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Facet-defining triangle inequalities for the quadratic linear ordering problem

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Abstract

The quadratic linear ordering problem models a large number of applications in a variety of different domains. To solve it exactly, polyhedral methods have been proposed but their development is still in its beginning. Specifically, while it is evident that only a fraction of the triangle inequalities, which are most commonly known from the boolean quadric polytope, take part in a minimal linear description of the polytope associated with a canonical formulation of the quadratic linear ordering problem, it is broadly unclear to which of these inequalities this applies and how to distinguish them from the others. At the same time, these inequalities are essential to build strong polyhedral and semidefinite programming relaxations. Addressing these open questions and potentials, we reveal the desired combinatorial pattern that enables to identify the triangle inequalities which are facet-inducing and deduce a corresponding exact polynomial-time separation algorithm.

Keywords Binary quadratic programming · Integer programming · Linear ordering · Separation algorithm · Branch-and-cut · Polyhedral combinatorics

Mathematics Subject Classification 68R01 · 90C05 · 90C09 · 90C10 · 90C20 · 90C22 · 90C27 · 90C30

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1 Introduction

Given a finite set of items, w.l.o.g. indexed by $[n] := \{1, \dots, n\}$, suppose that there is a reward of $c_{ij} \in \mathbb{R}$ for all $i, j \in [n]$, $i \neq j$, obtained when ranking item i before j , and a reward $q_{ijk\ell} \in \mathbb{R}$ for $i, j, k, \ell \in [n]$, $i \neq j$ and $k \neq \ell$, obtained when ranking i before j and k before ℓ *simultaneously*. The determination of a permutation $\pi : [n] \rightarrow [n]$, i.e. a mapping of each item $i \in [n]$ to a unique position $\pi(i) \in [n]$, that maximizes the total sum of these rewards is called the *quadratic linear ordering problem* (QLOP).

Given its generality, the QLOP has numerous important applications in different domains. For instance, the single-row facility layout problem embodies a prominent special case of the QLOP [1] that covers a variety of challenging operations research problems such as the layout of machines in flexible manufacturing systems [2] or the assignment of flights to terminal gates in an airport [3]. Another special case of the QLOP is the minimum linear arrangement problem [4] which is used e.g. in the design of error correcting codes [5]. More directly, the QLOP has been used to minimize crossings in layered graph drawings [6], and more recently to model the computation of the cutwidth parameter of an undirected graph [7]. Also in a more general sense, the QLOP relates to and inherits applications from combinatorial optimization problems that involve “betweenness” relations [8]. More fundamentally, the QLOP is a natural generalization of the classical linear ordering problem (LOP) which is well-known to be $\mathcal{NP}$ -hard [9], whence so is the QLOP.

Despite the relevance and broad applicability of the QLOP, only little is known about its combinatorial structure such as to exploit it in exact algorithms. In a seminal work, Buchheim, Wiegeler and Zheng [6] propose an integer linear programming (ILP) formulation, they introduce the corresponding polytope P_{QLO}^n , and they determine a minimal equation system associated with its linear description. Apart from that, the latter is however broadly unknown, except for the cases $n = 3$ and $n = 4$ which have been studied by DeVries in her PhD thesis [10]. Therein, she further presents a lifting theorem stating that every facet of the polytope associated with order n is also a facet of the polytope associated with order $n + 1$. Particularly, her work reveals that a minimal description of P_{QLO}^n , $n \geq 4$, comprises a restricted subset of the *triangle inequalities*, as known from the Boolean Quadric Polytope. However, since only P_{QLO}^3 and P_{QLO}^4 were studied, only triangle inequalities involving variables that refer to four distinct indices in total could be taken into account, and it also remained so far unexplained how to distinguish those that define facets of P_{QLO}^n , $n \geq 4$, i.e., that take part in an irredundant description of it, from those that do not.

In this paper, we extend these results by revealing a combinatorial pattern that enables to identify *all* the facet-defining triangle inequalities for P_{QLO}^n , including those that arise when $n \geq 5$ or $n \geq 6$. As we further clarify, these inequalities are also the only ones among the more general class of odd-cycle inequalities that induce facets of P_{QLO}^n , $n \geq 4$. These findings hence also provide evidence that a plain adoption of separation algorithms for the triangle or odd-cycle inequalities, as commonly used for unconstrained binary quadratic programming, can only deliver additional inequalities that induce lower-dimensional faces of P_{QLO}^n . Conversely, they suggest

that a cutting plane (respectively branch-and-cut) approach for the QLOP can profit from tailored separation algorithms for the triangle inequalities, and we present such an algorithm for an exact separation based on the identified facet-inducing configurations. This is also motivated by the experimental results in [10] which indicate a major relevance of the triangle inequalities for the computation of strong upper bounds by means of the linear relaxation of the ILP formulation from [6]. Furthermore, since triangle inequalities are of extensive relevance and use in semidefinite programming relaxations for (applications of) the QLOP, as proposed e.g. in [4, 6, 7], these are affected by the here provided distinction of irredundant and redundant inequalities as well.

The paper is organized as follows. In Sect. 2, we formally define the QLOP and report on prevalent results that build the basis for, or are extended in, this work. As a preparation for the presentation of our results, we provide in Sect. 3 some novel characterizations of the decision variables of the QLOP and their associated index sets. The determination and so enabled separation of facet-defining triangle inequalities is the subject of Sect. 4. Finally, a brief conclusion is given in Sect. 5.

