With $\bar{n} = 6$ and therefore $n \geq 8$ it follows that node 2 is not adjacent to node k in (**i4**).
- Tours in step (**i6**): in all tours created in (**i1**)–(**i3**) there is exactly one node between node k and node $k+1$ and in (**i4**),(**i5**) the 2-edges $\tilde{e}_k^i$ used here are forbidden.
- Tours in steps (**i7**), (**i8**), (**i9**): the respective single 2-edges do not appear in the tours (**i**j) with smaller j.
- Tours in steps (**i10**), (**i11**): in all tours created in (**i1**)–(**i9**) the nodes n and k are separated by node $k+1$ on the one side and by at least two nodes on the other.

This completes the proof of Claim 2.

Note that (8) holds for $\tilde{C}_{dim}^{\bar{n},1} \dot{\cup} \tilde{C}_{dim}^{\bar{n},2}$, so by invoking Claim 2 of the proof of Theorem 2.3 we can make use of (**L1**)–(**L8**) if these admit tours as realizations that are roots of (14).

Claim 3: For each step (**L1**)–(**L8**) there is a tour having node 1 adjacent to node 2 or exactly one node between these two.

Proof of Claim 3. Choose $w_1, w_2, w_3 \in \{3, \ldots, n-2\}$.

- (**L1**), (**L7**): Either $\{a, b\} = \{1, 2\}$, *i. e.*, there is exactly node $n-1$ between the two nodes, or they can be placed next to each other.
- (**L2**)–(**L6**): put node 1 next to node 2.
- (**L8**): If $a \notin \{1, 2\}$ put nodes 1,2 next to each other, otherwise force a 2-edge $\langle 1, n, 2\rangle$.

In comparison to the proof of Theorem 2.3 we create exactly one tour less in the first step and the same number in steps two and three. This proves Theorem 3.7. □

The idea used for Theorem 3.7 can be extended, see Figure 3.

Theorem 3.8 *For $n \geq 6$ the inequalities*

$$x_{ij} + \sum_{ikj \in V^{\langle 3\rangle}, k \in S} y_{ikj} + \sum_{kil \in V^{\langle 3\rangle}, k,l \in T} y_{kil} \leq 1 \qquad (16)$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $ij \in V^{\{2\}}$ and for all $S \cup T = V \setminus \{i, j\}, S \cap T = \emptyset, |S| \geq 1, |T| \geq 3$.

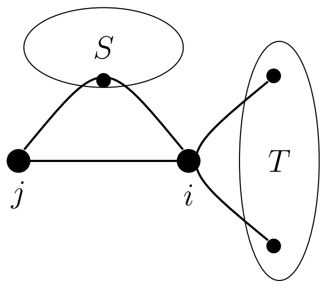


Figure 3: One can choose at most one out of this edge (straight line) and the 2-edges (curved lines).

Proof. We set, w. l. o. g., $i = n, j = n-1$ and use the notation $T = \{t_1, \ldots, t_{|T|}\}, S = \{s_1, \ldots, s_{|S|}\}$ with $|T| \geq 3, |S| \geq 1$. Roots of (16) satisfy

$$x_{\{n-1,n\}} + \sum_{\langle n-1,k,n\rangle \in V^{\langle 3\rangle}, k\in S} y_{\langle n-1,k,n\rangle} + \sum_{\langle k,n,l\rangle \in V^{\langle 3\rangle}, k,l\in T} y_{\langle k,n,l\rangle} = 1.$$

Thus, either the edge $\{n-1, n\}$ is contained in the tour, or there is exactly one node between nodes $n-1$ and n and this node belongs to set S, or n lies between two nodes which belong to set T. For $n = 6, |S| = 1, |T| = 3$ we verified the assumption using a linear algebra package. For $n \geq 7$ the proof is similar to the proof of Theorem 2.3, we use the same notation and only explain the necessary adaptations.

All tours which belong to $C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2}$ contain the edge $\{n-1, n\}$ and therefore it remains to adapt the third step. Setting $\{w_1, w_2, w_3\} = \{t_1, t_2, t_3\}$ steps (**L1**)–(**L4**) can be performed without any problems because node n lies between two nodes belonging to set T. The next steps (**ST1**)–(**ST6**) replace (**L5**)–(**L8**) and for $|S| \geq 1, |T| \geq 3$ these constructions are possible.

(**ST1**) $\ldots (n-1)\, \underline{s_1\, n\, a} \ldots$, for $a \in (S \cup T) \setminus \{s_1\}$
(the 2-edge $\langle n-1, s_1, n\rangle$ is not used as an e_L^i),

(**ST2**) $\ldots \underline{(n-1)\, a\, n}\, s_1 \ldots$, for $a \in S \setminus \{s_1\}$,

(**ST3**) $\begin{cases} \ldots (n-1)\, \underline{a\, n\, b} \ldots, & \text{for } a, b \in S \setminus \{s_1\}, a < b, \\ \ldots (n-1)\, \underline{a\, n\, b} \ldots, & \text{for } a \in S \setminus \{s_1\}, b \in T, \end{cases}$

(**ST4**) $\ldots (n-1)\, s_1\, \underline{a\, n\, b} \ldots$, for $a, b \in T, \{a, b\} \nsubseteq \{w_1, w_2, w_3\}, a < b$,

(**ST5**) $\ldots s_1\, \underline{(n-1)\, a\, n}\, m \ldots$, for $a \in T$ with $m \in T, m \neq a$,

(**ST6**) $\begin{cases} \ldots \underline{w_1\, (n-1)\, w_2}\, n\, w_3 \ldots, \\ \ldots \underline{w_1\, (n-1)\, w_3}\, n\, w_2 \ldots, \\ \ldots \underline{w_2\, (n-1)\, w_3}\, n\, w_1 \ldots . \end{cases}$

Because all tours in $C_{dim}^{\bar{n},1} \cup C_{dim}^{\bar{n},2}$ contain the edge $\{n-1, n\}$ the underlined 2-edges of (**ST1**)–(**ST6**) have not been used in these steps. Furthermore the e_L^i of tours built during one of these steps are in conflict. It remains to show Claim 1.
Claim 1: The 2-edges e_L^i of step (**ST**j) are not contained in tours in (**L1**)–(**L4**) and (**ST**l), $l < j$.
Proof of Claim 1.

- Tours in step (**ST1**): in all tours of (**L1**)–(**L4**) node n lies between two of the nodes $w_1, w_2, w_3 \in T$.
- Tours in step (**ST2**): in all tours of (**L1**)–(**L4**) two nodes lie between n and $n-1$ and the tours in (**ST1**) contain the 2-edge $\langle n-1, s_1, n\rangle$.
- Tours in step (**ST3**): in all tours of (**L1**)–(**L4**) node n lies between two of the nodes $w_1, w_2, w_3 \in T$ and the tours in (**ST1**)–(**ST2**) contain the 2-edge $\{s_1, n\}$.
- Tours in step (**ST4**): in all tours of (**L1**)–(**L4**) node n lies between two of the nodes $w_1, w_2, w_3 \in T$ and in the tours in (**ST1**)–(**ST3**) node n is adjacent to some node $s \in S$.
- Tours in step (**ST5**): in all tours of (**L1**)–(**L4**), (**ST4**) two nodes lie between n and $n-1$, and in the tours of (**ST1**)–(**ST3**) a node $s \in S$ lies between nodes $n-1, n$.
- Tours in step (**ST6**): in all tours of (**L1**)–(**L4**) the 2-edges $\langle w_1, n-1, w_2\rangle$, $\langle w_1, n-1, w_3\rangle$, $\langle w_2, n-1, w_3\rangle$ are forbidden explicitly. In all tours of (**ST1**)–(**ST5**) node $n-1$ is adjacent to at least one node $s \in S$.

This proves Claim 1.
Claim 2: We build exactly one tour less than in the proof of Theorem 2.3.
Proof of Claim 2. It suffices to compare $|C_{dim}^{\bar{n},3}| = n^2 - 4n + 3$ with the number of tours created in steps (**L1**)–(**L4**), (**ST1**)–(**ST6**). The number of tours equals

$$\underbrace{\binom{n-4}{2}}_{\textbf{(L1)}} + \underbrace{(1+1)}_{\textbf{(L2)}} + \underbrace{(n-5)}_{\textbf{(L3)}} + \underbrace{(n-5)}_{\textbf{(L4)}}$$

$$+ \underbrace{(|S|-1+|T|)}_{\textbf{(ST1)}} + \underbrace{(|S|-1)}_{\textbf{(ST2)}} + \underbrace{\left[\binom{|S|-1}{2} + (|S|-1)|T|\right]}_{\textbf{(ST3)}} + \underbrace{\left[\binom{|T|}{2} - 3\right]}_{\textbf{(ST4)}} + \underbrace{|T|}_{\textbf{(ST5)}} + \underbrace{3}_{\textbf{(ST6)}}$$

$$= \tfrac{1}{2}n^2 - \tfrac{5}{2}n + 2 + \tfrac{1}{2}(\underbrace{|S|+|T|}_{n-2})^2 + \tfrac{1}{2}(\underbrace{|S|+|T|}_{n-2}) - 1 = n^2 - 4n + 2 = |C_{dim}^{\bar{n},3}| - 1.$$

This completes the proof. □

In the case $|T| = 2$ further strengthenings are possible.

Theorem 3.9 *For $n \geq 6$ the inequalities*

$$x_{ij} + \sum_{ikj \in V^{\langle 3 \rangle}, k \in S} y_{ikj} + y_{t_1 i t_2} + y_{t_1 j t_2} \leq 1 \tag{17}$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $ij \in V^{\{2\}}$ and for all $S \cup T = V \setminus \{i, j\}$, $S \cap T = \emptyset$, $T = \{t_1, t_2\}$.

Proof. Validity holds because all edges contained in the inequality are in pairwise conflict. We set, w. l. o. g., $i = 1, j = 2, T = \{n-1, n\}, S = \{3, \ldots, n-2\}$. Roots of (17) satisfy

$$x_{12} + \sum_{1k2 \in V^{\langle 3 \rangle}, k \in S} y_{1k2} + y_{(n-1)1n} + y_{(n-1)2n} = 1. \tag{18}$$

Such a tour either contains the edge $\{1, 2\}$, or there is exactly one node $s \in S$ between nodes 1,2, or one of the nodes 1,2 lies between the nodes $(n-1)$ and n. For $n = 6, 7$ we verified the assumption by means of a linear algebra package and for $n \geq 8$ the proof is similar to the proofs of Theorem 2.3 and Theorem 3.7, so we use the same notation. We start with setting up an appropriate $\bar{n}$-permutation block with $\bar{n} = 6$. As in (15), in all tours of this block either node 1 is adjacent to node 2 or exactly one node $\bar{s} \in \{3, 4, 5, 6\} \subseteq S$ lies between them and in each case these first six elements are followed by $(\bar{n}+1)\, \varpi_{\bar{n}}\, n$. Like in the proof of Theorem 3.7, the resulting number of linearly independent tours is one less than $|C^{\bar{n},1}_{dim}|$ of the proof of Theorem 2.3. Furthermore, the iterative part (**i1**)–(**i11**) of the proof of Theorem 3.7 is also applicable here, because $T = \{n-1, n\}$ and so by claims 1 and 2 of the proof of Theorem 3.7 the number of tours equals $|C^{\bar{n},2}_{dim}|$. It remains to adapt the third step constructing the set $\tilde{C}^{\bar{n},3}_{dim}$.

(**S2.1**) $\ldots \underline{a\,(n-1)\,b}\,3\,n\,4\,1\,2 \ldots$, for $a, b \in \{5, \ldots, n-2\}, a < b$
(we do not use the 2-edge $\langle 3, n, 4 \rangle$ as an e^i_L),

(**S2.2**) $\begin{cases} \ldots 5\,(n-1)\,6\,\underline{3\,n\,2}\,1 \ldots, \\ \ldots 5\,(n-1)\,6\,\underline{4\,n\,2}\,1 \ldots, \end{cases}$

(**S2.3**) $\begin{cases} \ldots \underline{a\,(n-1)\,3}\,4\,n\,2\,1 \ldots, \\ \ldots \underline{a\,(n-1)\,4}\,3\,n\,2\,1 \ldots, \end{cases}$ for $a \in \{5, \ldots, n-2\}$,

(**S2.4**) $\begin{cases} \ldots 6\,(n-1)\,4\,\underline{3\,n\,5}\,1\,2 \ldots, \\ \ldots 6\,(n-1)\,3\,\underline{4\,n\,5}\,1\,2 \ldots, \end{cases}$

(**S2.5**) $\begin{cases} \ldots 2\,\underline{1\,(n-1)\,a}\,m\,n\,o \ldots, \\ \ldots 1\,\underline{2\,(n-1)\,a}\,m\,n\,o \ldots, \end{cases}$ $\begin{cases} \text{for } a \in \{3, \ldots, n-2\} \\ \text{with } m, o \in \{3, 4, 5\} \setminus \{a\}, m \neq o, \end{cases}$

(**S2.6**) $\ldots \underline{a\,n\,b}\,1\,2\,(n-1) \ldots,$ $\begin{cases} \text{for } a, b \in \{3, \ldots, n-2\}, a < b, \\ \{a, b\} \notin \{\{3, 4\}, \{3, 5\}, \{4, 5\}\}, \end{cases}$

(**S2.7**) $\ldots 5\,n\,6\,\underline{3\,(n-1)\,4}\,1\,2 \ldots,$

(**S2.8**) $\begin{cases} \dots 2\,\underline{1\,n\,a}\,m\,(n-1)\dots, & \text{for } a \in \{3,\dots,n-2\} \\ \dots 1\,\underline{2\,n\,a}\,m\,(n-1)\dots, & \text{for } a \in \{5,\dots,n-2\} \end{cases}$ with $m \in \{3,4\} \setminus \{a\}, 3 \in \{a,m\}$,

(**S2.9**) $\dots \underline{(n-1)\,a\,n}\,1\,2\dots$, for $a \in \{3,\dots,n-2\}$,

(**S2.10**) $\begin{cases} \dots 3\,\underline{(n-1)\,1\,n}\,4\dots, \\ \dots 3\,\underline{(n-1)\,2\,n}\,4\dots, \end{cases}$

(**S2.11**) $\begin{cases} \dots n\,\underline{1\,(n-1)\,2}\dots, \\ \dots (n-1)\,\underline{1\,n\,2}\dots. \end{cases}$

For $\bar{n} = 6, n \geq 8$, these yield tours whose incidence vectors satisfy (18). Indeed, the tours in (**S2.1**)–(**S2.9**) contain edge $\{1,2\}$ and in (**S2.10**)–(**S2.11**) all tours contain the 2-edge $\langle n-1,1,n\rangle$ or $\langle n-1,2,n\rangle$.

Claim 1: Each underlined 2-edge e_L^i has not appeared in previous tours.

Proof of Claim 1. Because n and $n-1$ are adjacent in all previous tours, we only have to show that a 2-edge e_L^i used in step (**S2.**j) is not used in tours of steps (**S2.**l), $l < j$.

- Tours in step (**S2.2**): the tours in (**S2.1**) contain the 2-edge $\langle 3,n,4\rangle$.
- Tours in step (**S2.3**): in the tours of (**S2.1**), (**S2.2**) the edges $\{3,n-1\}$ and $\{4,n-1\}$ are forbidden.
- Tours in step (**S2.4**): in (**S2.1**)–(**S2.3**) node n is adjacent to two of the nodes 2,3,4.
- Tours in step (**S2.5**): in all tours in (**S2.1**)–(**S2.4**) the edges $\{1,n-1\}, \{2,n-1\}$ are forbidden.
- Tours in step (**S2.6**): in the tours in (**S2.1**)–(**S2.5**) only the 2-edges $\langle 3,n,4\rangle$, $\langle 3,n,5\rangle$, $\langle 4,n,5\rangle$ are used.
- Tours in step (**S2.7**): in the tours in (**S2.1**)–(**S2.6**) at least one of the nodes 3,4 is not adjacent to node $n-1$.
- Tours in step (**S2.8**): in the tours in (**S2.1**)–(**S2.7**) node 1 is not adjacent to node n, in (**S2.1**), (**S2.4**)–(**S2.7**) node 2 is not adjacent to node n and in (**S2.2**)–(**S2.3**) the tours contain the 2-edges $\langle 2,n,3\rangle$, $\langle 2,n,4\rangle$.
- Tours in steps (**S2.9**), (**S2.10**): in the tours in (**S2.1**)–(**S2.8**) there are at least two nodes between nodes $n-1, n$.
- Tours in step (**S2.11**): the tours in step (**S2.1**)–(**S2.9**) contain edge $\{1,2\}$ and in (**S2.10**) the two edges of (**S2.11**) do not appear.

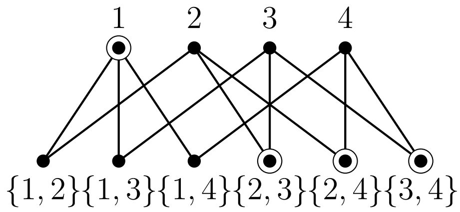


Figure 4: The graph $\tilde{G}$ for $n = 6$ and $i = 5, j = 6$ with marked solution $S = \{1\}, T = \{2, 3, 4\}$.

