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Box-constrained quadratic programs with fixed charge variables

Tin-Chi Lin · Dieter Vandenbussche

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Abstract Recent work has demonstrated the potential for globally optimizing nonconvex quadratic programs using a reformulation based on the first order optimality conditions. We show how this reformulation may be generalized to account for fixed cost variables. We then extend some of the polyhedral work that has been done for bound constrained QPs to handle such fixed cost variables. We show how to lift known classes of inequalities for the case without fixed cost variables and propose several new classes. These inequalities are incorporated in a branch-and-cut algorithm.

Keywords Branch-and-cut · Quadratic programming · Global Optimization

1 Introduction

In this paper, we study a mixed integer nonlinear program of the form

$$\begin{aligned} \max \quad & \frac{1}{2}x^T Qx + c^T x - f^T \delta, \\ \text{subject to} \quad & 0 \leq x \leq \delta \\ & x \in \mathbb{R}^n, \delta \in \{0, 1\}^n. \end{aligned} \tag{FCQP}$$

We refer to this problem as the Fixed Cost Quadratic Program (FCQP). We assume that $Q \in \mathbb{R}^{n \times n}$ and that $c, f \in \mathbb{R}^n$. Even with all the fixed cost variables, δ, fixed to one, this problem remains $\mathcal{NP}$-hard, see for instance [12]. Vandenbussche and Nemhauser [30,31] studied a branch-and-cut approach to this problem with the fixed cost variables fixed to 1. Their work is motivated by a classical reformulation by Giannessi and Tomasin [9] of a general Quadratic Program (QP) to a linear program with linear complementarity constraints. In this paper, we show how this reformulation can be extended to QPs with some type of fixed

T.-C. Lin · D. Vandenbussche (✉)
University of Illinois,
Urbana, IL, USA
e-mail: dieterv77@gmail.com

cost or capacity expansion variables. We apply this reformulation to FCQP and develop a number of useful polyhedral results that are incorporated into a branch-and-cut algorithm.

A key observation is that we do not assume that the matrix Q be negative semidefinite, and hence the difficulties with solving this problem stem not only from the fact that we have binary integer variables, but also that the objective is a nonconcave maximization. The main objective of this paper is to propose a general technique that can tackle both these difficulties. In the case the objective is concave, one can take advantage of this structure using the barrier-based branch-and-cut algorithm in CPLEX or various mixed-integer nonlinear programming techniques such as those described in Ref. [10]. Hence, we will restrict our attention to problems with indefinite Q.

Nonconcave QPs have many applications, including finding maximum cliques in graphs [16] and in water resource management [25]. A significant body of work studying pure 0–1 quadratic problems and their applications exists, as is evidenced by Huang et al. and Pardalos et al. [13,19,21–23] and the references therein. A variety of global optimization techniques can be used to solve QPs without integer variables, see for instance [5,18,24,29] and many others. They can also be solved with a general global optimization solver such as BARON [27]. Another approach uses the reformulation proposed in Ref. [9], which states that a bounded QP defined as

$$\max \ \frac{1}{2}x^T Qx + c^T x \text{ subject to } Ax \le b$$

is equivalent to

$$\begin{aligned} \max \quad & \tfrac{1}{2}\left(c^T x + b^T y\right) \\ \text{subject to} \quad & Ax \le b \quad y \ge 0 \\ & y^T(b - Ax) = 0 \\ & A^T y - Qx = c. \end{aligned}$$

The advantage of this reformulation is that it is linear, except for a finite number of complementarity constraints. To take advantage of this, Giannessi and Tomasin [9] suggest a finite, linear programming based branch-and-bound algorithm that recursively enforces the complementarity constraints, $y^T(b - Ax) = 0$. Alternatively, Balas [3] proposed a cutting plane approach to solve this reformulation. Vandenbussche and Nemhauser [30,31] studied the reformulation for the case where $Ax \le b$ corresponds to $0 \le x \le e$ and developed valid inequalities for the convex hull of complementary solutions. They incorporated these into a branch-and-cut algorithm which was demonstrated to be computationally advantageous.

Except for general purpose global optimization solvers, the techniques we have mentioned are not designed to solve QPs that also include binary integer variables. Our goal with this work is to develop a finite branch-and-cut algorithm for nonconcave QPs with fixed charge variables, such as FCQP. The main results of this work include:

- A generalization of the above reformulation of QPs that allows for fixed charge variables on the variables and constraints.
- The development of cutting planes to help tackle this reformulation using branch-and-cut. More specifically, we obtain a polyhedral description of a subset of the constraints in the reformulation. A particularly interesting aspect is the lifting of continuous variables in inequalities valid for the case without fixed charge variables, to obtain facet-inducing inequalities for the problem of interest (see e.g. proposition 12).
- Computational results presented in Sect. 8 that demonstrate the significant computational advantages of using a branch-and-cut approach to solve the reformulation of FCQP.

Constraints of the form $x \leq \delta$ with $\delta \in \{0, 1\}^n$ appear very often in the optimization literature, often referred to as fixed charge constraints [20]. They are fundamental constraints in standard linear integer programming models such as facility location and lot-sizing (see for instance [1] and [4]). These types of constraints have received a great deal of attention in the Integer Programming literature, and many different types of valid inequalities have been developed to deal with these structures, see for instance [2,11,20]. We point out here that we do not intend to improve upon this integer programming literature, rather this work attempts to study how one can accommodate the binary variables when dealing with the nonconcave objective.

The paper is organized as follows. In Sect. 2, we extend the reformulation of QP by Giannessi and Tomasin [9] to account for the binary fixed cost variables. In Sect. 3, we define a subset of the constraints of the reformulation that we will refer to as a one-row relaxation. This set is the main object of our investigation. In this section, we summarize the main theoretical results that characterize the facial structure of this one-row relaxation. Sections 4–7 detail the proofs of these results. Section 8 describes some computational results obtained from incorporating the polyhedral results into a branch-and-cut algorithm.

2 Reformulation

As mentioned above, Giannessi and Tomasin [9] showed that QPs, if bounded, can always be reformulated as linear programs with linear complementarity constraints. We now show that this reformulation can be generalized to a class of QPs with binary variables, of which FCQP is a special case.

We formulate this generalized QP as

$$\begin{aligned} \max \quad & \frac{1}{2}x^T Qx + c^T x - f^T \delta, \\ \text{subject to} \quad & Ax \leq b + \bar{b} \circ \delta \\ & \delta \in \{0, 1\}^m, \end{aligned} \tag{GenQP}$$

where $\circ$ represents the usual Hadamard product. Note that this formulation includes constraints such as $x \leq \delta$ but also allows one to model issues such as capacity expansion. Note also that if $\bar{b}_i = 0$, then we may eliminate δ_i from the formulation.

Theorem 1 *If GenQP is bounded, then it is equivalent to*

$$\begin{aligned} \max \ & \frac{1}{2}c^T x + \frac{1}{2}b^T y^0 + \frac{1}{2}(b + \bar{b})^T y^1 - f^T \delta \\ \text{subject to } & A^T y^0 + A^T y^1 - Qx = c \qquad && Ax \leq b + \bar{b} \circ \delta \\ & (y^0)^T (b - Ax) = 0 && (y^1)^T (b + \bar{b} - Ax) = 0 \\ & y^0, y^1 \geq 0 && \delta \in \{0, 1\}^m. \end{aligned} \tag{1}$$

Proof For any fixed $\delta \in \{0,1\}^n$, we can use the result from Ref. [9] to reformulate the resulting QP as

$$\begin{aligned} \max \quad & \frac{1}{2}c^T x + \frac{1}{2}\left(b + \bar{b}\circ\delta\right)^T y \\ \text{subject to} \quad & A^T y - Qx = c \\ & Ax \le b + \bar{b}\circ\delta \quad y \ge 0 \\ & y^T(b + \bar{b}\circ\delta - Ax) = 0. \end{aligned}$$

By introducing the variables $y^1 = \delta \circ y$ and $y^0 = (e - \delta)\circ y$, we easily obtain a solution to (1) with the same objective value. Hence, the optimal value of (1) is at least the optimal value of GenQP.

Conversely, suppose we have an optimal solution (x, δ, y^0, y^1) to (1). Using the equality $A^T y^0 + A^T y^1 - Qx = c$ and the complementarity constraints, one can see that

$$\frac{1}{2}c^T x + \frac{1}{2}b^T y^0 + \frac{1}{2}(b + \bar{b})^T y^1 = \frac{1}{2}x^T Qx + c^T x.$$

Hence, the optimal value of GenQP is at least the optimal value (1). □

Note that this formulation essentially introduces two multipliers for each constraint i, one for each possible right hand side, b_i or $b_i + \bar{b}_i$. Applying Theorem 1 to FCQP, we obtain

$$\max \quad \tfrac{1}{2}c^T x + \tfrac{1}{2}e^T y^1 - f^T\delta \tag{2}$$

$$\text{subject to} \quad y^1 + y^0 - Qx - z = c \quad \delta \in \{0,1\}^n \tag{3}$$

$$y^1, y^0, z \ge 0 \quad 0 \le x \le \delta \tag{4}$$

$$z^T x = 0 \quad (e - x)^T y^1 = 0 \quad x^T y^0 = 0 \tag{5}$$

Note that we did not need additional multipliers for the $x \ge 0$ constraints since these have no binary variables in the right hand side. Otherwise, by setting $A = I$, $b = 0$, and $\bar{b} = e$, the formulation for FCQP follows trivially from the theorem.