2 Related work

In order to formally define the QLOP, it is common to assume w.l.o.g. that the initially mentioned rewards are normalized as follows. First, for all $i, j \in [n]$, $i \neq j$, we expect $q_{ijij} = 0$ (can be moved to c_{ij}) and $q_{ijji} = 0$. Then, the rewards c_{ij} where $j < i$, and the rewards q_{ijkl} where either $j < i$, $\ell < k$, or both, can instead be captured by introducing a constant and adjusting c_{ij} and q_{ijkl} where $i < j$ and $k < \ell$, see also [6, 10]. Further exploiting commutativity in the sense that q_{klij} can be interchanged with q_{ijkl} , $i, j, k, \ell \in [n]$, the relevant index-pairs and index-quadruples become $I_2 := \{(i, j) : i, j \in [n], i < j\}$ respectively $I := \{(i, j, k, \ell) : i, j, k, \ell \in [n], (i, j), (k, \ell) \in I_2, (i, j) \prec (k, \ell)\}$ where $\prec$ denotes the property of being strictly smaller in the lexicographic sense, i.e., $i < k$ or $i = k$ and $j < \ell$ in this particular case. The reward coefficients may thus be rearranged to form strictly upper triangular matrices $C \in \mathbb{R}^{n \times n}$ and $Q \in \mathbb{R}^{\binom{n}{2} \times \binom{n}{2}}$. We denote by $\Pi(n)$ the set of all permutations of $[n]$, and write $\pi(i) < \pi(j)$ if item $i \in [n]$ is ranked before item $j \in [n]$ in some fixed permutation $\pi \in \Pi(n)$. Consequently, the objective of the QLOP becomes:

$$\max_{\pi \in \Pi(n)} f(\pi) := \sum_{\substack{(i,j) \in I_2 \\ \pi(i) < \pi(j)}} c_{ij} + \sum_{\substack{(i,j,k,\ell) \in I \\ \pi(i) < \pi(j); \pi(k) < \pi(\ell)}} q_{ijkl}$$

In [6], Buchheim, Wiegele, and Zheng introduce the quadratic linear ordering polytope, P_{QLO}^n , which is given by the convex hull of properly defined incidence vectors that describe the feasible solutions to the QLOP of order $n \geq 3$. These incidence vectors consist of two parts. Since the feasible solutions are in one-to-one correspondence with the permutations $\pi \in \Pi_n$, the first part is given by the character-

istic vectors $\chi(\pi) \in \mathbb{R}^{\binom{n}{2}}$ customary from the LOP, where for all $(i, j) \in I_2$ one has $\chi(\pi)_{ij} = 1$ if $\pi(i) < \pi(j)$ and $\chi(\pi)_{ij} = 0$ if $\pi(j) < \pi(i)$. The second part has $m(n) := \binom{n}{2} = |I|$ components, one for each $(i, j, k, \ell) \in I$, which are equal to one if $\chi(\pi)_{ij} = 1$ and $\chi(\pi)_{k\ell} = 1$, and equal to zero otherwise, i.e. they represent the linearized product $\chi(\pi)_{ij} \cdot \chi(\pi)_{k\ell}$. Based on this representation, the quadratic linear ordering polytope of order n can be written as

$$P_{\text{QLO}}^n := \text{conv} \left\{ (x, y) \in \{0, 1\}^{\binom{n}{2} + m(n)} : \pi \in \Pi_n, x = \chi(\pi), \text{ and } y_{ijk\ell} = x_{ij}x_{k\ell} \forall (i, j, k, \ell) \in I \right\}.$$

As Buchheim, Wiegale and Zheng show further, the equations

$$y_{ijik} + y_{ikjk} - y_{ijjk} - x_{ik} = 0 \text{ for all } i, j, k \in [n] : i < j < k \quad (1)$$

suffice to enforce that $x = \chi(\pi)$ holds for some $\pi \in \Pi_n$ provided that x and y are consistent binary vectors, and they constitute a *minimal equation system* for P_{QLO}^n , $n \geq 3$ [6].

Consequently, the dimension of P_{QLO}^n is $\dim P_{\text{QLO}}^n = \binom{n}{2} + m(n) - \binom{n}{3}$, and it is apparent that the following integer linear program is an exact formulation for the QLOP.

$$\begin{aligned} \max \quad & \sum_{(i,j) \in I_2} c_{ij}x_{ij} + \sum_{(i,j,k,\ell) \in I} q_{ijk\ell}y_{ijk\ell} & (\text{QLOP-ILP}) \\ \text{s.t.} \quad & y_{ijik} + y_{ikjk} - y_{ijjk} - x_{ik} = 0 \quad \text{for all } i, j, k \in [n] : i < j < k \end{aligned}$$

$$y_{ijk\ell} - x_{ij} \leq 0 \quad \text{for all } (i, j, k, \ell) \in I \quad (2)$$

$$y_{ijk\ell} - x_{k\ell} \leq 0 \quad \text{for all } (i, j, k, \ell) \in I \quad (3)$$

$$x_{ij} + x_{k\ell} - y_{ijk\ell} \leq 1 \quad \text{for all } (i, j, k, \ell) \in I \quad (4)$$

$$\begin{aligned} y_{ijk\ell} &\geq 0 & \text{for all } (i, j, k, \ell) \in I \\ x_{ij} &\in \{0, 1\} & \text{for all } (i, j) \in I_2 \end{aligned} \quad (5)$$

Indeed, given a permutation $\pi \in \Pi_n$ expressed in the binary variables x_{ij} , $(i, j) \in I_2$, the inequalities (2)–(5) implement the “standard” linearization (see [11, 12]) for the products $y_{ijk\ell} = x_{ij}x_{k\ell}$, $(i, j, k, \ell) \in I$.

In her PhD thesis [10], DeVries provides a linear description of P_{QLO}^3 and P_{QLO}^4 in a reduced variable space. This space is obtained by employing the Eq. (1) in order to eliminate variables (and themselves). For instance, one may substitute for the identity $y_{ijjk} = y_{ijik} + y_{ikjk} - x_{ik}$ for all $i, j, k \in [n] : i < j < k$. DeVries further observes that, in the presence of (1), for each triple $i, j, k \in [n] : i < j < k$, only half of the twelve inequalities appearing as (2)–(5) for (i, j, i, k) , (i, j, j, k) , $(i, k, j, k) \in I$ are irredundant. More precisely, for each of the three y -variables, one may choose either

the pair (2), (3) or the pair (4), (5), ensuring that in total each pair is selected at least once. An according selection and Eq. (1) then fully describe P_{QLO}^3 , while for $n \geq 4$ additional facet-defining inequalities are required to describe P_{QLO}^n . Specifically, besides the according instances of (2)–(5), a minimal description of P_{QLO}^4 comprises inequalities that DeVries grouped into four additional classes. One of these, which has been identified to be of major importance to compute strong relaxations of QLOP-ILP, consists of the triangle inequalities which are in the center of this paper.

Notably, DeVries further derives the following lifting theorem that we use repeatedly.