It remains to calculate $|\tilde{C}_{dim}^{\bar{n},3}|$.

$$|\tilde{C}_{dim}^{\bar{n},3}| = \underbrace{\left[\binom{n-2}{2} - 1\right]}_{(\textbf{S2.1})+(\textbf{S2.3})+(\textbf{S2.5})+(\textbf{S2.7})} + \underbrace{\left[\binom{n-2}{2} - 2\right]}_{(\textbf{S2.2})+(\textbf{S2.4})+(\textbf{S2.6})+(\textbf{S2.8})} + \underbrace{(n-2)}_{(\textbf{S2.9})+(\textbf{S2.10})} + \underbrace{2}_{(\textbf{S2.11})}$$
$$= n^2 - 4n + 3 = |C_{dim}^{\bar{n},3}|$$

With the introductory considerations Theorem 3.9 follows. □

While (14) and (17) only comprise a polynomial number of inequalities, there are exponentially many inequalities of type (16) and it is not clear in advance if one can separate them in polynomial time. The answer to this is given next.

Theorem 3.10 *The separation problem for the conflicting edges inequalities (16) can be solved in polynomial time.*

Proof. We are given a fractional solution $(\bar{x}, \bar{y})$ of a relaxation of $\mathbf{SQTSP}_n$. Fix $i, j \in V, i \neq j$. Then we want to find $S, T \subset V$ as in inequality (16) maximizing the sum

$$\sum_{ikj \in V^{\langle 3 \rangle}:\, k \in S} \bar{y}_{ikj} + \sum_{kil \in V^{\langle 3 \rangle}:\, k,l \in T} \bar{y}_{kil}.$$

For this purpose we construct two node sets $\tilde{V}_1 = V \setminus \{i, j\}$ and $\tilde{V}_2 = \{\{k, l\} \colon k, l \in V \setminus \{i, j\}, k \neq l\}$ and from this we build an undirected bipartite graph $\tilde{G} = (\tilde{V}, \tilde{E})$ with node set $\tilde{V} = \tilde{V}_1 \cup \tilde{V}_2$ and edge set $\tilde{E} = \big\{\{m, \{k, l\}\} \colon m \in \{k, l\} \in \tilde{V}\big\}$ (see Figure 4 for an illustration). The selection of node $v \in \tilde{V}_1$ corresponds to the assignment of v to S and choosing a node $\{k, l\} \in \tilde{V}_2$ to the assignment of k and l to T. Setting the weight of each node $v \in \tilde{V}_1$ to $\bar{y}_{ivj}$ and of $\{k, l\} \in \tilde{V}_2$ to $\bar{y}_{kil}$ the separation problem reduces to the problem of finding a maximum weight independent set in a bipartite graph. This problem is known to be solvable in polynomial time, see, *e. g.*, [9]. □

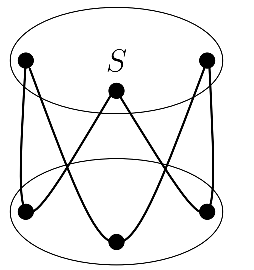


Figure 5: Case $n = 6, |S| = 3$: For this tour, the sum appearing in inequality (20) is zero.

3.3 The extended subtour elimination constraints

In the description of the formulations for $P_{\mathbf{SQTSP}_n}$, inequalities (3) are the subtour elimination constraints. These require that any tour has to leave any subset $S \subset V$, $1 \leq |S| \leq n-1$, and may be rewritten, via (2), in terms of y-variables,

$$\sum_{\substack{ijk \in V^{\langle 3 \rangle}: \\ i \in S, j,k \in V \setminus S}} y_{ijk} + 2 \cdot \sum_{\substack{ijk \in V^{\langle 3 \rangle}: \\ i,k \in S, j \in V \setminus S}} y_{ijk} \geq 2. \tag{19}$$

In some cases (19) can be improved. *E. g.*, the 2-edges immediately reentering set S after visiting one exterior node, *i. e.*, $y_{ijk}, i, k \in S, j \in V \setminus S$, may be considered as not exiting S after all and may be excluded from the left hand side if $|S| < \frac{n}{2}$. The condition $|S| < \frac{n}{2}$ is needed because in the case of $|S| \geq \frac{n}{2}$ some tours over n nodes may visit all exterior nodes only by such reentering 2-edges (see Figure 5). This leads to Theorem 3.11.

Theorem 3.11 *For $n \geq 6$ the inequalities*

$$\sum_{\substack{ijk \in V^{\langle 3 \rangle}: \\ i \in S, j,k \in V \setminus S}} y_{ijk} \geq 2 \tag{20}$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $S \subset V, 2 \leq |S| < \frac{n}{2}$.

Proof. Any tour must visit at least two nodes outside S consecutively because $|S| < \frac{n}{2}$. The two 2-arcs entering a corresponding exterior segment of the tour show the validity of the inequality. For $S = \{i, j\}$ the inequality is facet defining by Theorem 3.7, because

$$\begin{aligned}
& \sum_{ikl \in V^{\langle 3 \rangle}, j \notin \{k,l\}} y_{ikl} + \sum_{jkl \in V^{\langle 3 \rangle}, i \notin \{k,l\}} y_{jkl} \geq 2 \\
\overset{(2)}{\iff} & \underbrace{\sum_{ik \in V^{\{2\}}, k \neq j} x_{ik}}_{=2-x_{ij} \text{ (by (1))}} - \sum_{ikj \in V^{\langle 3 \rangle}} y_{ikj} + \underbrace{\sum_{jk \in V^{\{2\}}, k \neq i} x_{jk}}_{=2-x_{ij} \text{ (by (1))}} - \sum_{ikj \in V^{\langle 3 \rangle}} y_{ikj} \geq 2 \\
\iff & x_{ij} + \sum_{ikj \in V^{\langle 3 \rangle}} y_{ikj} \leq 1.
\end{aligned}$$

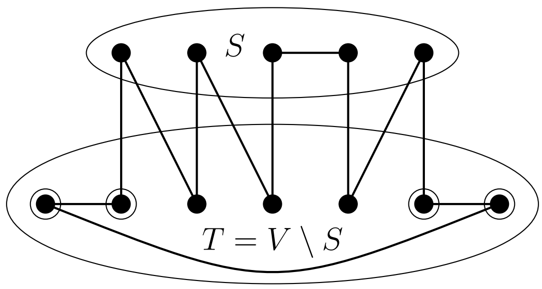


Figure 6: The incidence vector of the shown tour fulfills $\sum_{ijk \in V^{\langle 3 \rangle}:\, i \in S, j,k \in V \setminus S} y_{ijk} = 2$. The marked nodes belong to the only block of nodes in $V \setminus S$ with more than one node.

Thus we may assume $|S| \geq 3$ and $n \geq 7$. For $n = 7$ we verified the statement with a computer algebra system, so let $n \geq 8$ and consider, w. l. o. g., $T := \{t_1 = 1, t_2 = 2, \dots, t_{|T|} = |T|\}$, $|T| > \frac{n}{2}$ and $S := V \setminus T = \{s_1 = |T|+1, \dots, s_{|S|-1} = n-1, s_{|S|} = n\}$. Again, we use the proof-framework of Theorem 2.3 with its notation and explain the differences only. An incidence vector of a tour satisfies (20) with equality, $\sum_{ijk \in V^{\langle 3 \rangle}:\, i \in S, j,k \in V \setminus S} y_{ijk} = 2$, if deleting S from the tour decomposes the tour into isolated nodes and exactly one path consisting of at least two nodes (like in Figure 6), *i. e.*, the tours have the structure

$$\overbrace{\underbrace{t_{i_1}, t_{i_2}, \dots t_{i_m}}_{\substack{\text{block of } T\text{-nodes} \\ \text{of size } m \geq 2}} \; \underbrace{s_{j_1}, s_{j_2}, \dots s_{j_o}}_{\substack{\text{block of } S\text{-nodes} \\ \text{of size } o \geq 1}}} \; \overbrace{t_{i_{m+1}} \; \underbrace{s_{k_1}, s_{k_2}, \dots s_{k_p}}_{\substack{\text{block of } S\text{-nodes} \\ \text{of size } p \geq 1}}} \; \dots \; \overbrace{t_{i_{|T|}} \; \underbrace{s_{l_1}, s_{l_2}, \dots s_{l_q}}_{\substack{\text{block of } S\text{-nodes} \\ \text{of size } q \geq 1}}} \; .$$

Set $C_{dim}^{\bar{n},1}$ is constructed for $\bar{n} = 5$ in the same way as in the proof of Theorem 2.3. Because nodes 1 to 5 belong to set T ($n \geq 8, |S| \geq 3, |S| < \frac{n}{2}$), the desired T-block-structure is obtained automatically. In the inductive part the same is true for steps (**I1**)–(**I5**) as long as $k \in T$.

It remains to adapt the steps for nodes $k \in S$. We distinguish the two cases $k = s_1$ and $k > s_1$. For $k = s_1$ the three steps (**I1**)–(**I3**) can still be used and are then followed by steps (**SEC1.1**)–(**SEC1.3**) below. In this, (**SEC1.1**) and (**SEC1.3**) replace (**I4**), whereas (**SEC1.2**) deals with the 2-edges of (**I5**). They read

(**SEC1.1**) $\dots \underline{a\, b\, s_2}\, \varpi_k\, n\, 1\, s_1 \dots$, for $a, b \in T \setminus \{1\}, a \neq b$ (the 2-edge $\langle n, 1, s_1 \rangle$ in not used as an e_k^i),

(**SEC1.2**) $\dots m\, o\, s_2\, \varpi_k\, \underline{n\, a\, b} \dots$, for $a, b \in (T \cup \{s_1\}), s_1 \in \{a, b\}, (a, b) \neq (1, s_1)$, with $m, o \in T \setminus \{1\}, |\{a, b, m, o\}| = 4$,

(**SEC1.3**) $\dots \underline{a\, b\, s_2}\, \varpi_k\, n\, s_1 \dots$, for $a, b \in T, 1 \in \{a, b\}, a \neq b$.

Note that in comparison to (**I5**) the element $\langle n, 1, s_1 \rangle$ is lost in (**SEC1.1**),(**SEC1.2**).

For $k = s_i, 2 \leq i, k \leq n-2$ the procedure is almost identical to (**I1**)–(**I5**) up to the splitting of (**I4**) into the two steps (**SEC*i*.4**) and (**SEC*i*.5**) and the modifications ensuring the desired structure. To this end, the position of all nodes $s \in S$ that are not mentioned explicitly is represented by $\bar{S}$ with arbitrary internal order.

(**SEC*i*.1**) $\ldots \underline{a\, s_i\, 1}\, s_{i+1}\, \varpi_k\, n\, \bar{S} \ldots$, for $a \in \{2, \ldots, s_{i-1}\}$,

(**SEC*i*.2**) $\ldots 1\, \underline{s_i\, a\, s_{i+1}}\, \varpi_k\, n\, \bar{S} \ldots$, for $a \in \{2, \ldots, s_{i-1}\}$,

(**SEC*i*.3**) $\ldots \underline{a\, s_i\, b}\, s_{i+1}\, \varpi_k\, n\, \bar{S} \ldots$, for $a, b \in \{2, \ldots, s_{i-1}\}, a < b$,

(**SEC*i*.4**) $\ldots \underline{a\, b\, s_{i+1}}\, \varpi_k\, n\, m\, \bar{S}\, s_i \ldots$, for $a, b \in T, a \neq b$, with $m \in T, |\{a, b, m\}| = 3$ ($|\bar{S}| \geq 1$ because $s_1 \in \bar{S}$),

(**SEC*i*.5**) $\ldots \bar{S}\, \underline{a\, b\, s_{i+1}}\, \varpi_k\, n \ldots$, for $a, b \in \{1, \ldots, s_{i-1}\}, a \neq b, \{a, b\} \cap S \neq \emptyset$,

(**SEC*i*.6**) $\ldots \bar{S}\, s_{i+1}\, \varpi_k\, \underline{n\, a\, b} \ldots$, for $a, b \in \{1, \ldots, s_i\}, a \neq b, s_i \in \{a, b\}$.

The tours form roots of (20). The proof that the underlined 2-edges have not been used before is analogous to the proof of Claim 1 of the proof of Theorem 2.3 and skipped here. The number of tours of the entire second group is $|C_{dim}^{\bar{n},2}| - 1$.

For the tours in $C_{dim}^{\bar{n},3}$ we specify the position of $\bar{S}$, apart from that the procedure is identical to (**L1**)–(**L8**). Fix $w_1, w_2, w_3 \in T, |\{w_1, w_2, w_3\}| = 3$.

(**LSEC1**) $\ldots \underline{a\, (n-1)\, b}\, \bar{S}\, w_1\, n\, w_2 \ldots$, for $a, b \in \{1, \ldots, n-2\} \setminus \{w_1, w_2\}, a < b$,

(**LSEC2**) $\begin{cases} \ldots m\, (n-1)\, o\, \bar{S}\, \underline{w_1\, n\, w_3} \ldots, \\ \ldots m\, (n-1)\, o\, \bar{S}\, \underline{w_2\, n\, w_3} \ldots, \end{cases}$ with $m, o \in T \setminus \{w_1, w_2, w_3\}$, $m \neq o$,

(**LSEC3**) $\ldots \underline{w_1\, (n-1)\, a}\, \bar{S}\, w_2\, n\, w_3 \ldots$, for $a \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}$,

(**LSEC4**) $\ldots \underline{w_2\, (n-1)\, a}\, \bar{S}\, w_1\, n\, w_3 \ldots$, for $a \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}$,

(**LSEC5**) $\ldots \underline{a\, n\, b}\, \bar{S}\, m\, (n-1)\, o \ldots$, for $a, b \in \{1, \ldots, n-2\}, a < b, |\{a, b\} \cap \{w_1, w_2, w_3\}| = 1$, with $m, o \in T, \{m, o\} \not\subseteq \{w_1, w_2, w_3\}, |\{a, b, m, o\}| = 4$,

(**LSEC6**) $\begin{cases} \ldots n\, w_3\, \bar{S}\, \underline{w_1\, (n-1)\, w_2} \ldots, \\ \ldots n\, w_2\, \bar{S}\, \underline{w_1\, (n-1)\, w_3} \ldots, \\ \ldots n\, w_1\, \bar{S}\, \underline{w_2\, (n-1)\, w_3} \ldots, \end{cases}$

(**LSEC7**) $\ldots \underline{a\, n\, b}\, \bar{S}\, m\, (n-1) \ldots$, for $a, b \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}, a < b$, with $m \in \{1, \ldots, n-2\}, |\{a, b, m\}| = 3$,

(**LSEC8**) $\ldots \underline{(n-1)\, a\, n}\, \bar{S} \ldots$, for $a \in \{1, \ldots, n-2\}$.

Again, the tours form roots of (20) and, as in Claim 2 of the proof of Theorem 2.3, the underlined 2-edges have not been used before, so we obtain the same number of tours $|C_{dim}^{\bar{n},3}|$ in this third step.

In total the construction results in $|C_{dim}^{\bar{n}}| - 1$ affinely independent tours, which proves Theorem 3.11. □

It is well known that (3) can be separated in polynomial time by solving a min-cut-problem between each pair of nodes [17]. As we will see, the situation changes for the *extended subtour elimination constraints* (20).

Given a weighted undirected 2-graph $\tilde{G} = (\tilde{V}, \tilde{E}, \tilde{w})$ with node set $\tilde{V}$, set of 2-edges $\tilde{E}$ and weights $\tilde{w}_e \geq 0, e \in \tilde{E}$ ($\tilde{w}_e$ polynomially bounded in $|\tilde{V}|$), the task is to determine a partition of $\tilde{V}$ into the sets $2 \leq |S| < \frac{n}{2}$, $S \cap T = \emptyset$, $S \cup T = \tilde{V}$ so that the cut value is minimized. For the cut value the weights of 2-edges $ijk \in \tilde{V}^{\langle 3 \rangle}$ are counted if $(i \in S \wedge \{j,k\} \subseteq T)$ or $(k \in S \wedge \{i,j\} \subseteq T)$. Note, 2-edges $ijk \in \tilde{V}^{\langle 3 \rangle}$ with $\{i,k\} \subseteq S, j \in T$ are not counted. We first consider a more general problem, the **(st_1t_2-cut)**-problem, where such a minimum cut is sought for $S \subset \tilde{V}$ without the cardinality constraints but under the condition that three special nodes $\{s, t_1, t_2\} \subset \tilde{V}$ are fixed in advance with $s \in S$ and $t_1, t_2 \in T$.

Lemma 3.12 *The problem (st_1t_2-**cut**) on a weighted undirected 2-graph as described above is* **NP***-complete.*

Proof. We prove the statement by reduction from MAX-2-SAT. Given a 2-SAT-formula with m variables and $|C|$ clauses, the task is to find a truth assignment for the variables maximizing the number of fulfilled clauses. Consider a 2-graph $\tilde{G} = (\tilde{V}, \tilde{E})$ with node set $\tilde{V} = \{s, t_1, t_2\} \cup \{x_i, \neg x_i \colon i = 1, \dots, m\}$. The idea is to include 2-edges in $\tilde{G}$ so that an optimal solution of **(st_1t_2-cut)** corresponds to an optimal MAX-2-SAT solution where literals belonging to S are set to *true* and literals belonging to T are set to *false*. To this end we encode a clause $(a \vee b), a, b \in \{x_i, \neg x_i \colon i = 1, \dots, m\}$ with a 2-edge $\langle s, \neg a, \neg b \rangle$ as the clause is *false* if and only if both literals are set to *false*. These 2-edges are assigned costs of value one. In order to ensure that, for each $i \in \{1, \dots, m\}$, exactly one literal of x_i and $\neg x_i$, is contained in T we add the 2-edges $\langle s, x_i, \neg x_i \rangle, \langle s, \neg x_i, x_i \rangle$ with costs $|C|+1$. Similarly for set S we introduce 2-edges $\langle x_i, t_1, t_2 \rangle, \langle \neg x_i, t_1, t_2 \rangle$ with costs $|C|+1$. All transformations are possible in polynomial time, so it remains to show correctness.