We are interested in solving this reformulation to obtain a globally optimal solution to FCQP. Our main tool for this will be LP-based branch-and-cut. That is, we intend to relax the complementarity constraints given in (5) and the integer constraints $\delta \in \{0,1\}$ to obtain an LP relaxation. We will then use branching to enforce the relaxed constraints. However, this basic approach is not very effective, mostly because of the weak bounds provided by the LP relaxations. Hence, in the remainder of this paper, we develop several classes of valid inequalities that can be separated efficiently. At the end of the paper, we will demonstrate their effectiveness in some computational tests.

3 One-row relaxation

Note that the reformulation of FCQP implies that $z_i y_i^1 = 0$ and $y_i^1 y_i^0 = 0$ for all $i \in 1,\ldots,n$. Furthermore, given the structure of the problem, we may assume WLOG that $z_i y_i^0 = 0$. In order to develop valid inequalities for the reformulation, we propose to study the polyhedral structure of a subset of the constraints. This is a commonly used technique in the IP literature, see for instance the use of knapsack inequalities by Crowder et al. [7], and has also been used in the context of complementarity [8]. This approach was also used by Vandenbussche and Nemhauser [30] to find valid inequalities for the reformulation of box-constrained QPs. In fact, the set we study is closely related to the relaxation they studied. In particular, for any $i \in N := \{1, \ldots, n\}$, define a *one-row relaxation* as the set

$$R_i = \left\{ (y_i^0, y_i^1, z_i, x) \in \mathbb{R}^{n+3} \mid \begin{array}{c} y_i^0 + y_i^1 - z_i - \sum_{j \in N} q_{ij} x_j = c_i \\ y_i^1(1 - x_i) = 0 \quad z_i x_i = 0 \\ y_i^0 x_i = 0 \quad y_i^0 z_i = 0 \\ y_i^0, y_i^1, z_i \geq 0 \quad 0 \leq x \leq e \end{array} \right\}.$$

We also define the convex hull of this set as $PR_i = \text{conv}(R_i)$. Note that the set $R_i|_{y_i^0=0} := \{(y_i^0, y_i^1, z_i, x) \in R_i : y_i^0 = 0\}$ is the one-row relaxation studied by Vandenbussche and Nemhauser [30].

It is not difficult to see that the complementarity constraints imply that R_i is bounded, and hence PR_i is a polytope. Knowing this, we can compute upper bounds for y_i^0, y_i^1, and z_i. Define

- $\bar{y}_i^0 = c_i + \sum_{j \in N_i^+} q_{ij}$,
- $\bar{y}_i^1 = c_i + q_{ii} + \sum_{j \in N_i^+} q_{ij}$, and
- $\bar{z}_i = -c_i - \sum_{j \in N_i^-} q_{ij}$,

where $N_i^+ = \{j \in N \setminus i : q_{ij} \geq 0\}$ and $N_i^- = \{j \in N \setminus i : q_{ij} < 0\}$. It is easy to see that if $y_i^0 > 0$, then $y_i^0 < \bar{y}_i^0$, with similar conclusions for y_i^1 and z_i. To develop the results in this paper, we will use

Assumption 1 $\bar{y}_i^0, \bar{y}_i^1, \bar{z}_i > 0$ *as this is the most complex and significant case. WLOG, we also assume that* $q_{ij} \neq 0 \; \forall j \in N \setminus i$*, otherwise we may consider* R_i *to be a set of smaller dimension.*

In the remainder of this section, we will outline the polyhedral characterization of the set PR_i. We will state a number of results that define classes of nontrivial facets, i.e. inequalities not induced by bounds on the variables. We will postpone the proofs for these results to later sections.

For convenience, given a vector $\alpha \in \mathbb{R}^n$, we denote $A^0 = \{j \in N \backslash i : \alpha_j = 0\}$, $A^+ = \{j \in N \setminus i : \alpha_j > 0\}$, and $A^- = \{j \in N \setminus i : \alpha_j < 0\}$. Given a scalar a, we also denote $a^+ = \max(0, a)$.

To introduce the first class of inequalities, we choose some $B \subseteq N \setminus i$ and define

$$V := c_i + \sum_{j \in N_i^+ \backslash B} q_{ij} + \sum_{j \in N_i^- \cap B} q_{ij}$$

and

$$SEP^B = \left\{ (\alpha^0, \alpha) \in \mathbb{R}^{n+1} \mid \begin{array}{c} \alpha_i = V\alpha^0 \quad \alpha_i, \alpha^0 \geq 0 \\ \sum_{j \in N_i^+ \backslash B} \alpha_j - \sum_{j \in N_i^- \backslash B} \alpha_j + \alpha_i = \bar{z}_i \\ \alpha_j = -q_{ij}\alpha^0 \; \forall j \in B \\ \alpha_j \in \{0, q_{ij}\} \; \forall j \in N \setminus (B \cup i) \end{array} \right\}$$

Theorem 2 *Suppose* $\emptyset \neq B \subseteq N \setminus i$ *is such that* $V > 0$, $q_{ii} + V > 0$*, and suppose* $(\alpha^0, \alpha) \in SEP^B$ *with* $\alpha^0 > 0$*, then* $z_i + \alpha^0 y_i^0 + \sum_j \alpha_j x_j \leq \sum_j \alpha_j^+$ *defines a facet of* PR_i.

A different class of facets arises when $B = \emptyset$. Define

$$SEP^z = \left\{ (\alpha^0, \alpha) \in \mathbb{R}^{n+1} \mid \begin{array}{c} \sum_{j\in N_i^+} \alpha_j - \sum_{j\in N_i^-} \alpha_j + \alpha_i = \bar{z}_i \\ 0 \le \alpha_j \le q_{ij} \ \forall j \in N_i^+ \\ q_{ij} \le \alpha_j \le 0 \ \forall j \in N_i^- \\ \alpha_i \ge 0, \ \alpha^0 = \frac{\alpha_i}{\bar{y}_i^0} \end{array} \right\}$$

Theorem 3 *Suppose* (α^0, α) *is a vertex of* SEP^z *and assume that* $A^0 \neq \emptyset$, *then* $z_i + \alpha^0 y_i^0 + \sum_j \alpha_j x_j \le \sum_j \alpha_j^+$ *defines a facet of* PR_i.

To obtain the next class of facets, we define

$$SEP^1 := \left\{ \alpha \in \mathbb{R}^n \mid \begin{array}{c} \sum_{j\in N_i^-} \alpha_j - \sum_{j\in N_i^+} \alpha_j - \alpha_i = \bar{y}_i^1 \\ 0 \le \alpha_j \le -q_{ij} \ \forall j \in N_i^- \\ -q_{ij} \le \alpha_j \le 0 \ \forall j \in N_i^+ \\ \alpha_i \le 0 \end{array} \right\}.$$

Theorem 4 *Suppose* α *is a vertex of* SEP^1 *and assume that either*

- $\alpha_j \in \{0, -q_{ij}\} \ \forall j \in N \setminus i$, *or*
- $q_{ii} < 0$ *and* $c_i + \sum_{j\in A^+} q_{ij} + \sum_{j\in N_i^+\cap A^0} q_{ij} > 0$,

then $y_i^1 + \sum_j \alpha_j x_j \le \sum_j \alpha_j^+$ *defines a facet of* PR_i.

The last class of facets we introduce are defined by the following result:

Theorem 5 *Suppose that* α *is a vertex of*

$$SEP^0 = \left\{ \alpha \in \mathbb{R}^n \mid \begin{array}{c} \sum_{j\in N_i^-} \alpha_j - \sum_{j\in N_i^+} \alpha_j = \bar{y}_i^0 \\ 0 \le \alpha_j \le -q_{ij} \ \forall j \in N_i^- \\ -q_{ij} \le \alpha_j \le 0 \ \forall j \in N_i^+ \\ \alpha_i = 0 \end{array} \right\}$$

and that $c_i + q_{ii} + \sum_{j\in N_i^+\cap A^0} q_{ij} + \sum_{j\in A^+} q_{ij} > 0$, *then* $y_i^0 + \sum_j \alpha_j x_j \le \sum_j \alpha_j^+$ *defines a facet of* PR_i.