Theorem 1 (*Theorem 3.2.7 in [10]*) *Let $(a, b), (x, y) \in \mathbb{R}^{\binom{n}{2}+m(n)}$ and $(a', b'), (x', y') \in \mathbb{R}^{\binom{n+1}{2}+m(n+1)}$ with $a' = (a, 0)$, $b' = (b, 0)$. Then if $a^T x + b^T y \leq c$ is a facet of P_{QLO}^n , $a'^T x' + b'^T y' \leq c$ is a facet of P_{QLO}^{n+1} .*

In addition to the polyhedral perspective, in [4, 6, 7], semidefinite programming relaxations for the QLOP are formulated that naturally employ the equations (1) and triangle inequalities as well.

3 Preparations

For several considerations to follow, it is helpful to associate the QLOP of order n with a graph. To this end, let $G_n = (V, E)$ be the undirected graph such that there is a vertex for each pair $(i, j) \in I_2$ and the corresponding variable x_{ij} , i.e. $V := \{x_{ij} : (i, j) \in I_2\}$, and an edge for each quadruple $(i, j, k, \ell) \in I$ respectively variable y_{ijkl} , i.e. $E := \{y_{ijkl} : (i, j, k, \ell) \in I\}$. For instance, G_4 is precisely the graph shown in Fig. 1. More generally, the following observation is simple but relevant.

Observation 1 *For $n \geq 3$, G_n is a complete undirected graph.*

To precisely describe important conditions, we also introduce additional index notation. Thereby, we exploit that, when visualizing the graph G_n in an “upper-triangular fashion” like in Fig. 1, the elements of I that involve only three distinct indices decompose into horizontal (h), vertical (v), and transversal (t) edges. Accordingly, we define the index sets $I_3^h := \{(i, j, i, k) : i, j, k \in [n], i < j < k\}$, $I_3^v := \{(i, k, j, k) : i, j, k \in [n], i < j < k\}$, and $I_3^t := \{(i, j, j, k) : i, j, k \in [n], i < j < k\}$. If less distinction is needed, we refer to the set $I_3 := I_3^h \cup I_3^v \cup I_3^t$. Finally, we distinguish the set of quadruples involving four distinct indices as $I_4 := I \setminus I_3 = \{(i, j, k, \ell), (i, k, j, \ell), (i, \ell, j, k) : i, j, k, \ell \in [n], i < j < k < \ell\}$. From this description, it is immediate that the cardinality of I may be alternatively expressed as $m(n) = |I| = |I_3 \cup I_4| = 3\binom{n}{3} + 3\binom{n}{4}$.

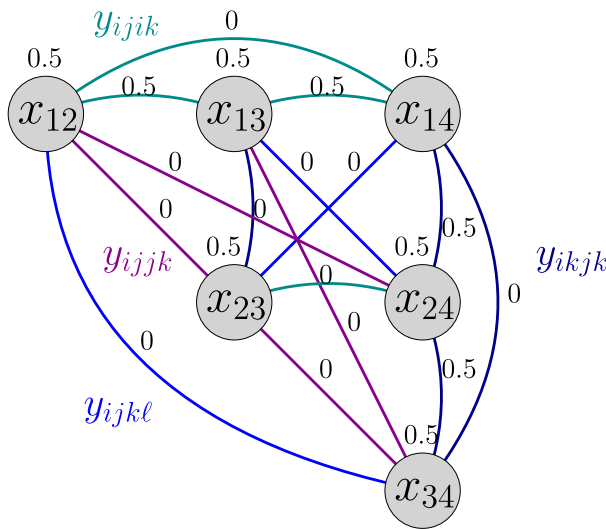


Fig. 1 A graph-based illustration where the vertices (edges) correspond to the x - (y -)variables for P_{QLO}^4 . The attached values reflect a feasible solution to the linear programming relaxation of QLOP-ILP that violates the (non-facet-inducing) triangle inequality $y_{1213} + y_{1314} - y_{1214} - x_{13} \leq 0$

4 Identification and separation of facet-defining triangle inequalities

In this section, we investigate the relation between the Eq. (1) and the triangle inequalities

$$y_{ijkl} - y_{klrs} + y_{ijrs} - x_{ij} \leq 0 \quad \text{for all } (i, j) \prec (k, \ell) \prec (r, s) \quad (6)$$

$$y_{ijkl} + y_{klrs} - y_{ijrs} - x_{k\ell} \leq 0 \quad \text{for all } (i, j) \prec (k, \ell) \prec (r, s) \quad (7)$$

$$-y_{ijkl} + y_{klrs} + y_{ijrs} - x_{rs} \leq 0 \quad \text{for all } (i, j) \prec (k, \ell) \prec (r, s) \quad (8)$$

$$-y_{ijkl} - y_{klrs} - y_{ijrs} + x_{ij} + x_{k\ell} + x_{rs} \leq 1 \quad \text{for all } (i, j) \prec (k, \ell) \prec (r, s) \quad (9)$$

where $(i, j), (k, \ell), (r, s) \in I_2$, and we precisely determine in which cases they induce a facet of P_{QLO}^n for all $n \geq 4$.

Specifically, for $n = 4$ only twelve of the according 80 instances of (6)–(9) define facets of P_{QLO}^4 [10], and it will become apparent that the distinction adheres to a non-trivial pattern for this case as well as for the instances that arise first for $n = 5$. As opposed to that, any instance of (6)–(9) defines a facet of the Boolean Quadric Polytope [13], which we will here, uncommonly, denote as $P_{\text{BQP}}^{(n)} := \text{conv} \left\{ (x, y) \in \{0, 1\}^{\binom{n}{2} + m(n)} : y_{ijkl} = x_{ij}x_{k\ell} \text{ for all } (i, j, k, \ell) \in I \right\}$,

so that the components of x and y are indexed in the same way as in the definition of P_{QLO}^n .