Let S be a solution of **(st_1t_2-cut)**. For each $i \in \{1, \dots, m\}$ at least one of the 2-edges $\langle s, x_i, \neg x_i \rangle, \langle s, \neg x_i, x_i \rangle, \langle x_i, t_1, t_2 \rangle$ and $\langle \neg x_i, t_1, t_2 \rangle$ is contained in the cut and causes costs of $|C| + 1$. Because $|\{x_i, \neg x_i\} \cap S| = 1$ if and only if exactly one of those 2-edges is contained in the cut, any solution corresponding to a proper assignment of the variables (*i. e.*, $\forall\, i \in \{1, \dots, m\} \colon |\{x_i, \neg x_i\} \cap S| = 1$) has costs at most $(|C|+1) \cdot m + |C|$ whereas the cut value of any other solution is at least $(|C|+1) \cdot (m+1)$. Therefore any optimal solution S^* corresponds to a proper assignment with as few 2-edges $\langle s, \neg a, \neg b \rangle$ as possible contained in the cut. Its objective value $(|C|+1) \cdot m + k$ corresponds to a solution of MAX-2-SAT with all literals in $S^* \setminus \{s\}$ set to *true* and k unsatisfied clauses.

For the converse direction we observe that for any 2-SAT assignment we can construct a solution of **(st_1t_2-cut)** with costs exactly $(|C|+1) \cdot m + k$ where k is the number of unsatisfied clauses by setting $S := \{s\} \cup \{x_i \colon x_i = true\} \cup \{\neg x_i \colon x_i = false\}$. This completes the proof. □

Lemma 3.12 is needed to prove Theorem 3.13 where the weight of a 2-edge is the value of the corresponding coordinate of a point contained in a relaxation of $\mathbf{SQTSP}_n$ fulfilling (1), (2), $x_{ij} \in [0,1]$ for all $ij \in V^{\{2\}}$ and $y_{ijk} \in [0,1]$ for all $ijk \in V^{\langle 3 \rangle}$.

Theorem 3.13 *The problem of finding a maximally violated extended subtour elimination constraint (20) for points* $(\bar{x}, \bar{y})$ *satisfying equality constraints (1), (2),* $x_{ij} \in [0,1]$ *for all* $ij \in V^{\{2\}}$ *and* $y_{ijk} \in [0,1]$ *for all* $ijk \in V^{\langle 3\rangle}$ *is* **NP***-complete.*

Proof. We prove this statement by reduction from **(**st_1t_2**-cut)**. Let $\overline{G} = (\overline{V}, \overline{E})$ be an undirected 2-graph with node set $\overline{V}, |\overline{V}| = \overline{n}$, and $\overline{E}$ the set of weighted undirected 2-edges with weights $w_e \geq 0$ polynomially bounded in $\overline{n}$ for all $e \in \overline{E}$. The set $\overline{V}$ contains three marked nodes $s, t_1, t_2 \in \overline{V}$. We construct a 2-graph $G' = (V', E')$ with node set

$$V' = \overline{V} \cup T' \cup \{s_1, s_2\} \cup (\overline{V} \times \{1, 2, 3\})$$

where T' is a set of artificial nodes to be introduced later and $\overline{E} \subset E'$. The inclusion of additional 2-edges in E' will ensure that in any optimal solution $(T' \cup \{t_1, t_2\}) \subset T$ and $\{s, s_1, s_2\} \subset S$. The challenge is to guarantee that all cost coefficients fulfill the degree constraints (1) and the flow constraints (2). As in (6) these can be transformed to

$$\sum_{ijk \in V'^{\langle 3\rangle}} w_{ijk} = 1, \text{ for all } j \in V', \tag{21}$$

and

$$\sum_{kij \in V'^{\langle 3\rangle}} w_{kij} = \sum_{ijk \in V'^{\langle 3\rangle}} w_{ijk}, \text{ for all } ij \in V'^{\{2\}}, \tag{22}$$

using only variables, here weights, corresponding to $V'^{\langle 3\rangle}$. We denote by

$$d(v) := \sum_{uvw \in V'^{\langle 3\rangle}} w_{uvw}$$

the *node degree* of $v \in V'$.

The node set T' and the 2-edge set E' are constructed by putting

$$T' := \{0_T, 1_T, \ldots, (18\overline{n} - 1)_T\}$$

and by successively adding 2-edges (and weights) to E'. In this construction, some 2-edges may be added more than once. In this case their weights are summed up.

(S1) In order to enforce $T' \subset T$, add 2-edges

$$E_{T'} := \bigcup_{k=0,6,\ldots,18\overline{n}-6} \Big\{ \langle a, b, c\rangle \colon a, b, c \in \{(k \bmod 18\overline{n})_T, \ldots, (k + 11 \bmod 18\overline{n})_T\}, \\ |\{a, b, c\}| = 3 \Big\}$$

with weights $w_e = 4 \sum_{f \in \overline{E}} w_f + 1 =: D$ for all $e \in E_{T'}$. Note, each k adds a complete 2-graph on the corresponding two successive blocks of 6 nodes, thereby forming a tightly linked giant cycle on these blocks of T'. This being done, all nodes in T' have a node degree $100D$.

(S2) Let $\langle i, j, k\rangle \in \overline{E}, i < k, w_{\langle i,j,k\rangle} > 0$. In order to ensure (22) for these original edges we complete them to a 2-cycle C_0 by inserting the 2-edges $\langle j, k, s_1\rangle, \langle k, s_1, s_2\rangle, \langle s_1, s_2, 0_T\rangle, \langle s_2, 0_T, 1_T\rangle, \langle 0_T, 1_T, 2_T\rangle, \dots, \langle (18\overline{n}-3)_T, (18\overline{n}-2)_T, (18\overline{n}-1)_T\rangle, \langle (18\overline{n}-2)_T, (18\overline{n}-1)_T, i\rangle, \langle (18\overline{n}-1)_T, i, j\rangle$, each with weight $w_{\langle i,j,k\rangle}$. In order to ensure the correct dependence of the objective value on the assignment of i, j, k to S or T two additional 2-cycles are needed:

1. Add $C_1 = \{\langle i, j, s_1\rangle, \langle j, s_1, s_2\rangle, \langle s_1, s_2, i\rangle, \langle s_2, i, j\rangle\}$, each with weight $\frac{w_{\langle i,j,k\rangle}}{2}$
2. and $C_2 = \{\langle j, k, 0_T\rangle, \langle k, 0_T, 1_T\rangle, \langle 0_T, 1_T, 2_T\rangle, \dots, \langle (18\overline{n}-3)_T, (18\overline{n}-2)_T, (18\overline{n}-1)_T\rangle, \langle (18\overline{n}-2)_T, (18\overline{n}-1)_T, j\rangle, \langle (18\overline{n}-1)_T, j, k\rangle\}$, each with weight $\frac{w_{\langle i,j,k\rangle}}{2}$.

Claim (S2).1 In any assignment of the nodes of V' to S and T with $T' \subset T, s_1, s_2 \in S$ the weights of the artificial 2-edges of (S2) in the cut sum up to $3w_{\langle i,j,k\rangle}$.

Proof of Claim (S2).1. Note that $\langle s_2, 0_T, 1_T\rangle \in C_0$ contributes $w_{\langle i,j,k\rangle}$ to each cut, so it remains to consider the other 2-edges.

- $i, j, k \in S$: The 2-edges $\langle i, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle \in C_0$ and $\langle j, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle, \langle k, 0_T, 1_T\rangle \in C_2$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $i, j \in S, k \in T$: $\langle i, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle \in C_0$ and $\langle j, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle, \langle j, k, 0_T\rangle \in C_2$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $i, k \in S, j \in T$: $\langle i, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle \in C_0$, $\langle k, j, (18\overline{n}-1)_T\rangle, \langle k, 0_T, 1_T\rangle \in C_2$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $i \in S, j, k \in T$: $\langle i, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle, \langle s_1, k, j\rangle \in C_0$ have weight $w_{\langle i,j,k\rangle} + w_{\langle i,j,k\rangle} = 2w_{\langle i,j,k\rangle}$.
- $j, k \in S, i \in T$: $\langle j, i, (18\overline{n}-1)_T\rangle \in C_0$ and $\langle j, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle, \langle k, 0_T, 1_T\rangle \in C_2$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $k \in S, i, j \in T$: $\langle s_2, i, j\rangle, \langle s_1, j, i\rangle \in C_1$ and $\langle k, j, (18\overline{n}-1)_T\rangle, \langle k, 0_T, 1_T\rangle \in C_2$ have weight $\frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $j \in S, i, k \in T$: $\langle j, i, (18\overline{n}-1)_T\rangle \in C_0$ and $\langle j, (18\overline{n}-1)_T, (18\overline{n}-2)_T\rangle, \langle j, k, 0_T\rangle \in C_2$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.
- $i, j, k \in T$: $\langle s_1, k, j\rangle \in C_0$ and $\langle i, j, s_1\rangle, \langle s_2, i, j\rangle \in C_1$ have weight $w_{\langle i,j,k\rangle} + \frac{w_{\langle i,j,k\rangle}}{2} + \frac{w_{\langle i,j,k\rangle}}{2} = 2w_{\langle i,j,k\rangle}$.

(S3) $t_1, t_2 \in T, s, s_1, s_2 \in S$ is enforced for optimal solutions by adding the 2-edges of the following 2-cycles, each 2-edge with weight D,

- $\langle t_1, 0_T, 1_T\rangle, \langle 0_T, 1_T, 2_T\rangle, \dots, \langle (18\overline{n}-2)_T, (18\overline{n}-1)_T), t_1\rangle, \langle (18\overline{n}-1)_T), t_1, 0_T\rangle$ and $\langle t_2, 0_T, 1_T\rangle, \langle 0_T, 1_T, 2_T\rangle, \dots, \langle (18\overline{n}-2)_T, (18\overline{n}-1)_T), t_2\rangle, \langle (18\overline{n}-1)_T), t_2, 0_T\rangle$,
- 2-triangles for $\{s, t_1, s_1\}$, *i. e.*, $\langle s, t_1, s_1\rangle, \langle t_1, s_1, s\rangle, \langle s_1, s, t_1\rangle$, and $\{s, t_2, s_2\}$,
- a 2-triangle for each $\{s_1, s_2, v\}$ with $v \in V' \setminus \{s_1, s_2\}$.

(S4) It remains to fulfill condition (21), *i. e.*, all node degrees need to have the same value K, so that dividing all weights by K yields (21) in the end. For this purpose, the artificial nodes $\overline{V} \times \{1,2,3\}$ were introduced. These will allow to compensate differences in degree via further 2-cycles. Currently, the node degrees read

node	current node degree
s	$< \underbrace{D}_{\overline{E} \text{ and } (S2)} + \underbrace{3D}_{(S3)}$
t_1, t_2	$< \underbrace{D}_{\overline{E} \text{ and } (S2)} + \underbrace{3D}_{(S3)}$
$v \in \overline{V} \setminus \{s, t_1, t_2\}$	$< \underbrace{D}_{\overline{E} \text{ and } (S2)} + \underbrace{D}_{(S3)}$
$v \in (\overline{V} \times \{1,2,3\})$	$= \underbrace{D}_{(S3)}$
s_1, s_2	$= \underbrace{\frac{3}{2} \cdot \sum_{f \in \overline{E}} w_f}_{(S2)} + \underbrace{D + 22 \cdot \overline{n} \cdot D}_{(S3)}$
$v \in T'$	$= \underbrace{100D}_{(S1)} + \underbrace{\frac{3}{2} \cdot \sum_{f \in \overline{E}} w_f}_{(S2)} + \underbrace{2D + D}_{(S3)}$

For $\overline{n} \geq 5$ the node degrees of s_1, s_2 which we denote by $K = \frac{3}{2} \cdot \sum_{f \in \overline{E}} w_f + D + 22 \cdot \overline{n} \cdot D$ are the highest ones. We increase the degree of $v \in \overline{V}$ by 2-cycles of length four with $\langle v, (v,1), (v,2) \rangle$, $\langle (v,1), (v,2), (v,3) \rangle$, $\langle (v,2), (v,3), v \rangle$, $\langle (v,3), v, (v,1) \rangle$. Then the degree of nodes in $(\overline{V} \times \{1,2,3\})$ can be filled up by 2-triangles for $\{(v,1), (v,2), (v,3)\}, v \in \overline{V}$. In the end, a 2-cycle over all elements in T' with weight $K - (100D + \frac{3}{2} \cdot \sum_{f \in \overline{V}^{\langle 3 \rangle}} w_f + 2D + D)$ completes the construction of G'.

It remains to show correctness. Recall, a 2-edge $\langle i,j,k \rangle \in V'^{\langle 3 \rangle}$ contributes its weight, if $((i \in S \wedge j,k \in T) \vee (k \in S \wedge i,j \in T))$.

First observe that for any feasible solution $S \subset V'$ with $3 \leq |S| < |V'|/2$, $(T' \cup \{t_1, t_2\}) \subseteq T$, $\{s, s_1, s_2\} \subseteq S$, $(\overline{V} \times \{1,2,3\}) \subseteq S$ and $\overline{V} \setminus \{s, t_1, t_2\}$ partitioned arbitrarily, the objective value is less than or equal to $4 \cdot \sum_{f \in \overline{E}} w_f$. Indeed, a constant offset of $3 \cdot \sum_{f \in \overline{V}^{\langle 3 \rangle}} w_f$ is caused by (S2) as proven in Claim (S2).1, all other artificial 2-edges do not contribute to the cut. For each node $v \in \overline{V}$ the three nodes $\{v\} \times \{1,2,3\}$ may jointly belong either to S or, if $v \in T$, to T. In both cases no costs arise. For solutions observing this structure the cut value is minimal for an optimal (st_1t_2-**cut**) solution on $\overline{V}$. Let z_{s,t_1,t_2} be the optimal value of (st_1t_2-**cut**) and denote by $z = z_{s,t_1,t_2} + 3 \cdot \sum_{f \in \overline{E}} w_f < D$ the value of a corresponding solution constructed within G'. We need to show that all solutions having not the described structure have higher objective value.

- $T' \subseteq T$: Consider a solution having a nonempty subset $T_s \subset T'$ with $T_s \subset S$. Then there is a $k \in \{0, 6, \ldots, 18\overline{n} - 6\}$ so that some of the nodes of $T_k := \{k, \ldots, k+5\}$ lie in S, *i. e.*, $T_k \cap S \neq \emptyset$. If $|T_k \cap S| \leq 4$ then costs of at least $D > 4 \cdot \sum_{f \in \overline{E}} w_f$ arise and this cannot be optimal. So consider the case $|T_k \cap S| > 4$. As T_k is completely

2-edge connected to $T_{(k+6 \mod 18\overline{n})}$ we may assume $|T_{(k+6 \mod 18\overline{n})} \cap S| > 4$ by the same argument. In the end we get $|T_k \cap S| > 4$ for all $k \in \{0, 6, \ldots, 18\overline{n}-6\}$ which contradicts $|S| < \frac{|V'|}{2}$. So we have $T' \subset T$ for any feasible solution with objective value less than D.

- $s_1, s_2 \in S$: Assume $s_1, s_2 \in T$ then costs of at least D arise because s_1, s_2 are connected via triangles to all other nodes by (S3) and there has to be at least one node $v \in V'$ with $v \in S$. So, w. l. o. g., the case $s_1 \in S, s_2 \in T$ remains. But this entails costs of at least D (and much higher) as s_1, s_2 are connected via triangles to all nodes $v \in T'$. This proves $s_1, s_2 \in S$.
- $t_1, t_2 \in T$: Assume, w. l. o. g., $t_1 \in S$. Because $0_T, 1_T \in T$, the 2-edge $\langle t_1, 0_T, 1_T \rangle$ produces costs of D by (S3) and this cannot be optimal.
- $s \in S$: Assume $s \in T$. Because $s_1 \in S, t_1 \in T$, the 2-edge $\langle s_1, s, t_1 \rangle$ produces costs of D by (S3) and this cannot be optimal.

Thus, any solution with objective value at most z has the desired structure and z is therefore the optimal value. Conversely, given an optimal solution with value z^* for G' the optimal value of **(st_1t_2-cut)** is $z^*_{s,t_1,t_2} = z^* - 3 \cdot \sum_{f \in \overline{E}} w_f$. □

Until now we have only considered subtour elimination constraint (19) for the case $|S| < \frac{n}{2}$. If $|S| \geq \frac{n}{2}$, inequality (20) fails to be valid for those tours that visit all external vertices via reentering 2-edges. Thus, to make (20) valid for all tours it suffices to add all reentering 2-edges over one fixed external node with weight 2. Alternatively, this may be viewed as a strengthening of (19), because all reentering 2-edges except for those running over one special vertex are dropped.