The inequalities defined in Theorems 3 and 4 are closely related to the inequalities defined by Vandenbussche and Nemhauser [30] for the set $R_i|_{y_i^0=0}$. In fact, as we will show, the facets of PR_i described in these two theorems can be obtained by lifting the variable y_i^0 into inequalities valid for $R_i|_{y_i^0=0}$. However, many of the facets of PR_i defined by Theorem 3 are obtained by lifting y_i^0 into a valid inequality that does *not* define a facet of $R_i|_{y_i^0=0}$. For those inequalities we cannot use maximal lifting to show they define facets. We point out also that the inequalities defined by Theorems 2 and 5 do not follow from such simple liftings. The proofs of these results will be provided in Sects. 4–7. Furthermore, in these sections we will also show that these theorems identify all the nontrivial facets of PR_i, i.e. if an inequality cannot be identified through one of these theorems, then it does not define a nontrivial facet.

Before proceeding with the proofs, we illustrate the results with an example.

Example 1 Suppose $n = 3$ and that we have $q_{1\cdot} = \begin{bmatrix} 3 & -4 & 5 \end{bmatrix}$ and $c_1 = 0$. One can check that $\bar{y}_1^1 = 8$, $\bar{z}_1 = 4$, and $\bar{y}_1^0 = 5$. Using PORTA [6], one can verify that the nontrivial facets of PR_1, organized by corresponding theorem, are

- Theorem 2
  $z_1 + 4y_1^0 + 4x_1 + 16x_2 \leq 20$. Note that in this case, we have $B = \{2\}$.
- Theorem 3
  $z_1 - 4x_2 \leq 0$
  $z_1 + 4x_3 \leq 4$
  $z_1 + \frac{4}{5}y_1^0 + 4x_1 \leq 4$
- Theorem 4
  $y_1^1 - 8x_1 \leq 0$
  $y_1^1 - 4x_1 + 4x_2 \leq 4$
- Theorem 5
  $y_1^0 - 5x_3 \leq 0$

4 Basic results

In this section, we develop some basic understanding of the polyhedral structure of PR_i. We begin by characterizing all valid inequalities for PR_i. An analogous result for $R_i|_{y_i^0=0}$ can be found in Ref. [30] and hence we omit the proof here.

Proposition 6 *The inequality*

$$\alpha^0 y_i^0 + \alpha^1 y_i^1 + \alpha^z z_i + \sum_{j \in N} \alpha_j x_j \leq \beta$$

is valid for PR_i if and only if $\exists\ \lambda^1, \lambda^2, \lambda^3, \lambda^4$ satisfying

$$\sum_{j \in N} (-q_{ij}\lambda^1 + \alpha_j)^+ \leq \beta + \lambda^1 c_i, \tag{6}$$

$$\sum_{j \in N \setminus i} (q_{ij}\lambda^2 + \alpha_j)^+ + q_{ii}\lambda^2 + \alpha_i \leq \beta - \lambda^2 c_i, \tag{7}$$

$$\sum_{j \in N \setminus i} (-q_{ij}\lambda^3 + \alpha_j)^+ \leq \beta + \lambda^3 c_i, \tag{8}$$

$$\sum_{j \in N \setminus i} (q_{ij}\lambda^4 + \alpha_j)^+ \leq \beta - \lambda^4 c_i, \tag{9}$$

$$\lambda^2 \geq \alpha^1 \quad \lambda^3 \geq \alpha^z \lambda^4 \geq \alpha^0. \tag{10}$$

The following lemma is also a trivial extension of a result in [30].

Lemma 7 *If*

$$\alpha^0 y_i^0 + \alpha^1 y_i^1 + \alpha^z z_i + \sum_{j \in N} \alpha_j x_j \leq \beta$$

is a facet of PR_i, then there exist λ^k, $k = 1, 2, 3, 4$ satisfying (6)–(10) such that $\lambda^2 = \alpha^1$, $\lambda^3 = \alpha^z$, and $\lambda^4 = \alpha^0$.

Note that we can always use the equality set of R_i to eliminate y_i^1 from any valid inequality. Hence we may write a general inequality as

$$\alpha^0 y_i^0 + \alpha^z z_i + \sum_{j \in N} \alpha_j x_j \leq \beta. \tag{11}$$

In order to prove the next result, it is useful to know the structure of the vertices of the polytope PR_i. Suppose we define LPR_i as the LP relaxation of R_i, that is LPR_i is the polyhedron defined by all constraints of R_i except the complementarity constraints. LPR_i has only one defining equality and hence, for any vertex of LPR_i, at most one variable will not be at one of its bounds. This is very useful thanks to the following trivial lemma whose proof we omit.

Lemma 8 *Any vertex of PR_i is also a vertex of LPR_i.*

From this lemma, we know that if we have a vertex of PR_i such that $y_i^0 > 0$, then we must have $y_i^1 = 0$, $z_i = 0$, and $x_j \in \{0, 1\}\ \forall j \in N$. Similar conclusions can be drawn if $y_i^1 > 0$ or $z_i > 0$. Recall that we define a *nontrivial facet* as a facet not induced by any of the bound constraints.

Proposition 9 *Given a nontrivial facet (11) of PR_i, then $\alpha^z \geq 0$. If $\alpha^z = 0$, then $\alpha^0 > 0$ and $\alpha_i = 0$.*

Proof Since the inequality is a nontrivial facet, there exist distinct vertices of PR_i, $(0, \tilde{y}_i^1, 0, x^1)$ and $(0, 0, \tilde{z}_i, x^2)$, that satisfy (11) at equality and such that $\tilde{y}_i^1 > 0$, $\tilde{z}_i > 0$, and $x^k \in \{0, 1\}^n$ for each $k = 1, 2$. Furthermore, because of complementarity, we have that $x_i^1 = 1$ and $x_i^2 = 0$. For notational convenience, denote $X^k = \{j \in N \setminus i : x_j^k = 1\}$ for each $k = 1, 2$.

We first show that $\alpha^z \geq 0$. Suppose $\alpha^z < 0$, rescaling (11) by $|\alpha^z|$ and redefining the coefficients, we obtain $\alpha^0 y_i^0 - z_i + \sum_{j \in N} \alpha_j x_j \leq \beta$. From the points on the facet, we have

$$\alpha_i + \sum_{j \in X^1} \alpha_j = \beta \text{ and } -\tilde{z}_i + \sum_{j \in X^2} \alpha_j = c_i + \sum_{j \in X^2} (q_{ij} + \alpha_j) = \beta,$$

which implies that $\alpha_i = -\tilde{z}_i + \sum_{j \in X^2 \setminus X^1} \alpha_j - \sum_{j \in X^1 \setminus X^2} \alpha_j$.

Note that if we were to decrease x_ℓ^1 for some $\ell \in X^1$ by $\epsilon > 0$ and chose ϵ small enough so that $y_i^1 = \tilde{y}_i^1 - q_{i\ell}\epsilon \geq 0$, then we still have a point in R_i that must satisfy the inequality and hence $\alpha_i + \sum_{j \in X^1 \setminus \ell} \alpha_j + \alpha_\ell(1 - \epsilon) \leq \beta$. This implies that $\alpha_\ell \geq 0$. Using this technique, one can show that

$$\alpha_j \geq 0\ \forall j \in X^1 \quad \alpha_j \leq 0\ \forall j \notin X^1 \quad \alpha_j \geq -q_{ij}\ \forall j \in X^2 \quad \alpha_j \leq -q_{ij}\ \forall j \notin X^2.$$

Using these inequalities, one can show that

$$-q_{ii} < c_i + \sum_{j \in X^1} q_{ij} \leq \alpha_i \leq c_i + \sum_{j \in X^2} q_{ij} = -\tilde{z}_i < 0,$$

where the first inequality follows because $\tilde{y}_i^1 = c_i + q_{ii} + \sum_{j \in X^1} q_{ij} > 0$. Reorganizing, we get that

$$0 < \frac{-c_i - \sum_{j \in X^1} q_{ij}}{q_{ii}} < 1$$

By setting x_i equal to this fraction and $x_j = 1\ \forall j \in X^1$, we obtain a point in R_i that violates (11) since $\alpha_i < 0$ and $\alpha_i + \sum_{j \in X^1} \alpha_j = \beta$. Because of this contradiction, we may conclude that $\alpha^z \geq 0$.

Now suppose that $\alpha^z = 0$. We may now conclude that $\sum_{j \in X^2} \alpha_j = \beta$, $\alpha_j \geq 0\ \forall j \in X^2$, and $\alpha_j \leq 0\ \forall j \notin X^2$. Furthermore, $\alpha_i = \sum_{j \in X^2 \setminus X^1} \alpha_j - \sum_{j \in X^1 \setminus X^2} \alpha_j$ implies that $\alpha_i = 0$, as required.

Now suppose that in this case, we also have that $\alpha^0 \leq 0$. Since $\sum_{j\in X^1} \alpha_j = \beta$, it is not difficult to see then that the inequality $\alpha^0 y_i^0 + \sum_{j\in N\setminus i} \alpha_j \leq \beta$ is a linear combination of the bound inequalities $-x_j \leq 0 \; \forall j \notin X^1$, $x_j \leq 1 \; \forall j \in X^1$, and $-y_i^0 \leq 0$. This contradicts the assumption that (11) is a nontrivial facet, and hence we may also assume that $\alpha^0 > 0$ if $\alpha^z = 0$. □

Consider the point $(0, \tilde{y}_i^1, 0, x^1)$ defined in the previous proof. Using $\lambda^2 = 0$ in (7), we have

$$\beta = \sum_{j\in X^1} \alpha_j + \alpha_i \leq \sum_{j\in N\setminus i} \alpha_j^+ + \alpha_i \leq \beta.$$

This implies (7) is tight if the given inequality is a nontrivial facet. Similar arguments can be used to show that (8) and (9) are tight. We will take advantage of this fact throughout the next few sections, where we divide facet-defining inequalities into different categories, depending on the sign of α^z and α_i.