As is pointed out in [6], each Eq. (1) immediately relates to the triangle inequality

$$y_{ijik} + y_{ikjk} - y_{ijjk} - x_{ik} \leq 0 \quad \text{for all } i, j, k \in [n] : i < j < k \quad (10)$$

which can be obtained as an instance of (7) for the according I_2 -pair configuration $(i, j) \prec (i, k) \prec (j, k)$, and consists of I_3 -edges only. It is thus not surprising that the $3\binom{n}{3}$ further associated triangle inequalities

$$y_{ijik} - y_{ikjk} + y_{ijjk} - x_{ij} \leq 0 \quad \text{for all } i, j, k \in [n] : i < j < k \quad (11)$$

$$-y_{ijik} + y_{ikjk} + y_{ijjk} - x_{jk} \leq 0 \quad \text{for all } i, j, k \in [n] : i < j < k \quad (12)$$

$$-y_{ijik} - y_{ikjk} - y_{ijjk} + x_{ij} + x_{jk} + x_{ik} \leq 1 \quad \text{for all } i, j, k \in [n] : i < j < k \quad (13)$$

do not define facets of P_{QLO}^n , $n \geq 3$, as the following theorem records.

Theorem 2 *Each instance of (11), (12), and (13) is obtained as a linear combination of (1) and a weakening of the inequalities (2)–(5), and thus does not define a facet of P_{QLO}^n , $n \geq 3$.*

Proof Substituting for y_{ijjk} by $y_{ijik} + y_{ikjk} - x_{ik}$ in (11) gives $2y_{ijik} - x_{ij} - x_{ik} \leq 0$ which is implied by (2) and (3). Analogously, substituting for y_{ijjk} by $y_{ijik} + y_{ikjk} - x_{ik}$ in (12) gives $2y_{ikjk} - x_{ik} - x_{jk} \leq 0$ which is implied by (2) and (3). Finally, substituting for x_{ik} by $y_{ijik} + y_{ikjk} - y_{ijjk}$ in (13) gives $x_{ij} + x_{jk} - 2y_{ijjk} \leq 1$ which is implied by (4) and (5). $\square$

It follows that (11), (12), and (13) are implied in the presence of (1) and (2)–(5) which as such has been independently observed in [7] while expressing these constraints in the matrix notation that is common to its semidefinite programming context (see Lemma 2.1).

For $n \geq 4$, there are $4\binom{n}{4}$ further triangles built exclusively from I_3 -edges as well, but that involve four distinct indices in total. These triangles are induced by the configurations stated in the following theorem, and the according $16\binom{n}{4}$ triangle inequalities are *not* implied by (1) and (2)–(5)¹, but they still do not define facets.

Theorem 3 *Let $n \geq 4$, $i, j, k, \ell \in [n]$, and $i < j < k < \ell$. Then the triangle inequalities associated with the triangles built (i) from three I_3^h -edges for $(i, j) \prec (i, k) \prec (i, \ell)$, (ii) from three I_3^o -edges for $(i, \ell) \prec (j, \ell) \prec (k, \ell)$, (iii) from two I_3^t -edges and one I_3^o -edge for $(i, k) \prec (j, k) \prec (k, \ell)$, and (iv) two I_3^t -edges and one I_3^h -edge for $(i, j) \prec (j, k) \prec (j, \ell)$, do not define facets of P_{QLO}^n , $n \geq 4$.*

¹A concrete example configuration $(\bar{x}, \bar{y})$ for $n = 4$ that satisfies (1) and (2)–(5) but violates the triangle inequality considered in the proof of Theorem 3 with $(i, j, k, \ell) = (1, 2, 3, 4)$ is shown in Fig. 1.

Proof Each of the specified triangle inequalities can be obtained as a linear combination of the equations (1) and facet-defining triangle inequalities (as portrayed below).

If the inequality is an instance of (6)–(8), but with the exceptions of (8) for category (iii) and (6) for category (iv), the according procedure is as follows and exemplified in parenthesis for the inequality $y_{ijk} + y_{ikl} - y_{ijl} - x_{ik} \leq 0$ which is (7) for category (i). Identify the unique y -variable with a negative coefficient (y_{ijl}) and the unique instance of (1) with a non-zero coefficient for this variable ($y_{ijl} + y_{ikl} - y_{ijj} - x_{il} = 0$). In this equation, consider the unique I_2 -pair that is not related to the identified y -variable (which is (j, ℓ) in the example). Determine the two triangles that combine this pair with the other two I_2 -pairs of the triangle inequality under consideration (these are once (i, j) and (i, k) , and once (i, k) and (i, ℓ) in the example). To finally obtain the inequality as a linear combination, add the two according facet-defining inequalities (these are $y_{ikl} + y_{ilj} - y_{ikj} - x_{il} \leq 0$ and $y_{ijk} + y_{ikl} - y_{ijj} - x_{ik} \leq 0$ in the example, see Table 1 below) and subtract the identified equation from the result.

If the inequality is an instance of (9) and of category (iii) or (iv), the linear combination is obtained by starting at the facet-defining inequality $-y_{ijk} - y_{jkk} - y_{ijk} + x_{ij} + x_{jk} + x_{kl} \leq 1$ (see again Table 1 below), by then adding $y_{ijk} - y_{ikk} + y_{ijk} - x_{ij} \leq 0$, respectively $-y_{ijj} + y_{jkl} + y_{ijk} - x_{kl} \leq 0$, and by finally subtracting the unique equation of (1) that refers to three of the indices i, j, k, ℓ and that has a non-zero coefficient for the so-far missing x -variable present in the inequality.

For the remaining cases, i.e. an inequality that is either (9) for category (i) or (ii), (8) for category (iii) or (6) for category (iv), the linear combination is obtained by adding six facet-defining triangle inequalities from Table 1, by subtracting twice the unique equation that refers to three of the indices i, j, k, ℓ and that has a zero coefficient for all the three y -variables present in the inequality, and by subtracting once each of the other three instances of (1) that refer to three of the indices i, j, k, ℓ . $\square$

As an intermediate result that is in line with the findings by DeVries in [10], we conclude that a facet-defining triangle inequality must contain at least one I_4 -edge. The set I_4 has three quadruples for all $i, j, k, \ell \in [n]$, $i < j < k < \ell$, giving the twelve configurations in Table 1 for triangles with exactly one I_4 -edge.