Theorem 3.14 *For $n \geq 6$ the inequalities*

$$\sum_{\substack{ijk \in V^{\langle 3 \rangle}: \\ i \in S, j,k \in V \setminus S}} y_{ijk} + 2 \cdot \sum_{\substack{i\bar{t}k \in V^{\langle 3 \rangle}: \\ i,k \in S}} y_{i\bar{t}k} \geq 2 \qquad (23)$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $S \subset V, \frac{n}{2} \leq |S| \leq n-3, \bar{t} \in V \setminus S$.

Proof. Validity holds, because for tours that visit two nodes of $V \setminus S$ consecutively the first sum yields at least 2 while all other tours use one of the 2-edges in the second sum when visiting $\bar{t}$. Theorem 3.2 proves the statement for $|S| = n-3$, because for $V \setminus S = \{i, j, \bar{t} = k\}$

$$\sum_{m \in S} [y_{mij} + y_{mji} + y_{mik} + y_{mki} + y_{mjk} + y_{mkj}] + \underbrace{2 \sum_{mko \in V^{\langle 3 \rangle}: m,o \in S} y_{mko}}_{2(1 - \sum_{m \in S}[y_{mki} + y_{mkj}] - y_{ikj}) \text{ by (6)}} \geq 2$$

$$\iff \underbrace{\sum_{m \in S} [y_{mij} + y_{mji}]}_{2x_{ij} - y_{jik} - y_{ijk} \text{ by (1)}} + \underbrace{\sum_{m \in S} [y_{mik} - y_{mki}]}_{x_{ik} - y_{jik} - x_{ik} + y_{ikj}} + \underbrace{\sum_{m \in S} [y_{mjk} - y_{mkj}]}_{-y_{ijk} + y_{ikj}} - 2y_{ikj} \geq 0$$

$$\iff 2x_{ij} - 2y_{jik} - 2y_{ijk} \geq 0 \iff x_{ij} \geq y_{kij} + y_{ijk}.$$

We first consider the case $\frac{n}{2} \leq |S| \leq n-5$ and defer the case $|S| = n-4$ to the end of the proof. Set, w.l.o.g., $S = \{s_1 = n-|S|+1, \ldots, s_{|S|-1} = n-1, s_{|S|} = n\}, V \setminus S = T = \{1 = t_1, 2 = t_2, \ldots, t_{|T|-1}, t_{|T|} = \bar{t}\}$. Deleting S in a tour corresponding to a root of inequality (23) decomposes the tour into isolated nodes in T and at most one path in T that must contain $\bar{t}$. We use the same proof structure and notation as in the proofs of Theorem 2.3 and Theorem 3.11. In particular, $|T| \geq 5$ so we may use the same $\bar{n}$-permutation block with $\bar{n} = 5$. As long as $k \in T$ in the iterative steps, (**I1**)–(**I5**) may be used without modification. The steps have to be adapted for $k \in S$, starting with a specific ordering for $k = s_1$ which is then followed by the usual iterative scheme for $k = s_i$, $2 \leq i < |S|-1$. The case $k = s_1$ proceeds along (**I1**)–(**I3**) and (**SEC1.1**)–(**SEC1.3**) but the positioning of node $\bar{t}$ requires additional care.

(**SUB1.1**) $\ldots \underline{a\, s_1\, 1}\, s_2\, \varpi_k\, n \ldots$, for $a \in T \setminus \{1\}$,
(the 2-edge $\langle s_1, 1, s_2\rangle$ is not used as an e_k^i.),

(**SUB1.2**) $\ldots 1\, \underline{s_1\, a\, s_2}\, \varpi_k\, n \ldots$, for $a \in T \setminus \{1, \bar{t}\}$
(the missing $\langle s_1, \bar{t}, s_2\rangle$ is compensated later in (**SUB$\bar{t}$1**)),

(**SUB1.3**) $\ldots \underline{a\, s_1\, b}\, s_2\, \varpi_k\, n \ldots$, for $a, b \in T \setminus \{1\}, a > b$ (this ensures $\bar{t}$ in the T-path),

(**SUB1.4**) $\ldots \underline{a\, b\, s_2}\, \varpi_k\, n\, 1\, s_1 \ldots$, for $a, b \in T \setminus \{1\}, a \neq b$
(the 2-edge $\langle n, 1, s_1\rangle$ is not used as an e_k^i and is the one 2-edge that is lost),

(**SUB1.5**) $\ldots m\, o\, s_2\, \varpi_k\, \underline{n\, a\, s_1} \ldots$, for $a \in T \setminus \{1, \bar{t}\}$ with $m, o \in T \setminus \{1\}, |\{a, m, o\}| = 3$
(the missing $\langle n, \bar{t}, s_1\rangle$ is compensated later in (**SUB$\bar{t}$1**)),

(**SUB1.6**) $\ldots m\, o\, s_2\, \varpi_k\, \underline{n\, s_1\, a} \ldots$, for $a \in T$ with $m, o \in T \setminus \{1\}, |\{a, m, o\}| = 3$,

(**SUB1.7**) $\ldots \underline{a\, b\, s_2}\, \varpi_k\, n\, s_1 \ldots$, for $a, b \in T, 1 \in \{a, b\}, a \neq b$.

For $k = s_i$, $2 \leq i < |S|-1$ the structure follows (**SEC*i*.1**)–(**SEC*i*.6**) of the proof of Theorem 3.11 with the same $\bar{S}$ defined there:

(**SUB*i*.1**) $\ldots \underline{a\, s_i\, 1}\, s_{i+1}\, \varpi_k\, n\, \bar{S} \ldots$, for $a \in \{2, \ldots, s_{i-1}\}$,

(**SUB*i*.2**) $\ldots 1\, \underline{s_i\, a\, s_{i+1}}\, \varpi_k\, n\, \bar{S} \ldots$, for $a \in \{2, \ldots, s_{i-1}\} \setminus \{\bar{t}\}$
(the missing $\langle s_i, \bar{t}, s_{i+1}\rangle$ is compensated later in (**SUB$\bar{t}$1**)),

(**SUB*i*.3**) $\begin{cases} \ldots \underline{a\, s_i\, b}\, s_{i+1}\, \varpi_k\, n\, \bar{S} \ldots, & \text{for } a, b \in \{2, \ldots, s_{i-1}\} \setminus \{\bar{t}\}, a < b, \\ \ldots \underline{\bar{t}\, s_i\, a}\, s_{i+1}\, \varpi_k\, n\, \bar{S} \ldots, & \text{for } a \in \{2, \ldots, s_{i-1}\} \setminus \{\bar{t}\}, \end{cases}$

(**SUB*i*.4**) $\ldots \underline{a\, b\, s_{i+1}}\, \varpi_k\, n\, m\, \bar{S}\, s_i \ldots$, for $a, b \in T, a \neq b$, with $m \in T \setminus \{\bar{t}\}, |\{a, b, m\}| = 3$,

(**SUB*i*.5**) $\ldots \bar{S} \underline{a\, b\, s_{i+1}}\, \varpi_k\, n \ldots$, for $a, b \in \{1, \ldots, s_{i-1}\} \setminus \{\bar{t}\}, a \neq b, \{a, b\} \cap S \neq \emptyset$
(the missing $\langle s_j, \bar{t}, s_{i+1}\rangle$, $1 \leq j < i$, is compensated later in (**SUB$\bar{t}$1**) and $\langle \bar{t}, s_j, s_{i+1}\rangle$, $1 \leq j < i$, is compensated in (**SUB*i*.7**)),

(**SUB*i*.6**) $\ldots m\,\bar{S}\,s_{i+1}\,\varpi_k\,\underline{n\,a\,b}\ldots$, for $a, b \in \{1, \ldots, s_i\}, a \neq \bar{t}, a \neq b, s_i \in \{a, b\}$ with $m \in T \setminus \{\bar{t}\}, |\{a, b, m\}| = 3$
(the missing $\langle n, \bar{t}, s_i\rangle$, $1 \le j < i$, is compensated later in (**SUB$\bar{t}$1**)),

(**SUB*i*.7**) $\ldots \underline{\bar{t}\,a\,s_{i+1}}\,\varpi_k\,n\,\bar{S}\ldots$, for $a \in \{s_1, \ldots, s_{i-1}\}$.

For the nodes $n-1, n$ we have specific steps that are organized close to (**L1**)–(**L8**) ((**L5**) and (**L7**) are subsumed in (**SUBL5**) and so (**L8**) corresponds to (**SUBL7**)). Fix $w_1, w_2, w_3 \in S \setminus \{n-1, n\}, |\{w_1, w_2, w_3\}| = 3$.

(**SUBL1**)
$$\begin{cases} \ldots a\,(n-1)\,b\,\bar{S}\,w_1\,n\,w_2\ldots, \text{ for } a, b \in T, a > b, \\ \ldots \overline{a\,(n-1)\,b}\,\bar{S}\,w_1\,n\,w_2\ldots, \text{ for } a, b \in S \setminus \{w_1, w_2, n-1, n\}, a > b, \\ \ldots \overline{\underline{a\,(n-1)\,b}}\,\bar{S}\,w_1\,n\,w_2\ldots, \text{ for } a \in T, b \in S \setminus \{w_1, w_2, n-1, n\} \end{cases}$$
(the 2-edge $\langle w_1, n, w_2\rangle$ is not used as an e_L^i),

(**SUBL2**)
$$\begin{cases} \ldots t_1\,(n-1)\,t_2\,\bar{S}\,\underline{w_1\,n\,w_3}\ldots, \\ \ldots t_1\,(n-1)\,t_2\,\bar{S}\,\underline{w_2\,n\,w_3}\ldots, \end{cases}$$

(**SUBL3**) $\ldots \underline{a\,(n-1)\,w_1}\,w_2\,n\,w_3\,\bar{S}\ldots$, for $a \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}$,

(**SUBL4**) $\ldots \underline{a\,(n-1)\,w_2}\,w_1\,n\,w_3\,\bar{S}\ldots$, for $a \in \{1, \ldots, n-2\} \setminus \{w_1, w_2, w_3\}$,

(**SUBL5**)
$$\begin{cases} \ldots \underline{a\,n\,b}\,\bar{S}\,(n-1)\ldots, \text{ for } a, b \in T, a > b, \\ \ldots \underline{a\,n\,b}\,\bar{S}\,(n-1)\ldots, \text{ for } a, b \in S \setminus \{n-1, n\}, \{a, b\} \not\subset \{w_1, w_2, w_3\}, a > b, \\ \ldots \underline{a\,n\,b}\,\bar{S}\,(n-1)\ldots, \text{ for } a \in T, b \in S \setminus \{n-1, n\}, \end{cases}$$

(**SUBL6**)
$$\begin{cases} \ldots n\,w_3\,\underline{w_1\,(n-1)\,w_2}\,\bar{S}\ldots, \\ \ldots n\,w_2\,\underline{w_1\,(n-1)\,w_3}\,\bar{S}\ldots, \\ \ldots n\,w_1\,\underline{w_2\,(n-1)\,w_3}\,\bar{S}\ldots, \end{cases}$$

(**SUBL7**) $\ldots \underline{(n-1)\,a\,n}\,\bar{S}\ldots$, for $a \in \{1, \ldots, n-2\} \setminus \{\bar{t}\}$
(the missing $\langle n-1, \bar{t}, n\rangle$, $1 \le j < i$, is compensated later in (**SUB$\bar{t}$1**)).

The only 2-edges missing in these lists in comparison to the proof of Theorem 3.11 are the 2-edges $\langle s_i, \bar{t}, s_j\rangle$ for $1 \le i < j \le |S|$, *i. e.*, those that require tours with no two consecutive T-nodes in order to form roots of (23). As none of these 2-edges have appeared in the tours above, the construction of this case is completed by the following last step.

(**SUB$\bar{t}$1**) $\underline{s_i\,\bar{t}\,s_j}\,\omega_{ij}$ for $1 \le i < j \le |S|$ where ω_{ij} denotes an appropriately completed alternating sequence of the remaining nodes in $T \setminus \{\bar{t}\}$ and in $S \setminus \{s_i, s_j\}$.

The construction above generates $|C_{dim}^{\bar{n}}| - 1$ affinely independent tours, that are roots of (23), and proves the statement for the case $\frac{n}{2} \le |S| \le n-5$.

For the remaining case $|S| = n-4$ we verified the case $n = 8$ by means of a computer algebra system and consider $n \ge 9$ in the following. For $|T| = 4$ the approach with an initial permutation block having $\bar{n} = 5$ can still be applied, but the block has to be set up with care so as to ensure that all generated tours are indeed roots of (23). In particular, using the same notation as before, the permutations having s_1 in the middle as well as the permutations $(\bar{t}, s_1, t_i, t_j, t_k)$ and $(t_i, t_j, t_k, s_1, \bar{t})$ with $i, j, k \in \{1, 2, 3\}$, $|\{i, j, k\}| = 3$ may not be used. This reduces the rank by 3 to 51. In exchange, the iterative process may start with (**SUB*i*.1**)–(**SUB*i*.7**) immediately, because the switch to the first element of S is already covered by the initial permutation block. As before the construction is completed by (**SUBL1**)–(**SUBL7**) and (**SUB$\bar{t}$1**) without further modifications. In counting the number of tours, we may use the formulas of Claim 3 of the proof of Theorem 2.3 if we reassign the 2-edges of (**SUB$\bar{t}$1**) to the corresponding steps where they were omitted. The latter is possible for all except the 2-edges $\langle s_1, \bar{t}, s_2\rangle$ and $\langle s_1, \bar{t}, n\rangle$ omitted in the missing initial iterative step for s_1, so we assign them to $r_{\bar{n}}$. All in all we obtain for $\bar{n} = 5$

$$\tfrac{1}{2}n^3 - 2n^2 + \tfrac{1}{2}n + 2 + (2 + 51) - \tfrac{1}{2}5^3 + \tfrac{3}{2}5 = \tfrac{1}{2}n^3 - 2n^2 + \tfrac{1}{2}n = f(n)$$

affinely independent tours, which completes the proof. □

The facets of Theorem 3.11 and Theorem 3.14 were originally derived from the subtour elimination constraints of $P_{\mathbf{STSP}_n}$ by a strengthening approach that can be applied to any valid inequality of $P_{\mathbf{STSP}_n}$ with nonnegative coefficients. It is based on the following simple concept which we state here for the current setting (there is an obvious generalization for arbitrary coefficients and arbitrary combinatorial problems).

Definition 3.15 *For a given $E' \subseteq V^{\{2\}}$, a family $\mathcal{F} = \{(F_e^2, F_e^3)\}_{e\in E'}$ of pairs of sets $F_e^2 \subseteq V^{\{2\}}, F_e^3 \subseteq V^{\langle 3\rangle}$ for $e \in E'$ is E'-*dominated *if for any tour $C \in \mathcal{C}_n$ there is a tour $\bar{C} \in \mathcal{C}_n$ with $\sum_{f\in F_e^2} x_f^C + \sum_{f\in F_e^3} y_f^C \leq x_e^{\bar{C}}$ for all $e \in E'$. It is *improving*, if $e \in F_e^2$ for $e \in E'$ and there is an $e \in E'$ with $F_e^2 \neq \{e\}$ or $F_e^3 \neq \emptyset$.*

Given a valid inequality of $P_{\mathbf{STSP}_n}$ with nonnegative coefficients any improving support-dominated family gives rise to a strengthened valid inequality for $P_{\mathbf{SQTSP}_n}$.

Observation 3.16 *Suppose $\sum_{e\in E'} a_e x_e \leq b$ is a valid inequality for $P_{\mathbf{STSP}_n}$ with $a_e \geq 0, e \in E'$ and let $\mathcal{F} = \{(F_e^2, F_e^3)\}_{e\in E'}$ be E'-dominated. Then the inequality*

$$\sum_{e\in E'} a_e\Big(\sum_{f\in F_e^2} x_f + \sum_{f\in F_e^3} y_f\Big) \leq b$$

is valid for $P_{\mathbf{SQTSP}_n}$.

Proof. For any $C \in \mathcal{C}_n$, there is, by Definition 3.15, a $\bar{C} \in \mathcal{C}_n$ so that

$$\sum_{e\in E'} a_e\Big(\sum_{f\in F_e^2} x_f^C + \sum_{f\in F_e^3} y_f^C\Big) \leq \sum_{e\in E'} a_e x_e^{\bar{C}} \leq b.$$

□

The facets of Theorem 3.11 make use of the following family.

Observation 3.17 *Given $E' \subset V^{\{2\}}$, suppose $|V(E')| < \frac{n}{2}$. Then*

$$\mathcal{F} = \left\{ (F^2_{ij} := \{ij\}, F^3_{ij} := \{ikj \in V^{\langle 3 \rangle} : ik \notin E', kj \notin E'\}) \right\}_{ij \in E'}$$

is E'-dominated. It is improving whenever $E' \neq \emptyset$.

Proof. If $\mathcal{F}$ is E'-dominated with $E' \neq \emptyset$, it is improving because any node $k \in V \setminus V(E')$ gives rise to a 2-edge $ikj \in F^3_{ij}$ for each $ij \in E'$. It remains to show that $\mathcal{F}$ is E'-dominated.

For $E' = \emptyset$ there is nothing to show, so we may assume $E' \neq \emptyset$ and thus $n \geq 5$. Given a tour $C \in \mathcal{C}_n$, we have to show the existence of a tour $\bar{C} \in \mathcal{C}_n$ satisfying the requirements of Definition 3.15.