5 Inequalities with $\alpha^z > 0$ and $\alpha_i \geq 0$

In this section, we study the facets of PR_i of the form $\alpha^0 y_i^0 + \alpha^z z_i + \sum_{j\in N} \alpha_j x_j \leq \beta$ with the property that $\alpha^z > 0$ and $\alpha_i \geq 0$. Hence, we can rescale an arbitrary inequality to read

$$z_i + \alpha^0 y_i^0 + \sum_{j\in N} \alpha_j x_j \leq \beta. \tag{12}$$

In this case, we can substitute $\lambda^2 = 0$ into (7), $\lambda^3 = 1$ into (8), and $\lambda^4 = \alpha^0$ into (9). Note that, since $\alpha_i \geq 0$, we may also set $\lambda^1 = 0$ in which case (6) becomes equivalent to (7). Hence, the conditions necessary for the validity of (12) are

$$\sum_{j\in N\setminus i} \alpha_j^+ + \alpha_i = \beta, \tag{13}$$

$$-c_i + \sum_{j\in N\setminus i} (-q_{ij} + \alpha_j)^+ = \beta, \tag{14}$$

$$c_i\alpha^0 + \sum_{j\in N\setminus i} (q_{ij}\alpha^0 + \alpha_j)^+ = \beta. \tag{15}$$

Lemma 10 *If (12) is a nontrivial facet and $\alpha_i \geq 0$, then $\alpha^0 \geq 0$, $\alpha_j \leq q_{ij} \; \forall j \in N_i^+$, $\alpha_j \geq q_{ij} \; \forall j \in N_i^-$, $\alpha_j \geq -q_{ij}\alpha^0 \; \forall j \in N_i^+$, and $\alpha_j \leq -q_{ij}\alpha^0 \; \forall j \in N_i^-$.*

Proof Suppose we have a facet with $\alpha^0 < 0$. From (13) and since $\alpha_i \geq 0$, it is easy to see that the same inequality with $\alpha^0 = 0$ is also valid, a contradiction. Hence, we know that $\alpha^0 \geq 0$.

Now suppose that $\alpha_j > q_{ij}$ for some $j \in N_i^+$. Since $\alpha^0 \geq 0$, that means the jth term contributes to the left hand side of all equalities (13)–(15). Hence, we can decrease α_j and β by a sufficiently small $\epsilon > 0$ and obtain another valid inequality. However, the original inequality is a now a linear combination of the new one and the bound $x_j \leq 1$, which implies the original cannot be a facet. A similar argument shows that $\alpha_j \geq q_{ij} \; \forall j \in N_i^-$.

Suppose that $\alpha_j + q_{ij}\alpha^0 < 0$ for some $j \in N_i^+$. Since this also implies that $\alpha_j < 0$, index j does not contribute to the left hand sides of any of the inequalities (13)–(15). Hence, we may increase α_j by a sufficiently small amount and remain valid, a contradiction. We omit the proof for the case $j \in N_i^-$. □

Given a nontrivial facet (12) with $\alpha_i \geq 0$, suppose we denote $B^+ = \{j \in N_i^+ : \alpha_j < 0\}$, $B^- = \{j \in N_i^- : \alpha_j > 0\}$, and $B = B^+ \cup B^-$. Using Lemma 10 and eliminating $\beta := \alpha_i + \sum_{j \in N \setminus i} \alpha_j^+ = \alpha_i + \sum_{j \in N_i^+ \setminus B} \alpha_j + \sum_{j \in B^-} \alpha_j$ from (13)–(15) to get

$$\sum_{j \in N_i^+ \setminus B} \alpha_j - \sum_{j \in N_i^- \setminus B} \alpha_j + \alpha_i = \bar{z}_i. \tag{16}$$

$$\bar{y}_i^0 \alpha^0 + \sum_{j \in B^+} \alpha_j - \sum_{j \in B^-} \alpha_j - \alpha_i = 0 \tag{17}$$

$$-q_{ij}\alpha^0 \leq \alpha_j \leq 0 \; \forall j \in B^+ \quad 0 \leq \alpha_j \leq q_{ij} \; \forall j \in N_i^+ \setminus B^+ \tag{18}$$

$$0 \leq \alpha_j \leq -q_{ij}\alpha^0 \; \forall j \in B^- \quad q_{ij} \leq \alpha_j \leq 0 \; \forall j \in N_i^- \setminus B^- \tag{19}$$

$$\alpha^0, \alpha_i \geq 0 \tag{20}$$

For any choice of B, the system (16) – (20) defines a polyhedron in $\mathbb{R}^{n+1}$. Clearly, any facet-defining inequality of the form (12) with $\alpha_i \geq 0$ must correspond to some vertex of this polyhedron for some choice of B. If for some vertex, we have $\alpha_j = 0$ for some $j \in B$, then without loss of generality we can remove that index from B. Hence, we may assume that $\alpha_j \neq 0 \; \forall j \in B$. At this point, it is convenient to consider two situations, $B \neq \emptyset$ and $B = \emptyset$. We begin with the former in the next section.

5.1 $B \neq \emptyset$

We now prove a brief lemma that further characterizes the vertices of the polyhedron defined by (16)–(20).

Lemma 11 *Suppose* (α^0, α) *is a vertex of* (16)–(20)*,* $B \neq \emptyset$*, and* $\alpha_j \neq 0 \; \forall j \in B$*, then*

- $\alpha^0 > 0$
- $\alpha_j = -\alpha^0 q_{ij} \; \forall j \in B$
- $\alpha_j \in \{0, q_{ij}\} \; \forall j \in N \setminus (B \cup i)$
- $V := c_i + \sum_{j \in N_i^+ \setminus B} q_{ij} + \sum_{j \in B^-} q_{ij} > 0$

Proof Since $B \neq \emptyset$, $\alpha_j \neq 0 \; \forall j \in B$, and $\alpha_i \geq 0$, (17) implies that $\alpha^0 > 0$.

To prove the second item, suppose that $-q_{ik}\alpha^0 < \alpha_k < 0$ for some $k \in B^+$. We now show that we can construct two points satisfying (16)–(20) such that α lies on the line-segment between these two points. We will perturb (α^0, α) by adding ϵ^0 to α^0 and adding ϵ_j to $\alpha_j \; \forall j \in B$. All other coefficients will remain unchanged. To ensure that (17) remains satisfied, we must have that

$$\epsilon_k + \sum_{j \in B^+ \setminus k} \epsilon_j - \sum_{j \in B^-} \epsilon_j + \bar{y}_i^0 \epsilon^0 = 0. \tag{21}$$

Furthermore, to ensure that the inequalities $-\alpha^0 q_{ij} \leq \alpha_j \; \forall j \in B^+ \setminus k$ and $\alpha_j \leq -\alpha^0 q_{ij} \; \forall j \in B^-$ continue to hold, we define $\epsilon_j = -q_{ij}\epsilon^0 \; \forall j \in B^- \cup B^+ \setminus k$. Hence (21) requires that $\epsilon_k = \left(\sum_{j \in B^+ \setminus k} q_{ij} - \sum_{j \in B^-} q_{ij} - \bar{y}_i^0 \right) \epsilon^0$. Since $\alpha_j \neq 0 \; \forall j \in B$, $-q_{ik}\alpha^0 < \alpha_k < 0$, and $\alpha^0 > 0$, we can choose ϵ^0 to be a small enough positive number so that the perturbed (α^0, α) still satisfies (16)–(20). Similarly, we can make ϵ^0 a negative number close enough to zero so that we obtain an opposite perturbation. Clearly, (α^0, α) will be a convex combination of these two perturbations and hence cannot be a vertex. A similar argument can be carried out if instead $\exists k \in B^-$ such that $0 < \alpha_k < -q_{ik}\alpha^0$.