In the remainder of this section, we will make repeated use of the following customary approach: For any triangle inequality, let $F = \{(x, y) \in P_{\text{QLO}}^n : a^T x + b^T y = c\}$ denote the corresponding face of P_{QLO}^n (F is non-empty since each of (6)–(9) is satisfied with equality for some vertices of P_{QLO}^n). Interpreting the incidence vectors (vertices of P_{QLO}^n) that lie on F as the rows of a matrix M , the dimension $\dim F$ of F is given by $\text{rank}(M) - 1$ if $(0, 0) \notin F$, which only applies to (9), and by $\text{rank}(M)$ if $(0, 0) \in F$, see e.g. [14]. Thus, comparing the dimensions of F and P_{QLO}^n , we may deduce whether the triangle inequality that defines F is facet-inducing.

Choosing $n = 4$, and carrying out this approach for each of the 48 triangle inequalities related to the twelve triangles defined by the configurations in Table 1, we find that *exactly one inequality per triangle* induces a face of dimension 16 and thus is facet-defining as $\dim P_{\text{QLO}}^4 = 17$. These inequalities provide the shapes

Table 1 Triangle configurations with *one* I_4 -edge and their facet-defining inequalities (F.-D. I.)

I_4	Configuration	I_3 -cases	F.-D. I	Plain Inequality
(i, j, k, ℓ)	$(i, j) \prec (i, k) \prec (k, \ell)$	(I_3^h, I_3^t)	(6)	$y_{ijk} - y_{ikk\ell} + y_{ijk\ell} - x_{ij} \leq 0$
(i, j, k, ℓ)	$(i, j) \prec (i, \ell) \prec (k, \ell)$	(I_3^h, I_3^v)	(7)	$y_{ij\ell} + y_{ikk\ell} - y_{ijk\ell} - x_{i\ell} \leq 0$
(i, j, k, ℓ)	$(i, j) \prec (j, k) \prec (k, \ell)$	(I_3^t, I_3^t)	(9)	$-y_{ijk} - y_{jkk\ell} - y_{ijk\ell} + x_{ij} + x_{jk} + x_{k\ell} \leq 1$
(i, j, k, ℓ)	$(i, j) \prec (j, \ell) \prec (k, \ell)$	(I_3^t, I_3^v)	(8)	$-y_{ijj\ell} + y_{j\ell k\ell} + y_{ijk\ell} - x_{k\ell} \leq 0$
(i, k, j, ℓ)	$(i, j) \prec (i, k) \prec (j, \ell)$	(I_3^h, I_3^t)	(7)	$y_{ijk} + y_{ikj\ell} - y_{ijk\ell} - x_{ik} \leq 0$
(i, k, j, ℓ)	$(i, k) \prec (i, \ell) \prec (j, \ell)$	(I_3^h, I_3^v)	(7)	$y_{ik\ell} + y_{\ell j\ell} - y_{ikj\ell} - x_{i\ell} \leq 0$
(i, k, j, ℓ)	$(i, k) \prec (j, \ell) \prec (k, \ell)$	(I_3^v, I_3^t)	(7)	$y_{ikj\ell} + y_{j\ell k\ell} - y_{ikk\ell} - x_{j\ell} \leq 0$
(i, k, j, ℓ)	$(i, k) \prec (j, k) \prec (j, \ell)$	(I_3^v, I_3^v)	(7)	$y_{ikjk} + y_{jkj\ell} - y_{kkj\ell} - x_{jk} \leq 0$
(i, ℓ, j, k)	$(i, j) \prec (i, \ell) \prec (j, k)$	(I_3^h, I_3^t)	(7)	$y_{ij\ell} + y_{i\ell jk} - y_{ijk\ell} - x_{i\ell} \leq 0$
(i, ℓ, j, k)	$(i, k) \prec (i, \ell) \prec (j, k)$	(I_3^h, I_3^v)	(6)	$y_{ik\ell} - y_{i\ell jk} + y_{ijk\ell} - x_{ik} \leq 0$
(i, ℓ, j, k)	$(i, \ell) \prec (j, k) \prec (j, \ell)$	(I_3^h, I_3^v)	(8)	$-y_{i\ell jk} + y_{jkj\ell} + y_{i\ell j\ell} - x_{j\ell} \leq 0$
(i, ℓ, j, k)	$(i, \ell) \prec (j, k) \prec (k, \ell)$	(I_3^t, I_3^v)	(6)	$y_{i\ell jk} - y_{jkk\ell} + y_{i\ell k\ell} - x_{i\ell} \leq 0$

of the according $12\binom{n}{4}$ instances arising more generally for $n \geq 4$ (and indices $i, j, k, \ell \in [n], i < j < k < \ell$), and are listed explicitly in Table 1. They are further in line with Table 3.4 in [10] that contains the same twelve triangle inequalities, though expressed in terms of a reduced variable space. While it has so far been unclear, however, how to derive the facet-defining inequality when given a triangle with one I_4 -variable, our analysis reveals that the number of I_3^t -elements present in the triangles can be used as a characteristic criterion, also for the case of two I_4 -variables. We first state the precise conditions for the case of triangle inequalities that involve exactly one I_4 -variable.

Theorem 4 *Let $n \geq 4$, and let $T \subset E$ be a triangle in G_n involving exactly one I_4 -edge. Suppose w.l.o.g. that the I_2 -pairs of the involved vertices are ordered lexicographically, and that $T = \{e, f, g\}$ where e joins the first two vertices, f joins the latter two vertices, and g joins the first and the third vertex according to this order. Then the inequality for T that defines a facet of P_{QLO}^n is (9) if the two non- I_4 -edges of T are both from I_3^t , whereas it is either (8) if only $e \in I_3^t$, or (6) if only $f \in I_3^t$, or (7) if only $g \in I_3^t$, and otherwise (no I_3^t -edge) it is either (8) if $e \in I_4$, or (6) if $f \in I_4$, or (7) if $g \in I_4$.*

Proof For $n = 4$, the facet-defining property is deduced from the approach outlined above, and it extends to $n \geq 5$ by Theorem 1. The correctness of the stated pattern is verified by explicitly comparing the entries in the columns “Configuration”, “ I_3 -cases” and “F.-D. I.” of each row in Table 1. For instance, the first configuration combines the I_4 -variable y_{ijkl} (g) with the I_3^h -variable y_{ijik} (e) and the I_3^t -variable $y_{ikk\ell}$ (f) to a triangle T whence the facet-defining inequality is given by (6), and the stated scheme applies consistently also for the other configurations. $\square$

While for $n \geq 5$, the facial structure of P_{QLO}^n has, in all conscience, not been explored in the literature, we now proceed to reveal the roles of any further possible triangle inequality.