For this let $F^C_2 = E' \cap C^{\{2\}}$ and $F^C_3 = \{ij \in E' : F^3_{ij} \cap C \neq \emptyset\}$. By the requirements on $\mathcal{F}$ and $n \geq 5$ we have $F^C_2 \cap F^C_3 = \emptyset$ (only for $n = 3$ a tour may contain the subsequences ij as well as ikj). Furthermore, for each $ij \in F^C_3$ there is a unique node k_{ij} with $\langle i, k_{ij}, j \rangle \in C$. We know

$$k_{ij} \notin V(F^C_2) \quad \text{for } ij \in F^C_3, \tag{24}$$

because $\{i, k_{ij}\} \in F^C_2 \subseteq E'$ or $\{j, k_{ij}\} \in F^C_2 \subseteq E'$ contradicts $\langle i, k_{ij}, j \rangle \in F^3_{ij}$.

Next, consider the graph $G^C_{\mathcal{F}} = (V, F^C_2 \cup F^C_3)$ and note that all its components are isolated nodes or paths. Indeed, consider a fixed node i appearing in C within the subsequence $\ldots a\,b\,i\,c\,d \ldots$, then only the two edges bi, ic and the two 2-edges abi, icd can give rise to edges $ij \in F^C_2 \cup F^C_3$. However, by (24) at most one of ai and bi and at most one of ic and id can be contained in $F^C_2 \cup F^C_3$, so the degree of i in $G^C_{\mathcal{F}}$ is at most two. Furthermore, i cannot lie on a cycle, because this would induce a subcycle of the tour C of length at most $2|V(F^C_2 \cup F^C_3)| < n$ as $V(F^C_2 \cup F^C_3) \subset V(E')$. Thus, by adding edges appropriately we may complete $F^C_2 \cup F^C_3$ to a tour $\bar{C}$ with $F^C_2 \cup F^C_3 \subset \bar{C}^{\{2\}}$.

This tour $\bar{C}$ satisfies the requirements of Definition 3.15. Indeed, suppose there is an $ij \in E'$ with $\xi_{ij} := \sum_{f \in F^2_{ij}} x^C_f + \sum_{f \in F^3_{ij}} y^C_f > 0$, then $\xi_{ij} = 1$ because by $n \geq 5$ either $ij \in C^{\{2\}}$ or $ikj \in C$ for a unique k. In both cases $ij \in F^C_2 \cup F^C_3 \subset \bar{C}^{\{2\}}$, therefore $\xi_{ij} = x^{\bar{C}}_{ij}$. □

The facets of Theorem 3.14 arise from the next family.

Observation 3.18 *Given $E' \subset V^{\{2\}}$, suppose $|V(E')| \geq \frac{n}{2}$ with some $\bar{t} \in V \setminus V(E')$. Then*

$$\mathcal{F} = \left\{ (F^2_{ij} := \{ij\}, F^3_{ij} := \{ikj \in V^{\langle 3 \rangle} : k \neq \bar{t}, ik \notin E', kj \notin E'\}) \right\}_{ij \in E'}$$

is E'-dominated. It is improving if and only if the graph $\bar{G} = (V \setminus \{\bar{t}\}, (V \setminus \{\bar{t}\})^{\{2\}} \setminus E')$ has a component that is not a clique. In particular, it is improving if $|V(E')| \leq n - 2$.

Proof. We first show that $\mathcal{F}$ is E'-dominated. The statement holds for $E' = \{e\}$ for some $e \in V^{\{2\}}$ because for any $C \in \mathcal{C}_n$ we have $\sum_{f \in F^2_e} x^C_f + \sum_{f \in F^3_e} y^C_f \leq 1$ by the choice of F^2_e and F^3_e and so any tour $\bar{C}$ with $e \in \bar{C}^{\{2\}}$ suffices for Definition 3.15. $|E'| \geq 2$

requires $n \geq 4$ and for $n = 4$ we have $\mathcal{F} = \{(e, \emptyset)\}_{e \in E}$, so each $C \in \mathcal{C}_4$ serves as its own $\bar{C}$ in Definition 3.15.

For $n \geq 5$ the proof is almost identical to the proof of Observation 3.17 and we use the same notation. Given a tour $C \in \mathcal{C}_n$ we may construct the graph $G^C_{\mathcal{F}} = (V, F^C_2 \cup F^C_3)$ and prove that all its nodes have degree at most two in exactly the same way. This time, however, $G^C_{\mathcal{F}}$ cannot contain a cycle, because it would induce a subcycle of C that does not visit $\bar{t}$ as $\bar{t} \notin V(F^3_{ij})$ for $ij \in E'$. From this point on the proof of $\mathcal{F}$ being E'-dominated can be completed as for Observation 3.17.

By definition, $\mathcal{F}$ is improving if and only if there is an edge $ij \in E'$ and a node $k \in V \setminus \{\bar{t}\}$ with $ik \notin E'$ and $jk \notin E'$. Such an edge ij does not exist if and only if any two nodes $i, j \in V(\bar{G})$ that are connected by a path of length two in $\bar{G}$ are adjacent in $\bar{G}$. The latter property holds if and only if every component of $\bar{G}$ is a clique. $\square$

We illustrate this technique for the *comb-inequalities* [7, 13, 14, 15], which are a large class of valid inequalities of $P_{\mathbf{STSP}_n}$ known to be facet defining in many cases. They are defined as follows.

$$\sum_{i=0}^{k} \sum_{l_1, l_2 \in W_i} x_{l_1 l_2} \leq |W_0| + \sum_{i=1}^{k} (|W_i| - 1) - \lceil \tfrac{k}{2} \rceil \tag{25}$$

with $W_i \subseteq V$, $i = 0, 1, \ldots, k$, satisfying

$$\begin{aligned} |W_0 \cap W_h| &\geq 1, & h &= 1, \ldots, k, \\ |W_h \setminus W_0| &\geq 1, & h &= 1, \ldots, k, \\ |W_h \cap W_m| &= 0, & 1 \leq h &< m \leq k, \\ k &\text{ odd.} \end{aligned}$$

The inequality remains valid if the first condition is changed to $|W_0 \cap W_h| = 1, h = 1, \ldots, k$, and the third condition may be dropped in this case. For the support

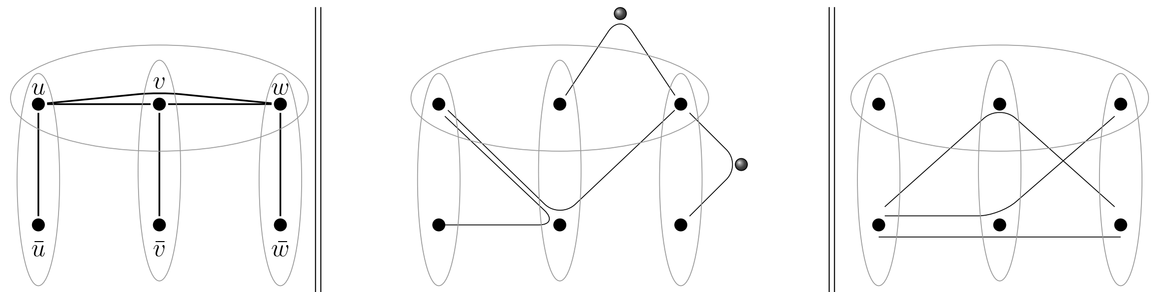
$$E' = \{ij \in V^{\{2\}} : \exists h \in \{0, 1, \ldots, k\} \text{ with } i, j \in W_h\}$$

and $|\bigcup_{h=0}^{k} W_h| < \frac{n}{2}$ Observation 3.17 gives rise to the strengthened valid inequality

$$\sum_{h=0}^{k} \sum_{ij \in W_h^{\{2\}}} x_{ij} + \sum_{h=0}^{k} \sum_{\substack{ij \in W_h^{\{2\}}, m \in V \setminus W_h : \\ im, mj \notin E'}} y_{imj} \leq |W_0| + \sum_{h=1}^{k} (|W_h| - 1) - \lceil \tfrac{k}{2} \rceil \tag{26}$$

and for $|\bigcup_{h=0}^{k} W_h| \geq \frac{n}{2}, \bar{t} \in V \setminus (\bigcup_{h=0}^{k} W_h)$ Observation 3.18 results in

$$\sum_{h=0}^{k} \sum_{ij \in W_h^{\{2\}}} x_{ij} + \sum_{h=0}^{k} \sum_{\substack{ij \in W_h^{\{2\}}, m \in V \setminus \{W_h \cup \{\bar{t}\}\} : \\ im, mj \notin E'}} y_{imj} \leq |W_0| + \sum_{h=1}^{k} (|W_h| - 1) - \lceil \tfrac{k}{2} \rceil$$



edges counted in comb-inequalities (25)	types of 2-edges that can be added to all comb-inequalities (see (26))	types of 2-edges added in the special case of Theorem 3.19

Figure 7: Visualization of the edges and the types of the 2-edges whose values are counted in Theorem 3.19

in all cases described above for the comb-inequalities. For $k = 1, |W_0| = 1$ they are equivalent to the extended subtour elimination constraints (20) and (23). The same relation is known to hold between comb-inequalities and subtour elimination constraints.

Even for rather small comb-inequalities, however, this strengthening may not be sufficient to preserve the property of being facet defining. Theorem 3.19 illustrates a case where further strengthenings are required as visualized in Figure 7.

Theorem 3.19 *For $n \geq 13$ the inequalities*

$$\sum_{h=0}^{3} \sum_{ij \in W_h^{\{2\}}} x_{ij} + \sum_{h=0}^{3} \sum_{\substack{ij \in W_h^{\{2\}}, m \in V \setminus W_h: \\ im, mj \notin E'}} y_{imj}$$
$$+ (y_{\bar{u}v\bar{w}} + y_{\bar{u}w\bar{v}} + y_{\bar{v}u\bar{w}}) + (y_{\bar{u}\bar{v}\bar{w}} + y_{\bar{u}\bar{w}\bar{v}} + y_{\bar{v}\bar{u}\bar{w}})$$
$$+ (y_{u\bar{v}\bar{w}} + y_{u\bar{w}\bar{v}} + y_{v\bar{u}\bar{w}} + y_{v\bar{w}\bar{u}} + y_{w\bar{u}\bar{v}} + y_{w\bar{v}\bar{u}}) \leq 4 \qquad (27)$$

define facets of $P_{\mathbf{SQTSP}_n}$ for all $W = \{u, v, w, \bar{u}, \bar{v}, \bar{w}\} \subset V, W_0 = \{u, v, w\}, W_1 = \{u, \bar{u}\}, W_2 = \{v, \bar{v}\}, W_3 = \{w, \bar{w}\}, |\{u, v, w, \bar{u}, \bar{v}, \bar{w}\}| = 6$ with $E' = \{uv, uw, vw, u\bar{u}, v\bar{v}, w\bar{w}\}$. For $7 \leq n \leq 12$ the inequality remains valid if we replace $m \in V \setminus W_h$ by $m \in V \setminus \{W_h \cup t\}$ with $t \in V \setminus W$ in the fourth summation symbol.

Proof. We first show validity. Put $E_1^+ := \{\bar{u}v\bar{w}, \bar{u}w\bar{v}, \bar{v}u\bar{w}\}$, $E_2^+ := \{\bar{u}\bar{v}\bar{w}, \bar{u}\bar{w}\bar{v}, \bar{v}\bar{u}\bar{w}\}$, $E_3^+ := \{u\bar{v}\bar{w}, u\bar{w}\bar{v}, v\bar{u}\bar{w}, v\bar{w}\bar{u}, w\bar{u}\bar{v}, w\bar{v}\bar{u}\}$, $E^+ := E_1^+ \cup E_2^+ \cup E_3^+$. For tours not using the 2-edges of E^+, validity follows from Observation 3.16 and Observation 3.17 (Observation 3.18). In discussing the other possibilities we will only consider *relevant configurations*, *i. e.*, in the given tour segments the number of elements appearing in (27) cannot be increased by simple exchange operations.

If a tour $C \in \mathcal{C}_n$ contains a 2-edge of E_1^+, w. l. o. g. $\bar{u}v\bar{w}$, this excludes all 2-edges of E_2^+. A tour with $\bar{u}v\bar{w} \in C$ can include at most one 2-edge of E_3^+. Consider, w. l. o. g., the case $\bar{u}\bar{v}w \in C$, then the relevant configurations are $\dots u\, [k_{uw}]\, w\, \bar{v}\, \bar{u}\, v\, \bar{w} \dots$

and $\ldots w\,\bar v\,\bar u\,v\,\bar w\,u\ldots$ where the notation [.] marks potential replacements for the direct edge between predecessor and successor. Both contain at most four elements of (27) (including $\bar v\bar u v$ and $v\bar w u$), so we may assume $E^+\cap C=\{\bar u v\bar w\}$. In a relevant tour of this type $\bar v$ has to be next to, w. l. o. g., $\bar u$ in order to keep the element $\bar v\bar u v$ (in all other configurations $\bar v$ does not contribute or by $E^+\cap C=\{\bar u v\bar w\}$ tours containing the 2-edge $u\bar v w$ can have at most 3 elements in (27)), so the only relevant cases are $\ldots\bar v\,\bar u\,v\,\bar w\,[k_{\bar w w}]\,w\,[k_{wu}]\,u\ldots$, $\ldots u\,\bar v\,\bar u\,v\,\bar w\,[k_{\bar w w}]\,w\ldots$, and $\ldots w\,[k_{wu}]\,u\,\bar v\,\bar u\,v\,\bar w\ldots$, each of them having at most 4 elements in (27). In the following we may assume $C\cap E_1^+=\emptyset$.

Next suppose $C\cap E_2^+\neq\emptyset$, then, w. l. o. g., $\{\bar u\bar v\bar w\}=C\cap E_2^+$. In this case only the elements $w\bar u\bar v,\bar v\bar w u$ of E_3^+ may be in C, as well. If both are active, then, w. l. o. g., $\ldots w\,\bar u\,\bar v\,\bar w\,u\,[k_{uv}]\,v\ldots$ is the only relevant configuration giving a count of at most 4. Suppose next, w. l. o. g., only $\bar v\bar w u\in C$, then the relevant configurations are, w. l. o. g., $\ldots\bar u\,\bar v\,\bar w\,u\,[k_{uw}]\,w\,[k_{wv}]\,v\ldots$, and $\ldots v\,\bar u\,\bar v\,\bar w\,u\,[k_{uw}]\,w\ldots$, both yielding at most 4 elements of (27). So consider $C\cap E^+=\{\bar u\bar v\bar w\}$. If v is next to, w. l. o. g., $\bar u$ then in view of the previous case the remaining relevant cases are, w. l. o. g., $\ldots u\,[k_{uv}]\,v\,\bar u\,\bar v\,\bar w\,[k_{\bar w w}]\,w\ldots$ and $\ldots w\,[k_{wu}]\,u\,[k_{uv}]\,v\,\bar u\,\bar v\,\bar w\ldots$. If v is neither next to $\bar u$ nor to $\bar w$, the remaining relevant cases are, w. l. o. g., $\ldots\bar u\,\bar v\,\bar w\,[k_{\bar w w}]\,w\,[k_{wv}]\,v\,[k_{vu}]\,u\ldots$ and $\ldots u\,[k_{u\bar u}]\,\bar u\,\bar v\,\bar w\,[k_{\bar w w}]\,w\,[k_{wv}]\,v\ldots$. Each of these induces at most 4 elements of (27).

Finally, suppose $C\cap(E_1^+\cup E_2^+)=\emptyset$ and assume, w. l. o. g., $\bar u\bar v w\in C$. All other elements of E_3^+ are then excluded from C. By $C\cap E_2^+=\emptyset$, $\bar w$ is not next to $\bar u$, so first suppose v is next to $\bar u$, then the relevant configuration is $\ldots u\,[k_{uv}]\,v\,\bar u\,\bar v\,w\,[k_{w\bar w}]\,\bar w\ldots$ ($\bar w\,v\,\bar u\in E_1^+$ may not be used). If u is next to $\bar u$ we have the relevant configurations $\ldots v\,\bar w\,u\,[k_{u\bar u}]\,\bar u\,\bar v\,w\ldots$ and $\ldots v\,[k_{vu}]\,u\,[k_{u\bar u}]\,\bar u\,\bar v\,w\,[k_{w\bar w}]\,\bar w\ldots$. In the last case, none of these nodes is next to $\bar u$, so the remaining relevant configurations are $\ldots\bar u\,\bar v\,w\,[k_{wv}]\,v\,\bar w\,u\ldots$ and $\ldots\bar u\,\bar v\,w\,[k_{wu}]\,u\,\bar w\,v\ldots$. In all cases the number of elements of (27) is at most 4, which completes the proof of validity.