Now define $V = c_i + \sum_{j \in N_i^+ \setminus B} q_{ij} + \sum_{j \in B^-} q_{ij}$. Since $\alpha_j = -q_{ij}\alpha^0 \ \forall j \in B$, we can rewrite (17) as $\alpha_i = V\alpha^0$. Clearly, we cannot have $V < 0$, otherwise we would violate $\alpha_i \geq 0$. Furthermore, if $V = 0$, then α^0 can take any nonnegative value and hence an extreme point solution would have $\alpha^0 = 0$. Hence, we may assume that $V > 0$. Consequently, we can also assume that $\alpha_i > 0$ and hence it is not difficult to see that any extreme point solution must have $\alpha_j \in \{0, q_{ij}\} \ \forall j \in N \setminus (B \cup i)$. □

Note that in order for inequality (12) to be facet-defining in this case, we must also have $q_{ii} + V > 0$, otherwise there is no point with $y_i^1 > 0$ that lies on the facet, contradicting the fact it is nontrivial. We now show that the necessary conditions derived up to this point are also sufficient. For convenience, we define

$$SEP^B = \left\{ (\alpha^0, \alpha) \in \mathbb{R}^{n+1} \mid \begin{array}{c} \alpha_i = V\alpha^0 \quad \alpha_i, \alpha^0 \geq 0 \\ \sum_{j \in N_i^+ \setminus B} \alpha_j - \sum_{j \in N_i^- \setminus B} \alpha_j + \alpha_i = \bar{z}_i \\ \alpha_j = -q_{ij}\alpha^0 \ \forall j \in B \\ \alpha_j \in \{0, q_{ij}\} \ \forall j \in N \setminus (B \cup i) \end{array} \right\}$$

We now restate and prove Theorem 2.

Theorem 2 *Suppose* $\emptyset \neq B \subseteq N \setminus i$ *is such that* $V > 0$, $q_{ii} + V > 0$, *and suppose* $(\alpha^0, \alpha) \in SEP^B$ *with* $\alpha^0 > 0$, *then* (12) *defines a facet of* PR_i.

Proof Define $\tilde{F}$ as an arbitrary face induced by

$$\mu^0 y_i^0 + \mu^1 y_i^1 + \mu^z z_i + \sum_{j \in N} \mu_j^x x_j \leq d \tag{22}$$

and assume $F \subseteq \tilde{F}$, where F is the face induced by (12), the inequality we want to prove is a facet. We will show that (22) is a linear combination of (12) and the equality set defining R_i. This will imply that (12) induces a facet.

For notational convenience, we will refer to points in R_i as (r, s, v, X) where r, s, v will represent the values of y_i^0, y_i^1, and z_i, respectively. X will refer to the index set $j \in N$ such that $x_j = 1$, with all other x's assumed to be 0.

It is not hard to check the following points are in R_i, and we will also show that they lie on F:

$$\begin{aligned} v^0 &= (\bar{y}_i^0, 0, 0, N_i^+) \\ v^1 &= (0, V + q_{ii}, 0, (N_i^+ \setminus B) \cup B^- \cup i) \\ v^2 &= (V, 0, 0, (N_i^+ \setminus B) \cup B^-) \\ v^z &= (0, 0, \bar{z}_i, N_i^-). \end{aligned}$$

To show that v^0 is in F, observe that

$$\begin{aligned} \bar{y}_i^0 \alpha^0 = \alpha_i + \sum_{j \in B^-} \alpha_j - \sum_{j \in B^+} \alpha_j &= \left(\alpha_i + \sum_{j \in B^-} \alpha_j + \sum_{j \in N_i^+ \setminus B} \alpha_j \right) - \sum_{j \in N_i^+} \alpha_j \\ &= \beta - \sum_{j \in N_i^+} \alpha_j \Rightarrow \bar{y}_i^0 \alpha^0 + \sum_{j \in N_i^+} \alpha_j = \beta. \end{aligned}$$

To show that $v^2 \in F$, recall that $\alpha^0 V = \alpha_i$ and hence

$$\alpha^0 V + \sum_{j \in (N_i^+ \setminus B) \cup B^-} \alpha_j = \alpha_i + \sum_{j \in (N_i^+ \setminus B) \cup B^-} \alpha_j = \beta.$$

The last equality also shows that $v^1 \in F$. Lastly, we have

$$\bar{z}_i + \sum_{j \in N_i^-} \alpha_j = \left(\sum_{j \in N_i^+ \setminus B} \alpha_j - \sum_{j \in N_i^- \setminus B} \alpha_j + \alpha_i \right) + \sum_{j \in N_i^-} \alpha_j = \beta,$$

which implies that $v^z \in F$. We now show a number of intermediate results:

$\mu_\ell^x = -q_{i\ell}\mu^0 \ \forall \ell \in B$
Suppose $\ell \in B^-$. We obtain another point by perturbing v^0 slightly, setting $x_\ell = \epsilon > 0$ and adding $q_{i\ell}\epsilon$ to y_i^0. By choosing ϵ small enough so that $\bar{y}_i^0 + q_{i\ell}\epsilon \geq 0$ and since $\alpha_\ell = -q_{i\ell}\alpha^0$, we have

$$\alpha^0 \left(\bar{y}_i^0 + \epsilon q_{i\ell} \right) + \sum_{j \in N_i^+} \alpha_j + \alpha_\ell \epsilon = \beta + \left(\alpha^0 \epsilon q_{i\ell} + \epsilon \alpha_\ell \right) = \beta,$$

which implies the perturbed point is also on F and hence $\tilde{F}$. By substituting v^0 and the perturbed point into $\tilde{F}$, we obtain $\mu_\ell^x = -q_{i\ell}\mu^0$.
Similarly, if $\ell \in B^+$, we can subtract $\epsilon > 0$ from x_ℓ to create a perturbed point that leads to the same conclusion.
$\mu_\ell^x = -q_{i\ell}\mu^1 \ \forall \ell \in A^0 := \{j \in N \setminus i : \alpha_j = 0\}$
Suppose $\ell \in N_i^+ \cap A^0$. We perturb v^1 by subtracting ϵ from x_ℓ and adjusting y_i^1 appropriately. Note that if ϵ is small enough, then $V + q_{ii} - \epsilon q_{i\ell} > 0$ and since $\ell \in A^0$, the perturbed point is also on F, and hence on $\tilde{F}$. Substituting both into the inequality defining $\tilde{F}$ and equating, we obtain the desired result. By increasing x_ℓ by ϵ if $\ell \in N_i^- \cap A^0$, one can derive the same result.
$\mu_\ell^x = q_{i\ell}\mu^z \ \forall \ell \in N \setminus \left(B \cup A^0 \cup i \right)$
Suppose that $\ell \in N_i^- \setminus \left(B^- \cup A^0 \right)$. We perturb v^z by subtracting small enough $\epsilon > 0$ from x_ℓ such that $z_i = \bar{z}_i + \epsilon q_{i\ell} \geq 0$. Since $\alpha_\ell = q_{i\ell}$, it is easy to see this point is in F. Again, we substitute both points into (22) to obtain the desired result. The other case is similar.

We now show that $\mu_i^x = (\mu^1 + \mu^z)\alpha_i - \mu^1 q_{ii}$. Substituting v^1 and v^z into (22) and eliminating common terms, we get

$$(V + q_{ii})\mu^1 + \mu_i^x + \sum_{j \in N_i^+ \setminus B} \mu_j^x = \bar{z}_i \mu^z + \sum_{j \in N_i^- \setminus B} \mu_j^x.$$

Substituting in the previous results as necessary, we obtain

$$\mu^1 \left(c_i + \sum_{j \in N_i^+ \setminus (B \cup A^0)} q_{ij} + \sum_{j \in B^-} q_{ij} \right) + \mu^1 q_{ii} + \mu_i^x + \sum_{j \in N_i^+ \setminus (B \cup A^0)} q_{ij}\mu^z$$
$$= \mu^z \left(-c_i - \sum_{j \in B^-} q_{ij} - \sum_{j \in N_i^- \cap A^0} q_{ij} \right) - \sum_{j \in N_i^- \cap A^0} q_{ij}\mu^1.$$

From (16), we have that

$$\alpha_i = -c_i - \sum_{j \in B^-} q_{ij} - \sum_{j \in N_i^- \cap A^0} q_{ij} - \sum_{j \in N_i^+ \setminus (B \cup A^0)} q_{ij}.$$

Hence, we may conclude that $\mu_i^x = -q_{ii}\mu^1 + (\mu^1 + \mu^z)\alpha_i$.