For $n \geq 5$, new triangles arise from each appropriate selection of two I_4 -edges and an I_3 -edge, i.e., five distinct indices $i, j, k, \ell, r \in [n], i < j < k < \ell < r$, are involved. For each of the $\binom{n}{5}$ choices of five such indices, this gives 30 distinct triangles each of which is represented by one configuration listed in Table 2. For these triangles, we have the following result.

Theorem 5 *Let $n \geq 5$, and let $T \subset E$ be a triangle in G_n involving exactly two elements of I_4 . Suppose w.l.o.g. that the I_2 -pair configuration of the involved vertices is ordered lexicographically, and that $T = \{e, f, g\}$ where e joins the first two vertices, f joins the latter two vertices, and g joins the first and the third vertex according to this order. Then there are two inequalities for T that define facets of P_{QLO}^n . If the unique non- I_4 -quadruple of T is from I_3^t , these are given by either (7) and (9) if $e, f \in I_4$, or by (6) and (9) if $e, g \in I_4$, or by (8) and (9) if $f, g \in I_4$. Otherwise, they are given by the pair built from (8) if $e \in I_4$, (6) if $f \in I_4$, and (7) if $g \in I_4$.*

Table 2 Triangle configurations with exactly $two I_4$ -edges and their facet-defining inequalities (F-D. I.) the first one of which is exemplified plainly

I_4	Configuration	I_3 -case	F-D. I	One plain inequality
$(i, j, k, \ell), (i, r, k, \ell)$	$(i, j) \prec (i, r) \prec (k, \ell)$	I_3^h	(6), (7)	$y_{ijr} - y_{ir}k\ell + y_{ijk\ell} - x_{ij} \leq 0$
$(i, j, k, \ell), (j, r, k, \ell)$	$(i, j) \prec (j, r) \prec (k, \ell)$	I_3^t	(8), (9)	$-y_{ijjr} + y_{jr}k\ell + y_{ijk\ell} - x_{k\ell} \leq 0$
$(i, j, k, \ell), (i, j, k, r)$	$(i, j) \prec (k, \ell) \prec (k, r)$	I_3^h	(7), (8)	$y_{ijk\ell} + y_{k\ell}kr - y_{ijk}r - x_{k\ell} \leq 0$
$(i, j, k, \ell), (i, j, \ell, r)$	$(i, j) \prec (k, \ell) \prec (\ell, r)$	I_3^t	(6), (9)	$y_{ijk\ell} - y_{k\ell}lr + y_{ij\ell}r - x_{ij} \leq 0$
$(i, j, k, r), (i, \ell, k, r)$	$(i, j) \prec (i, \ell) \prec (k, r)$	I_3^h	(6), (7)	$y_{ij\ell} - y_{\ell}kr + y_{ijk}r - x_{ij} \leq 0$
$(i, j, k, r), (i, \ell, k, r)$	$(i, j) \prec (j, \ell) \prec (k, r)$	I_3^t	(8), (9)	$-y_{ijj\ell} + y_{j\ell}kr + y_{ijk}r - x_{kr} \leq 0$
$(i, j, k, r), (i, j, \ell, r)$	$(i, j) \prec (k, r) \prec (\ell, r)$	I_3^v	(7), (8)	$y_{ijk}r + y_{kr\ell}r - y_{ij\ell}r - x_{kr} \leq 0$
$(i, j, \ell, r), (i, k, \ell, r)$	$(i, j) \prec (i, k) \prec (\ell, r)$	I_3^h	(6), (7)	$y_{ijk} - y_{ik\ell}r + y_{ij\ell}r - x_{ij} \leq 0$
$(i, j, \ell, r), (j, k, \ell, r)$	$(i, j) \prec (j, k) \prec (\ell, r)$	I_3^t	(8), (9)	$-y_{ijjk} + y_{j\ell}kr + y_{ijk}r - x_{\ell}r \leq 0$
$(i, k, j, \ell), (i, r, j, \ell)$	$(i, k) \prec (i, r) \prec (j, \ell)$	I_3^h	(6), (7)	$y_{ikir} + y_{ikj\ell} - y_{irj\ell} - x_{jk} \leq 0$
$(i, k, j, \ell), (j, \ell, k, r)$	$(i, k) \prec (j, \ell) \prec (k, r)$	I_3^t	(7), (9)	$y_{ikj\ell} + y_{j\ell}kr - y_{ikkr} - x_{j\ell} \leq 0$
$(i, k, j, \ell), (i, k, j, r)$	$(i, k) \prec (j, \ell) \prec (j, r)$	I_3^h	(7), (8)	$y_{ikj\ell} + y_{j\ell}jr - y_{ikjr} - x_{j\ell} \leq 0$
$(i, k, j, \ell), (i, k, \ell, r)$	$(i, k) \prec (j, \ell) \prec (\ell, r)$	I_3^t	(6), (9)	$y_{ikj\ell} - y_{j\ell}lr + y_{ik\ell}r - x_{ik} \leq 0$
$(i, k, j, r), (i, \ell, j, r)$	$(i, k) \prec (i, \ell) \prec (j, r)$	I_3^h	(6), (7)	$y_{ik\ell} - y_{\ell}jr + y_{ikjr} - x_{jk} \leq 0$
$(i, k, j, r), (j, r, k, \ell)$	$(i, k) \prec (j, r) \prec (k, \ell)$	I_3^t	(7), (9)	$y_{ikjr} + y_{jr}k\ell - y_{ik\ell} - x_{jr} \leq 0$
$(i, k, j, r), (i, k, \ell, r)$	$(i, k) \prec (j, r) \prec (\ell, r)$	I_3^v	(7), (8)	$y_{ikjr} + y_{jr\ell}r - y_{ik\ell}r - x_{jr} \leq 0$
$(i, k, \ell, r), (j, k, \ell, r)$	$(i, k) \prec (j, k) \prec (\ell, r)$	I_3^v	(6), (7)	$y_{ikjk} - y_{j\ell}kr + y_{ik\ell}r - x_{ik} \leq 0$
$(i, \ell, j, k), (i, r, j, k)$	$(i, \ell) \prec (i, r) \prec (j, k)$	I_3^h	(6), (7)	$y_{\ell ir} - y_{irjk} + y_{\ell}jk - x_{il} \leq 0$
$(i, \ell, j, k), (j, k, \ell, r)$	$(i, \ell) \prec (j, k) \prec (\ell, r)$	I_3^t	(7), (9)	$y_{\ell}jk + y_{j\ell}kr - y_{\ell}lr - x_{jk} \leq 0$
$(i, \ell, j, k), (i, \ell, j, r)$	$(i, \ell) \prec (j, k) \prec (j, r)$	I_3^h	(7), (8)	$y_{\ell}jk + y_{j\ell}jr - y_{\ell}jr - x_{jk} \leq 0$
$(i, \ell, j, k), (i, \ell, k, r)$	$(i, \ell) \prec (j, k) \prec (k, r)$	I_3^t	(6), (9)	$y_{\ell}jk - y_{j\ell}kr + y_{\ell}kr - x_{\ell} \leq 0$
$(i, \ell, j, r), (j, r, k, \ell)$	$(i, \ell) \prec (j, r) \prec (k, \ell)$	I_3^v	(6), (8)	$y_{\ell}jr - y_{jr}k\ell + y_{\ell}k\ell - x_{\ell} \leq 0$
$(i, \ell, j, r), (i, \ell, k, r)$	$(i, \ell) \prec (j, r) \prec (k, r)$	I_3^v	(7), (8)	$y_{\ell}jr + y_{jr}kr - y_{\ell}kr - x_{jr} \leq 0$
$(i, \ell, k, r), (j, \ell, k, r)$	$(i, \ell) \prec (j, \ell) \prec (k, r)$	I_3^v	(6), (7)	$y_{\ell}j\ell - y_{j\ell}kr + y_{\ell}kr - x_{\ell} \leq 0$