The proof that (27) is facet defining for $n\geq 13$ follows the structure and uses the notation of Theorem 2.3. We set, w. l. o. g., $u=1,v=2,w=3,\bar u=4,\bar v=5,\bar w=6$ and use an $\bar n$-permutation block with roots of (27) for $\bar n=9$. This results in $r_9=349$, so due to the comb-structure the rank is reduced by one in comparison to Theorem 2.3. The iterative steps creating the set $C_{dim}^{\bar n,2}$ need to be adapted so that the subsequences can indeed be completed to roots of (27), *i. e.*, we will show afterwards that there are realizations containing exactly four of the edges or 2-edges of inequality (27). Up to the exchange $1\leftrightarrow 7$ and the generation sequence, the steps cover exactly the same 2-edges as (**I1**)–(**I5**) and read

($\boldsymbol{I_C}$-**1**) $\ldots\underline{a\,k\,7}\,(k+1)\,\varpi_k\,n\ldots$, for $a\in\{8,\ldots,k-1\}$
(the 2-edge $\langle k,7,k+1\rangle$ is not used as an e_k^i),

($\boldsymbol{I_C}$-**2**) $\ldots 7\,\underline{k\,a\,(k+1)}\,\varpi_k\,n\ldots$, for $a\in\{8,\ldots,k-1\}$,

($\boldsymbol{I_C}$-**3**) $\ldots\underline{a\,k\,b}\,(k+1)\,\varpi_k\,n\ldots$, for $a,b\in\{8,\ldots,k-1\},a<b$,

($\boldsymbol{I_C}$-**4**) $\ldots m\,k\,\overline{a\,b\,(k+1)}\,\varpi_k\,n\ldots$, for $a,b\in\{7,\ldots,k-1\}$ with $m\in\{7,\ldots,k-1\}$, $|\{a,b,m\}|=3$,

($\boldsymbol{I_C}$-**5**) $\dots \underline{a\,k\,b}\,(k+1)\,\varpi_k\,n\dots$, for $a \in \{1,\dots 6\}, b \in \{7,\dots,k-1\}$,

($\boldsymbol{I_C}$-**6**) $\dots m\,o\,(k{+}1)\,\varpi_k\,n\,S\,\underline{a\,k\,b}\,S'\dots$, for $a, b \in \{1,\dots,6\}, a < b$, with $m, o \in \{7,\dots,k-1\}$, $m \neq o$, $S, S' \subset \{1,\dots,6\}\backslash\{a,b\}, S \neq \emptyset, S' \neq \emptyset, S \cap S' = \emptyset, |S \cup S' \cup \{a,b\}| = 6$,

($\boldsymbol{I_C}$-**7**) $\dots \underline{k\,a\,(k+1)}\,\varpi_k\,n\dots$, for $a \in \{1,\dots 6\}$,

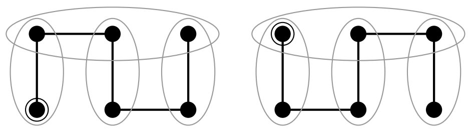
($\boldsymbol{I_C}$-**8**) $\dots \underline{a\,b\,(k+1)}\,\varpi_k\,n\,m\,o\dots$, for $a, b \in \{1,\dots,k-1\}, \{a,b\} \cap \{1,\dots,6\} \neq \emptyset$, with $m, o \in \{1,\dots,k-1\}, |\{a,b,m,o\}| = 4$,

($\boldsymbol{I_C}$-**9**) $\dots (k+1)\,\varpi_k\,\underline{n\,a\,b}\dots$, for $a, b \in \{1,\dots,k\}, a \neq b, k \in \{a,b\}$.

Because $\bar{n} = 9$ and $n \geq 13$ we have $|\{7,\dots,k-1\}| \geq 3$, so the constructions of steps ($\boldsymbol{I_C}$-**1**)–($\boldsymbol{I_C}$-**9**) are possible for all $\bar{n}+1 \leq k \leq n-2$. The rules ensure that each underlined 2-edge has not appeared in any tour constructed earlier. It remains to show that tours can be chosen so as to yield roots of (27).

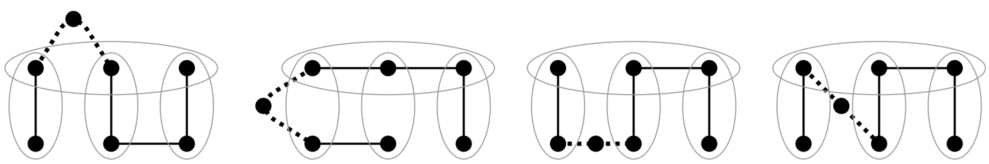
(**Case 1**) If k is not supposed to be adjacent to any node of $\{1,\dots,6\}$, we may place the subsequence $4\,1\,2\,3\,6\,5$ ($= \bar{u}\,u\,v\,w\,\bar{w}\,\bar{v}$) anywhere in the free area. This applies to tours in steps ($\boldsymbol{I_C}$-**1**)–($\boldsymbol{I_C}$-**4**), and step ($\boldsymbol{I_C}$-**9**) with $a, b \in \{7,\dots,k\}$.

(**Case 2**) If only one node $q \in \{1,\dots,6\}$ is supposed to be adjacent to a node $p \in \{7,\dots,k\}$ and there are no further requirements on the continuation of the tour in the region beyond q, the nodes of $\{1,\dots,6\}$ can be arranged consecutively with q in first or last position (see the marked node below).

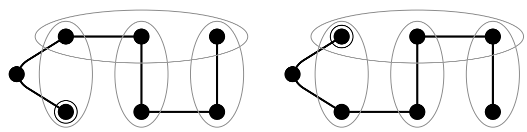


Thus, there are appropriate tours for step ($\boldsymbol{I_C}$-**5**), step ($\boldsymbol{I_C}$-**8**) with $a \in \{1,\dots,6\}, b \in \{7,\dots,k-1\}$ and in step ($\boldsymbol{I_C}$-**9**) with $a = k, b \in \{1,\dots,6\}$.

(**Case 3**) In step ($\boldsymbol{I_C}$-**6**) node k is required to be adjacent to at least two nodes of $\{1,\dots,6\}$ on either side. This is possible for any 2-edge akb with $a, b \in \{1,\dots,6\}$ as illustrated by the marked 2-edge below.

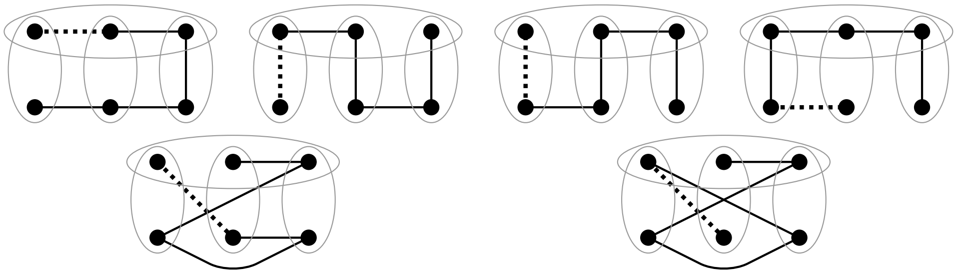


(**Case 4**) If a node $q \in \{1,\dots,6\}$ is supposed to lie between two nodes in $V \setminus \{1,\dots,6\}$ but on one side the continuation of the tour is free, the remaining nodes $\{1,\dots,6\} \setminus \{q\}$ can be arranged on the free side as follows (node q is marked).



Thus, appropriate tours are available in step ($\boldsymbol{I_C}$-**7**), in step ($\boldsymbol{I_C}$-**8**) with $a \in \{7, \dots, k-1\}, b \in \{1, \dots, 6\}$ and in step ($\boldsymbol{I_C}$-**9**) with $a \in \{1, \dots, 6\}, b = k$.

(**Case 5**) Finally, in step ($\boldsymbol{I_C}$-**8**) with $a, b \in \{1, \dots, 6\}$, it is required to provide the ordered pair ab with one side being free for any continuation. For each required pair the graphs below depict an appropriate ordering (ab is marked), that allows to arrange the nodes $\{1, \dots, 6\} \setminus \{a, b\}$ in an appropriate sequence on this free side.



Next, using the same arguments, the steps (**L1**)–(**L8**) are adapted so that for fixed $w_1, w_2, w_3 \in \{7, \dots, n-2\}, |\{w_1, w_2, w_3\}| = 3$ all required tours of $C_{dim}^{\bar{n},3}$ can be realized as roots of (27); in some cases the distance between nodes $n-1$ and n needs to be increased. The possible situations are similar to the ones for steps ($\boldsymbol{I_C}$-**1**)–($\boldsymbol{I_C}$-**9**).

- Tours in (**L1**): There are three cases.
  - $a, b \in \{7, \dots, n-2\}$: We can place the subsequence $4\,1\,2\,3\,6\,5$ right to w_2, see (**Case 1**).
  - $a \in \{1, \dots, 6\}, b \in \{7, \dots, n-2\}$: The continuation of the left side of a is free and can be done according to the sequences in (**Case 2**).
  - $a, b \in \{1, \dots, 6\}$: The situation equals (**Case 3**). With adapted tours $\dots S\, a\, \overline{(n-1)\, b\, S' w_1\, n}\, w_2 \dots,\ S, S' \subset \{1, \dots, 6\} \setminus \{a, b\}, |S| = 1, |S'| = 3, S \cap S' = \emptyset, S \cup S' \cup \{a, b\} = \{1, \dots, 6\}$ according to (**Case 3**) we get tours that are roots of (27) and there are still at least two nodes between $n-1$ and n.
- Tours in (**L2**): Using $m, o \in \{7, \dots, n-2\} \setminus \{w_1, w_2, w_3\}, m \neq o$ we place the subsequence $4\,1\,2\,3\,6\,5$ right to w_3.
- Tours in (**L3**), (**L4**), (**L5**): There are two cases. Note, in (**L5**) $b \notin \{1, \dots, 6\}$ by $a < b$ and definition of w_1, w_2, w_3.
  - $a \in \{7, \dots, n-2\}$: We can place the subsequence $4\,1\,2\,3\,6\,5$ left to a.
  - $a \in \{1, \dots, 6\}$: The continuation of the tour on the left side of a is free and so we can use one of the subsequences presented in (**Case 2**).
- Tours in (**L6**): We can place the subsequence $4\,1\,2\,3\,6\,5$ to the left of n, see (**Case 1**).
- Tours in (**L7**): There are three cases.

- $a, b \in \{7, \ldots, n-2\}$: We set $m = w_1$ and place the subsequence $4\,1\,2\,3\,6\,5$ to the right of $n-1$.
- $a \in \{1, \ldots, 6\}, b \in \{7, \ldots, n-2\}$: We set $m = w_1$ and continue the tour on the left side of a according to the sequences presented in (**Case 2**).
- $a, b \in \{1, \ldots, 6\}$: With adapted tours $\ldots S\,\underline{a\,n\,b}\,S'(n-1)\ldots,\ S, S' \subset \{1, \ldots, 6\} \setminus \{a, b\}, |S| = 1, |S'| = 3, S \cap S' = \emptyset, S \cup S' \cup \{a, b\} = \{1, \ldots, 6\}$ according to (**Case 3**) we get tours that are roots of (27) and there are still at least two nodes between $n-1$ and n.

- Tours in (**L8**): There are two cases.
  - $a \in \{7, \ldots, n-2\}$: We can place the subsequence $4\,1\,2\,3\,6\,5$ to the right of n.
  - $a \in \{1, \ldots, 6\}$: The continuation on both sides of the tour is free and so we can use one of the subsequences presented in (**Case 2**) on an arbitrary side.

In summary, we created exactly one tour less than in the proof of Theorem 2.3, hence Theorem 3.19 follows. □

4 Computational results

In order to provide some evidence that the new inequalities are indeed worth consideration in practical cutting plane approaches, we present a few computational results for random nonnegative costs, for random Angle-TSP in the plane and for randomly generated reload cost instances. We used the SCIP branch-and-cut framework [2] with CPLEX 12.1 [1] as linear solver on an Intel Core i7 CPU 920 with 2.67 GHz and 12 GB RAM in single processor mode. The basic relaxation (indicated by (I) in the tables below) is obtained by exact separation of the standard subtour elimination constraints (3) for the x_{ij} variables (we use the separator of SCIP). This is then extended to (II) by separating (10), (11), (17), (16) (this includes (14)) and, whenever a violated subtour inequality (3) is found, by adding the corresponding strengthened variants (20) or (23) instead of (3). For exact separation of inequalities (16) we solve the linear programming formulation using CPLEX by taking advantage of the total unimodularity of the corresponding constraint matrix and the warm-start-properties of the simplex-algorithm because the cost coefficients only change slightly if i is fixed and j varies.

We tested random instances for $5 \leq n \leq 25$. For general nonnegative cost instances, integral costs $c_e, e \in V^{\langle 3 \rangle}$, were chosen uniformly at random between 0 and 10000. Random Angle-TSP instances in the plane were generated by choosing points uniformly at random out of $\{0, \ldots, 1000\}^2$. Here the costs $c_{ijk}, ijk \in V^{\langle 3 \rangle}$, are computed by

$$c_{ijk} = \left\lfloor \frac{18000}{\pi} \arccos\left(\left(\frac{v_j - v_i}{\|v_j - v_i\|} \right)^T \left(\frac{v_k - v_j}{\|v_k - v_j\|} \right) \right) \right\rfloor \tag{28}$$

with $v_i \in \mathbb{R}^2$ denoting the coordinate vector of point i. In order to give a visual impression of such instances, the optimal solution of one such random instance with 30 points is displayed in Figure 8 together with an optimal solution for squared costs c_{ijk}^2 instead of c_{ijk}, which penalizes sharp turns even more.

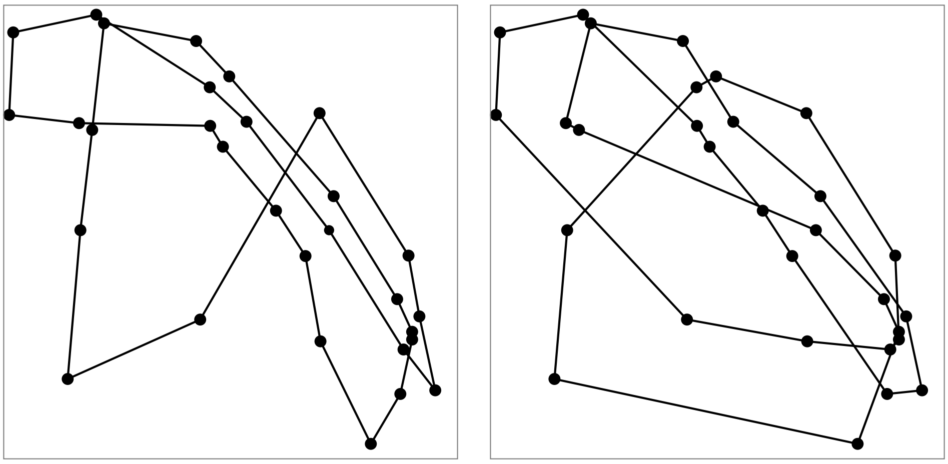


Figure 8: An optimal solution for a random Angular-Metric TSP instance on 30 nodes for costs equal to the change in direction (28) and the same costs squared.

For these two classes of random instances Figure 9 gives, for each n, the average of the root gap $(c^* - c_{relax})/c_{relax}$ over 10 instances.

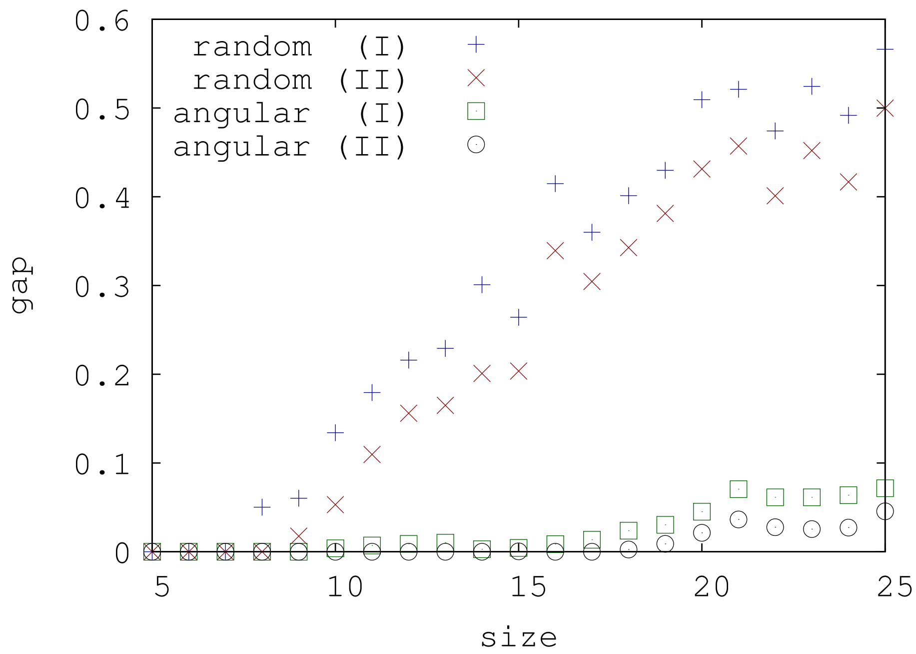


Figure 9: Average root gaps of random and random angular instances

For the reload cost instances we generated random graphs $\tilde{G} = (\tilde{V}, \tilde{E})$ by including each edge $e \in \tilde{E}$ independently with some fixed probability $p \in [0, 1]$ and randomly coloring these edges with colors $D = \{1, \ldots, d\}$. Two types of costs are used for the instances. In the instances RI_1 each color change causes costs of one, and in RI_2 the color change between two colors $i, j \in D, i \neq j$, causes costs d_{ij} with d_{ij} chosen uniformly at random in $\{1, \ldots, 10\}$. Because each color change causes costs of at least one, the 2-graph either contains a monochromatic Hamiltonian cycle (these have cost 0, so optimality gaps are meaningless) or the optimal value is at least two. Table 1 shows, for each choice of parameters, the average of optimal value and relaxation value over ten random instances (infeasible instances are skipped) for the two separation modes described above. In total we generated 360 instances, 349 of them were feasible. Via exploiting the special integrality property of these instances, approach (I) allowed to prove optimality of the solutions of 175 instances within the root node in comparison to 205 instances in case of approach (II).