Next, we show that $\mu^0 = \mu^1 + (\mu^1 + \mu^z)\alpha^0$. Using the fact that v^2 and v^1 are in $\tilde{F}$, we have

$$V\mu^0 + \sum_{j \in N_i^+ \setminus B} \mu_j^x + \sum_{j \in B^-} \mu_j^x = (V + q_{ii})\mu^1 + \sum_{j \in N_i^+ \setminus B} \mu_j^x + \sum_{j \in B^-} \mu_j^x + \mu_i^x.$$

Hence,

$$V(\mu^0 - \mu^1) = \mu^1 q_{ii} + \mu_i^x = (\mu^1 + \mu^z)\alpha_i = (\mu^1 + \mu^z)\alpha^0 V,$$

which, since $V > 0$, implies the desired result. From here, simple algebraic manipulations show that

$$d = \mu^1 c_i + (\mu^1 + \mu^z)\left(\alpha_i + \sum_{j \in N_i^+ \setminus B} \alpha_j + \sum_{j \in B^-} \alpha_j\right).$$

Combining all these results, we have shown that $\mu^1 \times (y_i^0 + y_i^1 - z_i - \sum_{j \in N} q_{ij} = c_i) + (\mu^1 + \mu^z) \times$(12) is equal to $\mu^0 y_i^0 + \mu^1 y_i^1 + \mu^z z_i + \sum_{j \in N} \mu_j^x x_j \le d$, as desired. □

5.2 $B = \emptyset$

If we assume that $B = \emptyset$, then (16)–(20) simplifies to define the following polytope

$$SEP^z = \left\{ (\alpha^0, \alpha) \in \mathbb{R}^{n+1} \mid \begin{array}{c} \sum_{j \in N_i^+} \alpha_j - \sum_{j \in N_i^-} \alpha_j + \alpha_i = \bar{z}_i \\ 0 \le \alpha_j \le q_{ij} \ \forall j \in N_i^+ \\ q_{ij} \le \alpha_j \le 0 \ \forall j \in N_i^- \\ \alpha_i \ge 0, \ \alpha^0 = \frac{\alpha_i}{\bar{y}_i^0} \end{array} \right\}$$

While any $(\alpha^0, \alpha) \in SEP^z$ induces a valid inequality of the form (12), clearly only vertices of SEP^z can induce facets of PR_i. In the remainder of this section, we will characterize those vertices of SEP^z that yield facets. We begin by identifying facets that result from lifting facet-defining inequalities of $R_i|_{y_i^0=0}$ introduced by Vandenbussche and Nemhauser [30]. Again, we define $A^+ = \{j \in N \setminus i : \alpha_j > 0\}$ and $A^0 = \{j \in N \setminus i : \alpha_j = 0\}$.

Proposition 12 *Suppose (α^0, α) is a vertex of SEP^z, then if*

- $\alpha_j \in \{0, q_{ij}\} \ \forall j \in N \setminus i$, *or*
- $q_{ii} < 0$ *and* $K := c_i + q_{ii} + \sum_{j \in A^+} q_{ij} + \sum_{j \in A^0 \cap N_i^-} q_{ij} < 0$,

then (12) *defines a facet of* PR_i.

Proof Vandenbussche and Nemhauser [30] showed that if either of the conditions of the proposition hold, then $z_i + \sum_{j \in N} \alpha_j x_j \le \sum_{j \in N} \alpha_j^+$ defines a facet of $\text{conv}(R_i|_{y_i^0=0})$. We will show that if we maximally lift y_i^0 into the inequality, its lifting coefficient is $\frac{\alpha_i}{\bar{y}_i^0}$, proving the desired result. The lifting problem reads

$$\theta = \min \left\{ \frac{\sum_j (\alpha_j^+ - \alpha_j x_j) - z_i}{y_i^0} \mid (y_i^1, y_i^0, z_i, x) \in R_i, y_i^0 > 0 \right\}.$$

Using the fact that $y_i^0 > 0$ implies that $x_i = 0$, $y_i^1 = 0$, and $z_i = 0$, the lifting problem may be simplified to

$$\theta = \min \left\{ \frac{\alpha_i + \sum_{j \in N_i^+} \alpha_j (1 - x_j) - \sum_{j \in N_i^-} \alpha_j x_j}{y_i^0} \mid (0, y_i^0, 0, x) \in R_i, y_i^0 > 0 \right\}.$$

It is easy to see that an optimal solution to this problem is to set $x_j = 1 \ \forall j \in N_i^+$ and $x_j = 0 \ \forall j \in N_i^- \cup i$, since this minimizes the numerator and maximizes the denominator. Hence, the lifting coefficient is $\theta = \frac{\alpha_i}{\bar{y}_i^0}$. □

Note that the argument used in the proof does not rely on the two conditions of the proposition. However, if neither of the conditions are satisfied, then the inequality does not define a facet of $\text{conv}(R_i|_{y_i^0=0})$ and hence we would not be able to guarantee that the lifted inequality defines a facet. We now restate Theorem 3 which shows that lifting some of these nonfacets does indeed yield facets of PR_i.

Theorem 3 *Suppose* (α^0, α) *is a vertex of* SEP^z. *If* $A^0 \neq \emptyset$, *then* (12) *defines a facet of* PR_i.

Proof Because of Proposition 12, we may assume that $\exists k \in N \setminus i$ such that $\alpha_k \notin \{0, q_{ik}\}$. Since (α^0, α) defines a vertex of SEP^z, this implies that $\alpha_i = 0$ since we cannot have two or more variables not at their bounds at a vertex. Hence, we also have that $\alpha^0 = 0$.

Since $\sum_{j \in N_i^+} \alpha_j - \sum_{j \in N_i^-} \alpha_j = \bar{z}_i$, it is not difficult to show that

$$K := c_i + q_{ii} + \sum_{j \in A^+} q_{ij} + \sum_{j \in A^0 \cap N_i^-} q_{ij} = |q_{ik} - \alpha_k| + q_{ii}.$$

If $K < 0$, it must be the case that $q_{ii} < 0$ and hence the second sufficient condition of Proposition 12 applies to show the inequality is a facet. Hence, we may now also assume that $K \geq 0$.

Define an arbitrary face $\tilde{F}$ as before and assume $F \subseteq \tilde{F}$, where F is the face induced by (12), the inequality we want to prove is a facet.

The rest of proof continues in much the same way as the proof of Theorem 2. We construct various points in F and $\tilde{F}$ that help characterize $(\mu^0, \mu^1, \mu^z, \mu, d)$ so that the inequality defining $\tilde{F}$ is nothing but a linear combination of (12) and the equality $y_i^0 + y_i^1 - z_i - \sum_j q_{ij} x_j = c_i$. Two key claims that must be shown state that $\mu_k^x = -\mu^1 q_{ik} + (\mu^1 + \mu^z)\alpha_k$ and that $\mu^0 = \mu^1$ (recall that since $\alpha_i = 0$, $\alpha^0 = 0$ as well). We refer the reader to Ref. [15] for the details. □

What remains in this section is to show that any inequalities that do not satisfy the sufficient conditions of Proposition 12 or Theorem 3 cannot define a facet of PR_i.

Proposition 13 *Suppose* (α^0, α) *is a vertex of* SEP^z. *If* $A^0 = \emptyset$, *then* (12) *does not define a facet of* PR_i.

Proof Observe that since $A^0 = \emptyset$, we have that $K = \bar{y}_i^1 > 0$. Furthermore, suppose $\alpha_j = q_{ij}$ for all $j \in N \setminus i$, then since $\sum_j |\alpha_j| = \bar{z}_j$, we have $\bar{y}_i^0 = 0$, contradicting Assumption 1. Hence the sufficient conditions of Proposition 12 do not apply. We begin by assuming that $k \in N_i^+$ is such that $0 < \alpha_k < q_{ik}$. We will show that (12) is not a facet by constructing two valid inequalities such that (12) is a convex combination of the two.

Define $\alpha^1 = \alpha + (q_{ik} - \alpha_k)e_k - (q_{ik} - \alpha_k)e_i$ and $\beta^1 = \beta$, where e_j is the j^{th} unit vector. We can have (α^1, β^1) satisfy (7) with $\lambda^2 = 0$ and (8) with $\lambda^3 = 1$. Recall that $(q_{ik} - \alpha_k) + q_{ii} = K$ and hence $-q_{ii} + \alpha_i^1 \leq 0$, which means we can satisfy (6) with $\lambda^1 = 1$.

We now show that we can satisfy (9) with $\lambda^4 = \frac{\alpha_i^1}{\bar{y}_i^0}$. Note that $(q_{ik} - \alpha_k) + q_{ii} = K = \bar{y}_i^1$ implies $-(q_{ik} - \alpha_k) = -\bar{y}_i^0$ and hence $\lambda^4 = -1$. This makes (9) equivalent to (8), which is already satisfied. This implies that the inequality $z_i + \frac{\alpha_i^1}{\bar{y}_i^0} y_i^0 + \sum_j \alpha_j^1 x_j \leq \beta^1$ is valid.

The second perturbation is defined by $\alpha^2 = \alpha - \alpha_k e_k + \alpha_k e_i$ and $\beta^2 = \beta$. Clearly, (7) and (8) are still satisfied. Since $\alpha_i^2 \geq 0$, we can satisfy (6) by setting $\lambda^1 = 0$. Lastly, we want to show that (9) holds for $\lambda^4 = \frac{\alpha_k}{\bar{y}_i^0} = \frac{\alpha_i^2}{\bar{y}_i^0}$. We have

$$\lambda^4 c_i + \sum_{j \in N \setminus i} (\lambda^4 q_{ij} + \alpha_j^1)^+ = \lambda^4 c_i + \sum_{j \in N_i^+} (\lambda^4 q_{ij} + \alpha_j^1)$$
$$= \lambda^4 \bar{y}_i^0 + \sum_{j \in N_i^+ \setminus k} \alpha_j = \alpha_k + \sum_{j \in N_i^+ \setminus k} \alpha_j = \beta. \quad (\text{since } \alpha_i = 0)$$

Hence, we have shown that $z_i + \frac{\alpha_i^2}{\bar{y}_i^0} y_i^0 + \sum_j \alpha_j^2 x_j \leq \beta^2$ is valid. It is now easy to see that $\frac{\alpha_k}{q_{ik}} \times (\alpha^1, \beta^1) + \frac{q_{ik} - \alpha_k}{q_{ik}} \times (\alpha^2, \beta^2) = (\alpha, \beta)$, which implies the original inequality is not a facet.