Table 2 (continued)

I_4	Configuration	I_3 -case	F.-D. I	One plain inequality
$(i, r, j, k), (j, k, \ell, r)$	$(i, r) \prec (j, k) \prec (\ell, r)$	I_3^v	(6), (8)	$y_{irjk} - y_{jklr} + y_{ir\ell r} - x_{ir} \leq 0$
$(i, r, j, k), (i, r, j, \ell)$	$(i, r) \prec (j, k) \prec (j, \ell)$	I_3^h	(7), (8)	$y_{irjk} + y_{jkl\ell} - y_{irj\ell} - x_{jk} \leq 0$
$(i, r, j, k), (i, r, k, \ell)$	$(i, r) \prec (j, k) \prec (k, \ell)$	I_3^t	(6), (9)	$y_{irjk} - y_{jkk\ell} + y_{irkk\ell} - x_{ir} \leq 0$
$(i, r, j, \ell), (j, \ell, k, r)$	$(i, r) \prec (j, \ell) \prec (k, r)$	I_3^o	(6), (8)	$y_{irj\ell} - y_{j\ell kr} + y_{irkr} - x_{ir} \leq 0$
$(i, r, j, \ell), (i, r, k, \ell)$	$(i, r) \prec (j, \ell) \prec (k, \ell)$	I_3^o	(7), (8)	$y_{irj\ell} + y_{j\ell k\ell} - y_{irkk\ell} - x_{j\ell} \leq 0$
$(i, r, k, \ell), (j, r, k, \ell)$	$(i, r) \prec (j, r) \prec (k, \ell)$	I_3^o	(6), (7)	$y_{irjr} - y_{jrk\ell} + y_{irkk\ell} - x_{ir} \leq 0$

Proof The correctness of the stated pattern is verified by comparing the entries in the columns “Configuration”, “ I_3 -case” and “F.-D. I.” of each row in Table 2. Following the same methodology as above, we choose $n = 5$ and find that *exactly two inequalities per triangle*, given by the referenced ones, induce a face of dimension 44 and thus are facet-defining as $\dim P_{\text{QLO}}^5 = 45$. This property then follows for $n \geq 6$ by Theorem 1. $\square$

To again ease an immediate application of the according shapes of the $60\binom{n}{5}$ inequalities for $n \geq 5$, we list the first of the two inequalities per configuration explicitly in Table 2. The respective other one is easily derived by adapting the sign pattern of the coefficients according to (6)–(9).

Finally, for $n \geq 6$, triangles composed of three I_4 -quadruples (which implies six distinct indices) enter the scene. For each of the $\binom{n}{6}$ choices of $i, j, k, \ell, r, s \in [n]$, $i < j < k < \ell < r < s$, there are 15 such triangles. By relating each of them to a lexicographically smallest contributing I_4 -quadruple, they can be irredundantly listed as is displayed in Table 3.

Theorem 6 *Let $n \geq 6$, and let $T := \{e, f, g\} \subset E$ be a triangle in G_n where $e, f, g \in I_4$. Order the six indices such that the I_2 -pair configuration is $(i, j) \prec (k, \ell) \prec (r, s)$. Then each of the according triangle inequalities (6)–(9) defines a facet of P_{QLO}^n .*

Proof When applying our approach to the triangles induced by the configurations listed in Table 3 and $n = 6$, it turns out that any triangle inequality induces a face of dimension 99 and is thus facet-defining as $\dim P_{\text{QLO}}^6 = 100$. This property follows for $n \geq 7$ by Theorem 1. $\square$

Here, the according 60 inequality shapes can be easily enumerated based on (6)–(9), whence we refrain from listing them explicitly.

Having now determined all the facet-defining configurations, we may exploit them to solve the *separation problem* for the triangle inequalities in the context of the QLOP, which we may formalize as follows: Given $(\bar{x}, \bar{y}) \in \mathbb{R}^{\binom{n}{2} + m(n)}$ that satisfies (1)–(5), either determine a triangle inequality that is violated by $(\bar{x}, \bar{y})$ or prove that no such inequality exists.