RI_1						RI_2					
p	d	n	opt.	(I)	(II)	p	d	n	opt.	(I)	(II)
$\frac{1}{2}$	5	10	6.000	6.000	6.000	$\frac{1}{2}$	5	10	26.300	26.175	26.300
		15	4.400	3.966	4.126			15	16.200	14.801	15.976
		20	4.100	2.378	2.988			20	11.400	6.021	7.077
	10	10	6.000	6.000	6.000		10	10	25.889	25.889	25.889
		15	7.500	7.250	7.458			15	24.200	23.348	23.608
		20	6.900	5.771	6.201			20	22.900	19.327	21.096
	20	10	8.000	8.000	8.000		20	10	34.000	34.000	34.000
		15	8.900	8.900	8.900			15	30.200	27.553	29.361
		20	9.700	9.328	9.430			20	28.700	23.733	25.597
1	5	10	2.000	1.471	1.742	1	5	10	5.800	2.862	4.563
		15	1.800	0.000	0.000			15	2.400	0.000	0.000
		20	0.800	0.000	0.000			20	0.200	0.000	0.000
	10	10	3.400	3.368	3.400		10	10	10.900	8.426	9.684
		15	3.100	1.404	1.952			15	6.100	2.094	3.151
		20	2.700	0.062	0.247			20	4.500	0.000	0.275
	20	10	5.000	5.000	5.000		20	10	12.900	11.330	12.350
		15	5.900	4.937	5.262			15	12.300	7.886	9.075
		20	5.000	2.881	3.603			20	10.500	5.092	5.936

Table 1: Average optimal and relaxation values for random reload cost instances with edge-probability p, d colors and n nodes

A natural next step is to investigate the quality of semidefinite relaxations. First experiments indicate that in many cases semidefinite approaches improve the lower bounds resp. gaps significantly. A detailed investigation, however, exceeds the current scope and will be the topic of a separate study.

References

[1] IBM ILOG CPLEX 12.1: Using the CPLEX callable library. Information available at `http://www-01.ibm.com/software/integration/optimization/cplex-optimizer/`.

[2] T. Achterberg. *Constraint Integer Programming*. PhD thesis, Technische Universität Berlin, 2007.

[3] A. Aggarwal, D. Coppersmith, S. Khanna, R. Motwani, and B. Schieber. The angular-metric traveling salesman problem. *SIAM J. Comput.*, 29:697–711, December 1999.

[4] E. Amaldi, G. Galbiati, and F. Maffioli. On minimum reload cost paths, tours, and flows. *NETWORKS*, 2010. To appear.

[5] D. L. Applegate, R. E. Bixby, V. Chvatal, and W. J. Cook. *The Traveling Salesman Problem: A Computational Study (Princeton Series in Applied Mathematics)*. Princeton University Press, January 2007.

[6] R. F. Bailey and B. Stevens. Hamiltonian decompositions of complete k-uniform hypergraphs. *Discrete Mathematics*, 310(22):3088 – 3095, 2010. Combinatorics 2008.

[7] V. Chvátal. Edmonds polytopes and weakly hamiltonian graphs. *Mathematical Programming*, 5:29–40, 1973.

[8] G. Dantzig, R. Fulkerson, and S. Johnson. Solution of a large-scale traveling-salesman problem. *Operations Research*, 2:393–410, 1954.

[9] U. Faigle and G. Frahling. A combinatorial algorithm for weighted stable sets in bipartite graphs. *Discrete Applied Mathematics*, 154(9):1380 – 1391, 2006.

[10] F. Fischer, G. Jäger, A. Lau, and P. Molitor. Complexity and algorithms for the traveling salesman problem and the assignment problem of second order. Preprint 2009-16, Fakultät für Mathematik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany, Oct. 2009.

[11] G. Galbiati, S. Gualandi, and F. Maffioli. On minimum reload cost cycle cover. *Electronic Notes in Discrete Mathematics*, 36:81 – 88, 2010.

[12] L. Gourvès, A. Lyra, C. Martinhon, and J. Monnot. The minimum reload s-t path, trail and walk problems. *Discrete Appl. Math.*, 158:1404–1417, July 2010.

[13] M. Grötschel and M. W. Padberg. Lineare Charakterisierungen von Travelling Salesman Problemen. *Zeitschrift für Operations Research, Series A*, 21(1):33–64, Feb. 1977.

[14] M. Grötschel and M. W. Padberg. On the symmetric travelling salesman problem I: inequalities. *Mathematical Programming*, 16:265–280, 1979.

[15] M. Grötschel and M. W. Padberg. On the symmetric travelling salesman problem II: lifting theorems and facets. *Mathematical Programming*, 16:281–302, 1979.

[16] G. Gutin, A. Punnen, A. Barvinok, E. K. Gimadi, and A. I. Serdyukov. *The Traveling Salesman Problem and Its Variations (Combinatorial Optimization)*. Springer, May 2002.

[17] S. Hong. *A Linear Programming Approach for the Traveling Salesman Problem*. PhD thesis, John Hopkins University, Baltimore, Maryland, USA, 1972.

[18] G. Jäger and P. Molitor. Algorithms and experimental study for the traveling salesman problem of second order. *Lecture Notes in Computer Science*, 5165:211–224, 2008.

[19] E. L. Lawler, J. K. Lenstra, , A. H. G. Rinnooy Kan, and D. B. Shmoys, editors. *The Traveling Salesman Problem: A Guided Tour of Combinatorial Optimization*. John Wiley & Sons, Chichester, 1985.

[20] M. Padberg. The boolean quadric polytope: some characteristics, facets and relatives. *Mathematical Programming*, 45:139–172, August 1989.

[21] H.-C. Wirth and J. Steffan. On minimum diameter spanning trees under reload costs. In P. Widmayer, G. Neyer, and S. Eidenbenz, editors, *Graph-Theoretic Concepts in Computer Science*, volume 1665 of *Lecture Notes in Computer Science*, pages 78–89. Springer Berlin/Heidelberg, 1999.

[22] X. Zhao, H. Huang, and T. P. Speed. Finding short DNA motifs using permuted markov models. *Journal of Computational Biology*, 12(6):894–906, 2005.

5 Appendix

Theorem 5.1 *The inequalities* (12) *define facets of* $P_{\mathbf{SQTSP}_n}$ *for all 2-cycles* $C \subset V^{\langle 3 \rangle}$ *with* $|C| = 5$ *if* $n \geq 5$.

Proof. For $5 \leq n \leq 9$ we verified the statement be means of a linear algebra package. For $n \geq 10$ the proof is similar to the proof of Theorem 2.3. We use the same notation and consider, w. l. o. g., the 2-cycle $C = \{123, 234, 345, 154, 215\}$. For $n \geq 10$ a tour satisfies $\sum_{e \in C^{\{2\}}} x_e - \sum_{e \in C} y_e = 2$ if and only if the intersection of its edges with $C^{\{2\}}$ results in at least two unconnected paths of at least one edge. Requiring this structure for the tours of the initial $\bar{n}$-permutation block with $\bar{n} = 5$ yields $r_5 - 1$ affinely independent tours for $\tilde{C}^{\bar{n},1}_{dim}$. In the construction of sets $\tilde{C}^{\bar{n},2}_{dim}$ and $\tilde{C}^{\bar{n},3}_{dim}$ ($\tilde{C}^{\bar{n}}_{dim} = \tilde{C}^{\bar{n},1}_{dim} \cup \tilde{C}^{\bar{n},2}_{dim} \cup \tilde{C}^{\bar{n},3}_{dim}$) the existence of tours with this structure can be ensured by the following slight adaptations of steps (**I1**)–(**I5**) for $\bar{n} < k < n - 1$ and (**L1**)–(**L8**) with $w_1, w_2, w_3 \in \{6, \ldots, n - 2\}$.

- Tours in (**I1**): There are three cases (once again, $\langle k, 1, k+1 \rangle$ is not used as an e^i_k).
  1. For $6 \leq a \leq k - 1$ we use the tours (note that 3 is followed by 5 and not 4)
  $$\ldots \underline{a\, k\, 1}\, (k+1)\, \varpi_k\, n\, 2\, 3\, 5\, 4 \ldots$$
  2. For nodes $a \in \{2, 5\}$ adjacent to node 1 in C, we construct tours
  $$\ldots 3\, \underline{2\, k\, 1}\, (k+1)\, \varpi_k\, n\, 4\, 5 \ldots \text{ resp. } \ldots 4\, \underline{5\, k\, 1}\, (k+1)\, \varpi_k\, n\, 3\, 2 \ldots$$
  3. For nodes $a \in \{3, 4\}$ not adjacent to node 1 in C, we construct tours
  $$\ldots 2\, \underline{3\, k\, 1}\, (k+1)\, \varpi_k\, n\, 4\, 5 \ldots \text{ resp. } \ldots 5\, \underline{4\, k\, 1}\, (k+1)\, \varpi_k\, n\, 3\, 2 \ldots$$
- Tours in (**I2**): For $a \in \{2, \ldots, 5\}$ we use the same technique as for (**I1**) above with the roles of node 1 and node a interchanged. For $a \in \{6, \ldots, k - 1\}$ appropriate tours are
  $$\ldots 2\, 1\, \underline{k\, a\, (k+1)}\, \varpi_k\, n\, 4\, 3\, 5 \ldots$$
- Tours in (**I3**): Whenever $\{a, b\} \cap \{1, \ldots, 5\} \neq \emptyset$ we can adapt the approach of (**I1**)–(**I2**) above by exchanging the roles of the nodes. In all other cases the following tours contain exactly two nonincident edges of $C^{\{2\}}$,
  $$\ldots \underline{a\, k\, b}\, (k+1)\, \varpi_k\, n\, 1\, 2\, 4\, 5\, 3 \ldots$$
- Tours in (**I4**): The situations that appear for $\{a, b\} \not\subset \{1, \ldots, 5\}$ have been discussed before. If $\{a, b\} \in C^{\{2\}}$ we place the nodes $\{1, \ldots, 5\} \setminus \{a, b\}$ next to node n in arbitrary order. The remaining cases satisfy $a, b \in \{1, \ldots, 5\}$ with $\{a, b\} \notin C^{\{2\}}$. The desired structure is obtained for, w. l. o. g., $a = 1, b = 3$ by tours
  $$\ldots k\, 2\, \underline{1\, 3\, (k+1)}\, \varpi_k\, n\, 4\, 5 \ldots$$

- Tours in (**I5**), (**L1**)–(**L4**), (**L6**), (**L8**): We can adapt the techniques above.
- Tours in (**L5**): We can use the techniques above setting $m \in \{w_1, w_2, w_3\} \setminus \{b\}$.
- Tours in (**L7**): If $\{a, b\} \in C^{\{2\}}$, w. l. o. g., for $a = 1, b = 2$ the tour

  $$\dots 4\,5\,\underline{1\,n\,2}\,3\,(n-1)\dots$$

  contains exactly two edges $45, 23 \in C^{\{2\}}$. If $\{a, b\} \notin C^{\{2\}}$, w. l. o. g., for $a = 1, b = 3$ the tour

  $$\dots 4\,5\,\underline{1\,n\,3}\,2\,(n-1)\dots$$

  contains exactly the edges $45, 23 \in C^{\{2\}}$, too.

This construction results in exactly one affinely independent tour less than in the proof of Theorem 2.3, and with the considerations therein, Theorem 5.1 follows. □

Theorem 5.2 *The inequalities* (13) *define facets of* $P_{\mathbf{SQTSP}_n}$ *for all* $S \subset V$ *with odd* $|S| = h \geq 3$ *and* $n \geq \frac{3}{2}(h+1)$.

Proof. Theorem 3.3 proves the case $h = 3$, so let $h \geq 5$ be odd with $n \geq \frac{3}{2}(h+1)$. The proof is similar to the proof of Theorem 2.3. We use the same notation and consider, w. l. o. g., $S = \{2\} \cup \{i, i+1 \colon i = 1 + 3k, k = 1, \dots, \frac{h-1}{2}\}$. A tour gives rise to a root of (13) if and only if the intersection of its edges with $S^{\{2\}}$ results in $\frac{h-1}{2}$ unconnected paths of at least two nodes. In this case either one node of S is isolated or exactly one of the $\frac{h-1}{2}$ paths contains three nodes; paths containing more than three nodes of S cannot arise from roots. To guarantee this structure for the tours, each edge $\{i, i+1\}, i = 1 + 3k, k = 2, \dots, \frac{h-1}{2}$, lies between two nodes not in S. Starting with the set $C_{dim}^{\bar{n},1}$ we use $\bar{n} = 5$ for the permutation block. Fulfilling (13) with equality requires that exactly one or two of the three edges $\{2,4\}, \{2,5\}, \{4,5\}$ have to be present in tours of the block. Due to this structure the rank of the initial block is reduced by one in comparison to Theorem 2.3.

In the inductive part with $\bar{n} < k < n-1$ we have to distinguish four cases.

1. $k \in V \setminus S$ with $(k+1) \in V \setminus S$: We can use steps (**I1**)–(**I5**) without any modifications of the decisive parts. We will show in Claim 2 below that the desired structure of the tours can be achieved easily.

2. $k \in V \setminus S$ with $(k+1) \in S$: For nodes of this type we use steps (**I1**)–(**I5**), but (**I4**) needs to be restricted to $a, b \in \{1, \dots, k-1\}, a \neq b, \{a, b\} \not\subset S$, because otherwise we would have a path formed by four nodes of S. In order to build tours for the missing 2-edges $\langle a, b, k+1 \rangle, a, b \in \{1, \dots, k-1\} \cap S, a \neq b$, the node $k+1$ needs to be separated from $k+2$, so all these will be built in an extra step (**C.14**) within the next iteration. Furthermore, in order to guarantee the existence of appropriate tours for (**I4**), the distance of node k and $k+1$ needs to be increased by one via inserting a suitable node, see also Claim 3 below.

3. $k \in \{i = 5+3l, l = 1, 2, \ldots, \frac{h-1}{2} - 1\}$: For nodes of this type we use steps (**I1**)–(**I5**) without any modifications of the decisive parts. By Claim 4 below the desired structure can be achieved easily.

4. $k \in \{i = 4+3l, l = 1, 2, \ldots, \frac{h-1}{2} - 1\}$: For these nodes we split the tour construction into many steps so as to simplify the exposition of appropriately constructed tours afterwards. The correspondence of this list of steps to (**Type-I1**)-(**Type-I4**) is explained in Claim 1, the existence of appropriate tours in Claim 5 below. Note, we have $5, k, (k+1) \in S$.