If alternatively we have $k \in N_i^-$ with $q_{ik} < \alpha_k < 0$, then we define

$$\begin{array}{ll} \alpha^1 = \alpha - |q_{ik} - \alpha_k| e_k - |q_{ik} - \alpha_k| e_i & \beta^1 = \beta - |q_{ik} - \alpha_k|, \text{ and} \\ \alpha^2 = \alpha + |\alpha_k| e_k + |\alpha_k| e_i & \beta^2 = \beta + |\alpha_k|. \end{array}$$

From here, the proof proceeds much like the case for $k \in N_i^+$ and we omit it here. □

6 Inequalities with $\alpha^z > 0$ and $\alpha_i < 0$

In the previous section, we have characterized those inequalities of the form (12) with $\alpha_i \geq 0$ that define nontrivial facets. Our objective in this section is to show that for any nontrivial facet (12) with $\alpha_i < 0$, we must have $\alpha^0 = -1$. From this fact, one can then easily show that all such facets are equivalent to a set of facets of $R_i|_{y_i^0 = 0}$ characterized by Vandenbussche and Nemhauser [30]. We begin with a simple lemma.

Lemma 14 *Suppose* (12) *is a nontrivial facet with* $\alpha_i < 0$ *and let* λ^ℓ *for* $\ell = 1, \ldots, 4$ *be obtained from Proposition* 6*, then* $-1 \leq -\lambda^1 \leq \alpha^0 < 0$, $0 \leq \alpha_j \leq q_{ij}$ $\forall j \in N_i^+$, *and* $q_{ij} \leq \alpha_j \leq 0$ $\forall j \in N_i^-$.

Proof From the results in Sect. 4, we know that we can set $\lambda^2 = 0$ in (7), $\lambda^3 = 1$ in (8), and $\lambda^4 = \alpha^0$ in (9). If $\alpha^0 = -1$, then (8) and (9) are equivalent. Hence, we may conclude that the

$\alpha^0 \geq -1$. Since the inequality is a nontrivial facet, we know there exist points $(\tilde{y}_i^0, 0, 0, X^0)$ and $(0, \tilde{y}_i^1, 0, X^1 \cup i)$ in R_i with $\tilde{y}_i^0, \tilde{y}_i^1 > 0$ that lie on the facet. Hence, we have that

$$\sum_{j \in X^1} \alpha_j + \alpha_i = \alpha^0 \left(c_i + \sum_{j \in X^0} q_{ij} \right) + \sum_{j \in X^0} \alpha_j.$$

It is easy to show that $\alpha_j + \alpha^0 q_{ij} \geq 0 \ \forall j \in X^0$ and $\alpha_j + \alpha^0 q_{ij} \leq 0 \ \forall j \notin X^0$. Hence, we may conclude that $\left(c_i + \sum_{j \in X^1} q_{ij}\right) \alpha^0 \leq \alpha_i < 0$. Now suppose that $\alpha^0 > 0$, then we may conclude that $0 < -c_i - \sum_{j \in X^1} q_{ij} < q_{ii}$. This then implies that $0 < \frac{-c_i - \sum_{j \in X^1} q_{ij}}{q_{ii}} < 1$. By setting x_i equal to this fraction and $x_j = 1 \ \forall j \in X^1$, we obtain a point that violates (12) since $\alpha_i < 0$. Hence, we have shown that $\alpha^0 \leq 0$. Furthermore, if $\alpha^0 = 0$, then since $\alpha_i < 0$, (7) and (9) cannot be tight simultaneously. But this is a contradiction, since the points $(\tilde{y}_i^0, 0, 0, X^0)$ and $(0, \tilde{y}_i^1, 0, X^1 \cup i)$ show that these two inequalities must be tight.

Note that if $\lambda^1 > 1 (< 0)$, then we may increase the coefficient of $z_i (y_i^1)$ and maintain validity. Hence, we have $0 \leq \lambda^1 \leq 1$. Furthermore, if $\lambda^1 = 0$, then (6) would contradict (7) since $\alpha_i < 0$.

Now suppose that $\alpha_j < 0$ for some $j \in N_i^+$. Since $\lambda^1 \geq 0$ and $\alpha^0 < 0$, we know that index j does not contribute to the left hand sides of (6)–(9). Hence, we can increase α_j without violating validity, a contradiction. If $\alpha_j > q_{ij}$ for some $j \in N_i^+$, then we can decrease α_j and β and maintain validity. A similar argument shows $q_{ij} \leq \alpha_j \leq 0 \ \forall j \in N_i^-$.

Finally, to show that $\alpha^0 \geq -\lambda^1$, note that if this were not the case, then we could use $-\lambda^1$ as the coefficient of y_i^0 and still have a valid inequality, a contradiction. □

We intend to show that if the inequality is to be a nontrivial facet, then we must have $\alpha^0 = -1$. We accomplish this with lemmas 16–18 that each handle a different case corresponding to the sign of $q_{ii}\alpha^0 + \alpha_i$. The proofs of these lemmas rely on the creation of two valid inequalities such that the original inequality is a convex combination of these two. The following lemma shows some sufficient conditions to obtain the required two valid inequalities.

Lemma 15 *Suppose $z_i + \alpha^0 y_i^0 + \sum_j \alpha_j x_j \leq \beta$ is a valid inequality for PR_i and define $\alpha^1 = \alpha + \sum_j \epsilon_j e_j$ and $\beta^1 = \sum_{j \in N_i^-} \epsilon_j$. Suppose that $0 \leq \alpha_j^1 \leq q_{ij} \ \forall j \in N_i^+$, $q_{ij} \leq \alpha_j^1 \leq 0 \ \forall j \in N_i^-$, and that*

$$\epsilon_i + \sum_{j \in N_i^+} \epsilon_j = \sum_{j \in N_i^-} \epsilon_j,$$

then

- *$\alpha_i^1 \geq 0$ implies that $z_i + \sum_j \alpha_j^1 x_j \leq \beta^1$ is valid,*
- *$-q_{ii} + \alpha_i^1 \leq 0$ implies that $z_i - y_i^0 + \sum_j \alpha_j^1 x_j \leq \beta^1$ is valid.*

Proof This lemma is a simple generalization of Proposition 11 found in [30]. □

For notational convenience, we denote $F = \{j \in N \setminus i : \alpha_j \notin \{0, q_{ij}\}\}$, $F^+ = F \cap N_i^+$, and $F^- = F \cap N_i^-$.

Lemma 16 *Suppose (12) is a valid inequality with $\alpha_i < 0$, $-1 < \alpha^0 < 0$, and $q_{ii}\alpha^0 + \alpha_i < 0$, then the inequality cannot be a facet of PR_i.*

Proof Note that in this case, we may set $\lambda^1 = -\alpha^0$ in order for (6) to hold. Now suppose that $q_{ik}\alpha^0 + \alpha_k < 0$ for some $k \in F^+$. Given that $\lambda^2 = 0$, $\lambda^3 = 1$ and $\lambda^4 = \alpha^0$, one can see that there exists $\epsilon > 0$ small enough so we may define $\tilde{\alpha} = \alpha - \epsilon e_i + \epsilon e_k$ and ensure that $\tilde{\alpha}$ satisfies (6)–(9). Hence the inequality $z_i + \alpha^0 y_i^0 + \sum_j \tilde{\alpha}_j x_j \leq \beta$ is valid. The opposite perturbation clearly also defines a valid inequality, which shows the original inequality cannot be a facet. Hence, we may assume that $q_{ij}\alpha^0 + \alpha_j \geq 0\ \forall j \in F^+$.

Now suppose that $q_{ik}\alpha^0 + \alpha_k > 0$ for some $k \in F^-$. Then we can define $\tilde{\alpha} = \alpha + \epsilon e_k + \epsilon e_i$ and $\tilde{\beta} = \beta + \epsilon$ for a small enough $\epsilon > 0$ so that $(\tilde{\alpha}, \tilde{\beta})$ satisfy (6)–(9). Hence, the inequality $z_i + \alpha^0 y_i^0 + \sum_j \tilde{\alpha}_j x_j \leq \tilde{\beta}$ is valid. Again the opposite perturbation also yields a valid inequality. Hence, $q_{ij}\alpha^0 + \alpha_j \leq 0\ \forall j \in F^-$.

Furthermore, a similar argument shows that we cannot have $k_1, k_2 \in F^+$ such that $q_{ik_\ell}\alpha^0 + \alpha_\ell > 0$ for $\ell = 1, 2$. Analogously, we cannot have $k_1, k_2 \in F^-$ such that $q_{ik_\ell}\alpha^0 + \alpha_\ell < 0$ for $\ell = 1, 2$. Lastly, one can also show that we cannot have some $k_1 \in F^+$ such that $q_{ik_1}\alpha^0 + \alpha_{k_1} > 0$ and some $k_2 \in F^-$ such that $q_{ik_2}\alpha^0 + \alpha_{k_2} < 0$.