Algorithm 1. Exact separation algorithm for the facet-defining triangle inequalities

Table 3 Triangle configurations with *three* I_4 -edges and their facet-defining inequalities (F-D. I). The I_4 -quadruple listed is the lexicographically smallest one

I_4	Configuration	F-D. I	I_4	Configuration	F-D. I
(i, j, k, ℓ)	$(i, j) \prec (k, \ell) \prec (r, s)$	(6)-(9)	(i, ℓ, j, s)	$(i, \ell) \prec (j, s) \prec (k, r)$	(6)-(9)
(i, j, k, r)	$(i, j) \prec (k, r) \prec (\ell, s)$	(6)-(9)	(i, r, j, k)	$(i, r) \prec (j, k) \prec (\ell, s)$	(6)-(9)
(i, j, k, s)	$(i, j) \prec (k, s) \prec (\ell, r)$	(6)-(9)	(i, r, j, ℓ)	$(i, r) \prec (j, \ell) \prec (k, s)$	(6)-(9)
(i, k, j, ℓ)	$(i, k) \prec (j, \ell) \prec (r, s)$	(6)-(9)	(i, r, j, s)	$(i, r) \prec (j, s) \prec (k, \ell)$	(6)-(9)
(i, k, j, r)	$(i, k) \prec (j, r) \prec (\ell, s)$	(6)-(9)	(i, s, j, k)	$(i, s) \prec (j, k) \prec (\ell, r)$	(6)-(9)
(i, k, j, s)	$(i, k) \prec (j, s) \prec (\ell, r)$	(6)-(9)	(i, s, j, ℓ)	$(i, s) \prec (j, \ell) \prec (k, r)$	(6)-(9)
(i, ℓ, j, k)	$(i, \ell) \prec (j, k) \prec (r, s)$	(6)-(9)	(i, s, j, r)	$(i, s) \prec (j, r) \prec (k, \ell)$	(6)-(9)
(i, ℓ, j, r)	$(i, \ell) \prec (j, r) \prec (k, s)$	(6)-(9)			

Input: $(\bar{x}, \bar{y}) \in \mathbb{R}^{\binom{n}{2}+m(n)}$ satisfying (1)–(5).

Output: A facet-defining triangle inequality (t. i.) violated by $(\bar{x}, \bar{y})$ if any.

```

1: for  $i$  from 1 to  $n$  do
2:   for  $j$  from  $i + 1$  to  $n$  do
3:     for  $k$  from  $j + 1$  to  $n$  do
4:       for  $\ell$  from  $k + 1$  to  $n$  do
5:         Inspect the configurations in Table 1 and, if a t. i. is violated, return it.
6:       for  $r$  from  $\ell + 1$  to  $n$  do
7:         Inspect the configurations in Table 2 and, if a t. i. is violated, return it.
8:       for  $s$  from  $r + 1$  to  $n$  do
9:         Inspect the configurations in Table 3 and, if a t. i. is violated, return it.
10: return  $\emptyset$ 

```

Algorithm 1 iteratively checks for a violated triangle inequality based on the irredundant cases displayed in Tables 1, 2 and 3 and returns it as soon as one is found. Since each inspection can be carried out in constant time, it is apparent that it has a worst-case running time of $\mathcal{O}(n^6)$ (while of course, the configurations respectively separation problems for triangles in involving four, five, and six distinct indices could also be treated separately). Asymptotically, Algorithm 1 is thus not faster than the enumeration of all triangle inequalities. However the employment of facet-inducing (triangle) inequalities is typically crucial for the practical performance of a cutting plane approach as has been demonstrated for the related Boolean Quadric Polytope in [15, 16]. In such an approach, relaxations of QLOP-ILP or an according semidefinite programming formulation are solved iteratively and thereby enriched with triangle inequalities that are violated by the respective current solution. The restriction to facet-defining inequalities then translates to the avoidance of redundant constraints that unnecessarily increase the size of the relaxation, without sacrificing strength in terms of pruning the solution space. In practice, Algorithm 1 may further be implemented so as to exploit that, for a given triangle, at most one inequality can be violated at a time [17, 18].

To conclude the present analysis, we address the class of odd-cycle inequalities that constitute a generalization of the triangle inequalities. They are defined as follows for $P_{\text{BQP}}^{\binom{n}{2}}$ and P_{QLO}^n , $n \geq 3$ [13]: Let $C \subseteq E$ be an arbitrary cycle in the graph

G_n . Then, any partition of C into $C_A \cup C_B$ such that $|C_A|$ is odd gives rise to the odd-cycle inequality

$$\sum_{(i,j) \in V_A} x_{ij} - \sum_{(i,j) \in V_B} x_{ij} - \sum_{(i,j,k,\ell) \in C_A} y_{ijkl} + \sum_{(i,j,k,\ell) \in C_B} y_{ijkl} \leq \left\lfloor \frac{|C_A|}{2} \right\rfloor \quad (14)$$

where we notationally treat edges from C , their I -quadruples and associated y -variables interchangeably, and where V_A (V_B) are the vertices (I_2 -pairs) incident to two edges in C_A (C_B).

An inequality (14) defines a facet of $P_{\text{BQP}}^{\binom{n}{2}}$, $n \geq 3$, if and only if C is simple and chordless [13, 19], giving a necessary condition also for P_{QLO}^n . However, by Obser-

vation 1, each cycle $C \subseteq E$ in G_n with $|C| \geq 4$ has a chord, whence we have the following result.

Theorem 7 *For $n \geq 4$, no odd-cycle inequality (14) other than the triangle inequalities referenced for the configurations displayed in Tables 1, 2 and 3, induces a facet of P_{QLO}^n .*

5 Conclusion

In this paper, we identified the triangle inequalities involving five and six distinct indices that define facets of the polytope induced by the feasible solutions to the quadratic linear ordering problem. Moreover, we revealed a so far unknown pattern that distinguishes the facet-defining triangle inequalities from the others in general. Based on this, we devised a polynomial-time algorithm that accurately separates these inequalities. Specifically, the configuration patterns that we found for triangles that involve four or five distinct indices suggest such a tailored algorithm because many triangle inequalities are actually redundant. As we further pointed out, the here identified triangle inequalities are also the only ones among the more general class of odd-cycle inequalities that define facets.

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Conflict of interest The authors have no conflict of interest to declare that are relevant to the content of this article.

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