   (**C.1**) $\ldots \underline{a\,k\,5}\,(k+1)\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \setminus S$ (the 2-edge $\langle k, 5, k+1\rangle$ is not used as an e_k^i),

   (**C.2**) $\ldots m\,5\,\underline{k\,a\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \setminus S$ with $m \in \{1, \ldots, k-1\} \setminus S, m \neq a$,

   (**C.3**) $\ldots m\,k\,5\,\underline{a\,b\,(k+1)}\,\varpi_k\,n\ldots$, for $a, b \in \{1, \ldots, k-1\} \setminus S, a \neq b$, with $m \in \{1, \ldots, k-1\} \setminus S, |\{a, b, m\}| = 3$,

   (**C.4**) $\ldots m\,5\,k\,\underline{a\,b\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \setminus S, b \in (\{1, \ldots, k-1\} \cap S) \setminus \{5\}$ with $m \in \{1, \ldots, k-1\} \setminus S, m \neq a$,

   (**C.5**) $\ldots m\,5\,k\,o\,p\,\underline{a\,b\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in (\{1, \ldots, k-1\} \cap S), b \in \{1, \ldots, k-1\} \setminus S$ with $m, o \in \{1, \ldots, k-1\} \setminus S, p \in (\{1, \ldots, k-1\} \cap S), |\{a, b, m, o, p, 5\}| = 6$,

   (**C.6**) $\ldots m\,5\,k\,o\,\underline{a\,b\,(k+1)}\,\varpi_k\,n\ldots$, for $a, b \in (\{1, \ldots, k-1\} \cap S) \setminus \{5\}, a \neq b$, with $m, o \in \{1, \ldots, k-1\} \setminus S, m \neq o$,

   (**C.7**) $\ldots m\,k\,\underline{5\,a\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \setminus S$ with $m \in \{1, \ldots, k-1\} \setminus S, m \neq a$,

   (**C.8**) $\ldots m\,\underline{5\,k\,a}\,o\,p\,(k+1)\,\varpi_k\,n\ldots$, for $a \in (\{1, \ldots, k-1\} \cap S)$ with $m, o \in \{1, \ldots, k-1\} \setminus S, p \in \{1, \ldots, k-1\} \cap S, |\{a, m, o, p, 5\}| = 5$,

   (**C.9**) $\ldots m\,\underline{a\,k\,b}\,o\,(k+1)\,\varpi_k\,n\ldots$, for $a \in (\{1, \ldots, k-1\} \cap S) \setminus \{5\}, b \in \{1, \ldots, k-1\} \setminus S$, with $m \in \{1, \ldots, k-1\} \setminus S, o \in \{1, \ldots, k-1\} \cap S, a \neq o, b \neq m$,

   (**C.10**) $\ldots \underline{a\,k\,b}\,m\,(k+1)\,\varpi_k\,n\ldots$, for $a, b \in \{1, \ldots, k-1\} \setminus S, a < b$ with $m \in \{1, \ldots, k-1\} \cap S, |\{a, b, m\}| = 3$,

   (**C.11**) $\ldots m\,o\,k\,\underline{a\,5\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \setminus S$ with $m \in \{1, \ldots, k-1\} \setminus S, o \in \{1, \ldots, k-1\} \cap S, m \neq a, o \neq 5$,

   (**C.12**) $\ldots m\,o\,k\,p\,\underline{a\,5\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \cap S, a \neq 5$ with $m, p \in \{1, \ldots, k-1\} \setminus S, o \in \{1, \ldots, k-1\} \cap S, |\{a, m, o, p, 5\}| = 5$,

   (**C.13**) $\ldots m\,o\,k\,p\,\underline{5\,a\,(k+1)}\,\varpi_k\,n\ldots$, for $a \in \{1, \ldots, k-1\} \cap S$ with $m, p \in \{1, \ldots, k-1\} \setminus S, o \in \{1 \ldots, k-1\} \cap S, |\{a, m, o, p, 5\}| = 5$,

   (**C.14**) $\ldots m\,\underline{k\,a\,b}\,o\,p\,(k+1)\,\varpi_k\,n\ldots$, for $a, b \in \{1, \ldots, k-2\} \cap S$ with $m, o \in \{1, \ldots, k-1\} \setminus S, m \neq o, p \in \{1, \ldots, k-1\} \cap S, |\{a, b, p\}| = 3$, (**C.15**) $\dots m\,\underline{a\,k\,b}\,o\,5\,(k+1)\,\varpi_k\,n\dots$, for $a,b \in \{1,\dots,k-1\}\cap S, a<b$, with $m,o \in \{1,\dots,k-1\}\setminus S, |\{a,b,m,o,5\}|=5$,

(**C.16**) $\dots m\,\underline{k\,a\,(k+1)}\,\varpi_k\,n\dots$, for $a \in (\{1,\dots,k-1\}\cap S)\setminus\{5\}$ with $m \in \{1,\dots,k-1\}\setminus S$.

After these steps we perform (**I5**). Note, (**C.14**) is only completing (**I4**) of the preceding iteration $k-1$, therefore it is also not counted in Claim 1.

Claim 1: In steps (**C.1**)–(**C.13**), (**C.15**)–(**C.16**), (**I5**) we build exactly $\frac{3}{2}k^2 - \frac{3}{2}k - 1$ tours for $k \in \{i = 4+3l, l = 1,2,\dots,\frac{h-1}{2}-1\}$.
Proof of Claim 1. We compare the underlined 2-edges with the 2-edges of (**Type-I1**)-(**Type-I4**) in the proof of Theorem 2.3

- (**Type-I1**): We get all 2-edges $\langle a,k,b\rangle, a,b \in \{1,\dots,k-1\}, a \neq b$, in steps (**C.1**), (**C.8**)–(**C.10**), (**C.15**).
- (**Type-I2**): The role of node 1 and node 5 changed. Apart from that we get all 2-edges $\langle k,a,k+1\rangle, a \in \{1,\dots,k-1\}\setminus\{5\}$ (in contrast to $\langle k,a,k+1\rangle, a \in \{1,\dots,k-1\}\setminus\{1\}$) in steps (**C.2**) and (**C.16**).
- (**Type-I3**): We get all 2-edges $\langle a,b,k+1\rangle, a,b \in \{1,\dots,k-1\}, a \neq b$, in steps (**C.3**)–(**C.7**), (**C.11**)–(**C.13**).
- (**Type-I4**): Because we use step (**I5**) we get all the 2-edges of that type.

This proves Claim 1.

It remains to prove that in all four cases above the desired structure can be achieved, *i. e.*, exactly $\frac{h-1}{2}$ unconnected paths of at least two nodes in S are present in each tour. To disconnect the nodes of a subset $S' \subset S$ in the desired way we need at least $\lfloor |S'|/2 \rfloor - 1$ nodes $v \in V\setminus S$; starting with two nodes of S' we place, next to them, one node of $V\setminus S$, then again two nodes of S', one of $V\setminus S$ and so on until in the end there may be three nodes of S' next to each other.
Claim 2: The desired structure described above can be achieved in (**I1**)–(**I5**) for nodes $k \in V\setminus S$ with $(k+1) \in V\setminus S$, $\bar{n} < k < n-1$.
Proof of Claim 2. By definition of S it follows $S = S \cap \{1,\dots,k-1\}$ and $|\{1,\dots,k-1\}\setminus S| \geq \frac{k}{3}$. It suffices to consider the case $k \in V\setminus S$, $(k+1) \in V\setminus S, (k-1) \in S$ because if there are more nodes in $V\setminus S$ we can simply place them next to each other. Thus, let $k = 3 + 3\frac{h-1}{2}$.

- Tours in (**I1**): If $a \in V\setminus S$ there remain $\frac{h-1}{2}-1$ nodes in $\{1,\dots,k\}\setminus(S\cup\{1,a,k\})$ that are not fixed to a position. With these nodes we can force $\frac{h-1}{2}$ unconnected paths of nodes in S (exactly one of these contains three nodes). In the case $a \in S$ we can either force a 2-edge $\langle m,o,a\rangle$ with $m \in \{1,\dots,k-1\}\setminus S, o \in S, o \neq a$ or force a 2-edge $\langle m,a,k\rangle$ with $m \in \{1,\dots,k-1\}\setminus S$, followed by alternating an edge $e \in S^{\{2\}}$ and a node in $\{1,\dots,k-1\}\setminus S$.

- Tours in (**I2**), (**I3**), (**I5**): We are in a similar situation as in (**I1**), at most one node $s \in S$ has to lie between two nodes in $V \setminus S$ and we have enough nodes in $\{1, \ldots, k-1\} \setminus S$ to force the desired structure.

- Tours in (**I4**): If $a, b \in S$ one of the desired edges is formed and next to node k we use the alternating order of edges in $S^{\{2\}}$ and nodes in $\{1, \ldots, k-1\} \setminus S$. In the case $\{a, b\} \not\subseteq S$ the situation equals (**I1**) with $a \in \{2, \ldots, k-1\} \setminus S$ apart from that an isolated node in S is forced if $\{a, b\} \cap S \neq \emptyset$.

Claim 3: The desired structure described above can be achieved for nodes $k \in V \setminus S$ with $(k+1) \in S$, $\bar{n} < k < n-1$.

Proof of Claim 3. As in Claim 2, there are at least $\frac{k}{3}$ nodes available in $\{1, \ldots, k-1\} \setminus S$ to separate $S \cap \{1, \ldots, k-1\}$ into $\frac{k}{3} - 1$ unconnected paths of at least two nodes each (and possibly one isolated node). So, except for (**I4**) with $a, b \in \{1, \ldots, k-1\} \cap S$ of this case, the same arguments as in Claim 2 prove this claim as well as the following two claims. Step (**I4**) cannot be performed for $a, b \in \{1, \ldots, k-1\} \cap S$ for this k because $a, b, k+1, k+2$ would be four consecutive nodes in S, so the construction is delayed to step (**C.14**) for $k+1$.

Claim 4: The desired structure described above can be achieved for nodes $k \in \{i = 5 + 3l \colon l = 1, 2, \ldots, \frac{h-1}{2} - 1\}$, $\bar{n} < k < n-1$.

Proof of Claim 4. The set $\{1, \ldots, k-1\}$ contains exactly $\frac{k+1}{3}$ nodes that belong to $V \setminus S$ and $(k+1) \in V \setminus S$. Therefore we have as many separating nodes as in the proof of Claim 2. In view of $(k+1), n \in V \setminus S$ only slight structural adaptations are needed to compensate $k \in S$, we skip the details here.

Claim 5: The desired structure described above can be achieved for nodes $k \in \{i = 4 + 3l \colon l = 1, 2, \ldots, \frac{h-1}{2} - 1\}$, $\bar{n} < k < n-1$.

Proof of Claim 5. The set $\{1, \ldots, k-1\}$ contains exactly $\frac{k+2}{3}$ nodes that belong to $V \setminus S$ and may thus serve to separate the nodes of $S \cap \{1, \ldots, k+1\}$ into $\frac{k-1}{3}$ unconnected paths of at least two nodes each (and possibly one isolated node if there is no path of length three). Note that $k+2 \in V \setminus S$ and that for each tour of (**C.1**)–(**C.16**) the specified part starts with a node $v \in \{1, \ldots, k-1\} \setminus S$ (in (**C.1**) and (**C.10**) this is a, otherwise it is m) and ends with $n \in V \setminus S$. Hence, the unspecified region can be filled up correctly whenever the number of nodes in $\{1, \ldots, k-1\} \setminus S$ within the specified segment from and including this node v to node $k+2$ exceeds the count of S-paths of at least 2 nodes within this segment by at most 2. Table 2 lists the forced isolated nodes in S, the edges in $S^{\{2\}}$ and 2-edges in $S^{\langle 3 \rangle}$ within these critical segments of steps (**C.1**)-(**C.16**). The requirements hold in all cases and are tight only for (**C.3**). Step (**I5**) can be treated in the same way as in Claims 2–4. This proves Claim 5.

It remains to adapt the concluding steps (**L1**)–(**L8**). How to do this depends on whether $(n-1) \notin S$ or $(n-1) \in S$. In both cases $n \notin S$, because by assumption $n \geq \frac{3}{2}(h+1) = 2 + 3\frac{h-1}{2} + 1$.

Claim 6: If $(n-1) \notin S$ the desired structure can be achieved within (**L1**)–(**L8**) for $w_1 = 2, w_2 = 4, w_3 = 5$ by restricting some of the open choices.

Proof of Claim 6. In this case $n > \frac{3}{2}(h+1)$, in particular $|V \setminus S| \geq \frac{1}{2}(h+3) + 1$. To separate the $\frac{h-1}{2}$ paths of at least two nodes of S we need at least $\frac{h-1}{2}$ nodes in $V \setminus S$.

step	isolated nodes of S	edges of $S^{\{2\}}$	2-edges of $S^{\langle 3\rangle}$	nodes of $V \setminus S$
(**C.1**)			$\langle k, 5, k+1\rangle$	a
(**C.2**)	$k+1$	$\{k, 5\}$		m, a
(**C.3**)	$k+1$	$\{k, 5\}$		m, a, b
(**C.4**)		$\{k, 5\}, \{b, k+1\}$		m, a
(**C.5**)	$k+1$	$\{k, 5\}, \{p, a\}$		m, o, b
(**C.6**)		$\{k, 5\}$	$\langle a, b, k+1\rangle$	m, o
(**C.7**)	$k+1$	$\{k, 5\}$		m, a
(**C.8**)		$\{p, k+1\}$	$\langle 5, k, a\rangle$	m, o
(**C.9**)		$\{a, k\}, \{o, k+1\}$		m, b
(**C.10**)	k	$\{m, k+1\}$		a, b
(**C.11**)		$\{o, k\}, \{5, k+1\}$		m, a
(**C.12**)		$\{o, k\}$	$\langle a, 5, k+1\rangle$	m, p
(**C.13**)		$\{o, k\}$	$\langle 5, a, k+1\rangle$	m, p
(**C.14**)		$\{p, k+1\}$	$\langle k, a, b\rangle$	m, o
(**C.15**)		$\{5, k+1\}$	$\langle a, k, b\rangle$	m, o
(**C.16**)			$\langle k, a, k+1\rangle$	m

Table 2: Specified edges and 2-edges of S and nodes of $V \setminus S$ in steps (**C.1**)–(**C.16**)

Therefore the structure can be achieved if at most three nodes in $V \setminus S$ are not used as separating nodes, *i. e.*, these may lie next to a further node in $V \setminus S$, and one isolated node belonging to S may lie between them. These rules can be satisfied in (**L1**)–(**L8**).

- For (**L1**): If $b \in S$ the nodes $n-1$ and n separate the path $b\,w_1$ of S, if $b \notin S$ then $n-1$, b and n are three nodes embracing an isolated node $w_1 \in S$.
- For (**L2**) choose $o \in S \setminus \{w_1, w_2, w_3\}$, then $n-1$ and n separate the path ow_1 of S.
- Because $\{w_1, w_2, w_3\} \subset S$, (**L3**),(**L4**),(**L6**),(**L8**) are not critical for any choice.
- For (**L5**) choose $o \in S \setminus \{w_1, w_2, w_3, a, b\}$ (one of a or b is in $\{w_1, w_2, w_3\}$, so this is feasible), then at most three nodes of a, n, b and m are not in S and they may separate one isolated node of S.
- For (**L7**) choose $m = w_1$. If $b \in S$ the path $b\,w_1$ of S is separated, otherwise a, n and b are at most three nodes in $V \setminus S$ separating the isolated node w_1 of S.

Claim 7: If $(n-1) \in S$ the desired structure can be achieved by appropriate adaptations of steps (**L1**)–(**L8**) with $w_1 = 1, w_2 = 2, w_3 = 3$.
Proof of Claim 7. We know that $|V \setminus S| = \frac{1}{2}(h+3)$. To separate the $\frac{h-1}{2}$ paths of at least two nodes of S we need at least $\frac{h-1}{2}$ nodes in $V \setminus S$. Therefore the structure can be achieved if at most two nodes in $V \setminus S$ are not used as separating node, *i. e.*, these may lie next to a further node in $V \setminus S$ and one isolated node belonging to S may lie between them. To achieve this, several adaptations are required in (**L1**)–(**L8**).

- Tours in (**L1**): There are four cases.
  - $a, b \in V \setminus S$: We use tours $\dots a\,(n-1)\,b\,m\,o\,w_1\,n\,w_2 \dots$ with $m, o \in (\{1, \dots, n-2\} \cap S) \setminus \{w_2\}, m \neq o$. These have the isolated node $n-1 \in S$ between $a, b \in V \setminus S$ and two adjacent nodes $w_1, n \in V \setminus S$, so these tours can be extended to the required structure.
  - $a \in V \setminus S, b \in S$: We use tours $\dots a\,(n-1)\,b\,w_1\,n\,w_2 \dots$ with two adjacent nodes $w_1, n \in V \setminus S$.
  - $a \in S, b \in V \setminus S$: We use tours $\dots a\,(n-1)\,b\,w_1\,n\,w_2 \dots$, these can be completed to have the three adjacent nodes $b, w_1, n \in V \setminus S$ but no isolated nodes.
  - $a, b \in S$: We use tours $\dots a\,(n-1)\,b\,w_1\,n\,w_2 \dots$ with two adjacent nodes $w_1, n \in V \setminus S$ and $a\,(n-1)\,b$ the only path of three nodes of S.

- Tours in (**L2**): Choose $m \in V \setminus (S \cup \{w_1, w_3, n\})$ and $o \in S \setminus \{n-1, w_2\}$, then the first row has three adjacent nodes $w_1, n, w_3 \in V \setminus S$ and can be completed without isolated nodes of S, while the second row has two adjacent nodes $n, w_3 \in V \setminus S$ and $(n-1)\,o\,w_2$ as the only path of three nodes of S.

- Tours in (**L3**): We use the tours $\dots \underline{a\,(n-1)\,w_1}\,m\,w_2\,n\,w_3 \dots$, $a \in \{1, \dots, n-2\} \setminus (\{w_1, w_2, w_3\}), m \in S \setminus \{w_2, a, n-1\}$ with adjacent nodes $n, w_3 \in V \setminus S$ and, if $a \notin S$, the isolated node $n-1$ between nodes $a, w_1 \in V \setminus S$.

- Tours in (**L4**): There are three adjacent nodes $w_1, n, w_3 \in V \setminus S$ and, if $a \in S$, the three nodes $a\,(n-1)\,w_2$ form the only path of three nodes of S.

- Tours in (**L5**): Choose $m \in S \setminus \{n-1, a, b\}$, $o \in V \setminus (S \cup \{n, a, b\}$, then for $b \in S$ the path $b\,m\,(n-1)$ is the only path of three nodes of S. For $b \notin S$ there are at most three adjacent nodes $a, n, b \in V \setminus S$ and no isolated nodes of S are needed.

- Tours in (**L6**): The tours $\dots n\,w_3\,\underline{w_1\,(n-1)\,w_2} \dots$ and $\dots n\,w_1\,w_2\,(n-1)\,w_3 \dots$ may be used as before. Modifying the remaining tour to $\dots n\,w_2\,4\,\underline{w_1\,(n-1)\,w_3} \dots$ yields one isolated node $n-1 \in S$ between $w_1, w_3 \in V \setminus S$.

- Tours in (**L7**): Set $m = w_2$, then this may induce at most three adjacent nodes $a, n, b \in V \setminus S$ or $b\,m\,(n-1)$ as the only path of three nodes of S.

- Tours in (**L8**) require at most two adjacent nodes $a, n \in V \setminus S$.

All in all we build exactly one tour less than in Theorem 2.3. This proves Theorem 5.2.□