This leaves us with three possible cases to consider:

Case 1 $\quad q_{ij}\alpha^0 + \alpha_j = 0\ \forall j \in F$
Case 2 $\quad q_{ik}\alpha^0 + \alpha_k > 0$ for some $k \in F^+$ and $q_{ij}\alpha^0 + \alpha_j = 0\ \forall j \in F \setminus k$
Case 3 $\quad q_{ik}\alpha^0 + \alpha_k < 0$ for some $k \in F^-$ and $q_{ij}\alpha^0 + \alpha_j = 0\ \forall j \in F \setminus k$

For the sake of brevity, we only prove this for case 2, as the other cases are very similar.

To prove the result for this case, we will create two valid inequalities such that the original is a convex combination of these two. To ensure their validity, we will define the two new inequalities so that they satisfy the necessary conditions defined by Lemma 15. To define the first inequality, we set

$$\alpha^1 = \alpha - e_k\epsilon_k - \sum_{j \in F^+ \setminus k} e_j\alpha_j - e_i\alpha_i - \sum_{j \in F^-} e_j\alpha_j$$

and

$$\beta^1 = \beta - \sum_{j \in F^-} \alpha_j.$$

In order to ensure that (α^1, β^1) satisfies the conditions set forth in Lemma 15, we need that $-\alpha_i - \sum_{j \in F^+ \setminus k} \alpha_j - \epsilon_k = -\sum_{j \in F^-} \alpha_j$, which uniquely defines ϵ_k. To show that $0 \leq \alpha_k^1 \leq q_{ik}$, we must perform some calculations.

After defining $A_q^+ = \{j \in N_i^+ : \alpha_j = q_{ij}\}$ and $A_0^- = \{j \in N_i^- : \alpha_j = 0\}$ and substituting appropriate values for λ^1, λ^2, and λ^3, we may rewrite (6)–(8) as

$$\alpha^0 c_i + \sum_{j \in A_0^-} \alpha^0 q_{ij} + \sum_{j \in A_q^+} (\alpha^0 + 1) q_{ij} + (\alpha^0 q_{ik} + \alpha_k) = \beta, \tag{23}$$

$$\alpha_i + \sum_{j \in A_q^+} q_{ij} + \sum_{j \in F^+} \alpha_j = \beta, \tag{24}$$

$$-c_i + \sum_{j \in A_0^-} (-q_{ij}) + \sum_{j \in F^-} (\alpha_j - q_{ij}) = \beta. \tag{25}$$

Combining equalities (23), (24), and (25) using multipliers -1, $1+\alpha^0$, and $-\alpha^0$, respectively and using the fact that $\alpha_j = -\alpha^0 q_{ij}\ \forall j \in F^-$, we get

$$-(\alpha^0 q_{ik} + \alpha_k) + (1+\alpha^0)\left(\alpha_k + \alpha_i + \sum_{j\in F^+\setminus k} \alpha_j - \sum_{j\in F^-} \alpha_j\right)$$

$$= -\alpha^0(q_{ik} - \alpha_k) + (1+\alpha^0)\left(\alpha_i + \sum_{j\in F^+\setminus k} \alpha_j - \sum_{j\in F^-} \alpha_j\right) = 0. \tag{26}$$

Note that the second part of (26) states that $-\alpha^0(q_{ik} - \alpha_k) + (1+\alpha^0)(-\epsilon_k) = 0$. Since $q_{ik} - \alpha_k > 0$, $-\alpha^0 > 0$, and $1 + \alpha^0 > 0$, we have that $\epsilon_k > 0$. Furthermore, since $\alpha^0 q_{ik} + \alpha_k > 0$, the first part of (26) shows that $\alpha_k - \epsilon_k > 0$. Hence the conditions of Lemma 15 are satisfied and we may conclude that the inequality $z_i + \sum_j \alpha_j^1 x_j \le \beta^1$ is valid since $\alpha_i^1 = 0$.

To generate the second inequality, we define

$$\alpha^2 = \alpha + e_k(q_{ik} - \alpha_k) + \sum_{j\in F^+\setminus k} e_j(q_{ij} - \alpha_j) - e_i\epsilon_i - \sum_{j\in F^-} e_j(\alpha_j - q_{ij})$$

and

$$\beta^2 = \beta - \sum_{j\in F^-}(\alpha_j - q_{ij}).$$

From Lemma 15, we require that $-\epsilon_i + \sum_{j\in F^+}(q_{ij} - \alpha_j) = -\sum_{j\in F^-}(\alpha_j - q_{ij})$. By applying $\alpha_j = -\alpha^0 q_{ij}\ \forall j \in F \setminus k$, we may rewrite (26) as

$$-\alpha^0\left((q_{ik} - \alpha_k) + \sum_{j\in F^+\setminus k}(q_{ij} - \alpha_j) + \sum_{j\in F^-}(\alpha_j - q_{ij})\right) + (1+\alpha^0)\alpha_i = 0. \tag{27}$$

This equation can also be written as $\alpha_i + \alpha^0(\alpha_i - \epsilon_i) = 0$. Adding and subtracting $q_{ii}\alpha^0$, we obtain $(\alpha_i + q_{ii}\alpha^0) + \alpha^0(\alpha_i - \epsilon_i - q_{ii})$. Since we have assumed that $\alpha_i + q_{ii}\alpha^0 < 0$, we have that $\alpha_i - \epsilon_i < q_{ii}$. Hence, Lemma 15 implies that the inequality $z_i - y_i^0 + \sum_j \alpha_j^2 x_j \le \beta^2$ is valid. From (26), (27), and $\alpha_j = -\alpha^0 q_{ij}\ \forall j \in F \setminus k$, we have

$$-\alpha^0 \begin{pmatrix}\alpha^2\\ \beta^2\end{pmatrix} + (1+\alpha^0)\begin{pmatrix}\alpha^1\\ \beta^1\end{pmatrix} = \begin{pmatrix}\alpha\\ \beta\end{pmatrix},$$

from which we can conclude that the original inequality is a convex combination of the two generated inequalities. □

Lemma 17 *Suppose* (12) *is a valid inequality with* $\alpha_i < 0$, $-1 < \alpha^0 < 0$, *and* $q_{ii}\alpha^0 + \alpha_i = 0$, *then the inequality cannot be a facet of* PR_i.

Proof Again, we may assume that $\lambda^1 = -\alpha^0$. Using perturbation arguments as in the previous lemma, we can show that we cannot have

- $k_1, k_2 \in F^+(F^-)$ such that $\alpha^0 q_{ik_\ell} + \alpha_{k_\ell} > 0$ for $\ell = 1, 2$,
- $k_1, k_2 \in F^+(F^-)$ such that $\alpha^0 q_{ik_\ell} + \alpha_{k_\ell} < 0$ for $\ell = 1, 2$,
- $k_1 \in F^+, k_2 \in F^-$ such that $\alpha^0 q_{ik_1} + \alpha_{k_1} > 0$ and $\alpha^0 q_{ik_2} + \alpha_{k_2} < 0$ or viceversa.

This leaves us with a limited set of possible situations:

(a) If $\exists\ k_1 \in F^+$ such that $\alpha^0 q_{ik_1} + \alpha_{k_1} > 0$, then there is at most one index $k_2 \in F$ such that $\alpha^0 q_{ik_2} + \alpha_{k_2} \neq 0$. Either $k_2 \in F^+$ with $\alpha^0 q_{ik_2} + \alpha_{k_2} < 0$ or $k_2 \in F^-$ with $\alpha^0 q_{ik_2} + \alpha_{k_2} > 0$.
(b) If $\exists\ k_1 \in F^-$ such that $\alpha^0 q_{ik_1} + \alpha_{k_1} < 0$, then there is at most one index $k_2 \in F$ such that $\alpha^0 q_{ik_2} + \alpha_{k_2} \neq 0$. Either $k_2 \in F^+$ with $\alpha^0 q_{ik_2} + \alpha_{k_2} < 0$ or $k_2 \in F^-$ with $\alpha^0 q_{ik_2} + \alpha_{k_2} > 0$.

For each of the possible resulting cases, one can show that two valid inequalities exist such that (12) is a convex combination of these two. These inequalities are different for each case but can be derived the same way as was done in the proof of Lemma 16 and so we omit the details here. We refer the reader to Ref. [15] for further details. □

Lemma 18 *Suppose* (12) *is a valid inequality with* $\alpha_i < 0$, $-1 < \alpha^0 < 0$, *and* $q_{ii}\alpha^0 + \alpha_i > 0$, *then the inequality cannot be a facet of* PR_i.

Proof In a certain sense, this is the most difficult case as we cannot assume that $\lambda^1 = -\alpha^0$. Note that if it were, (6) would contradict the fact that (9) is tight with $\lambda^4 = \alpha^0$. To proceed, we require some notation. Define

$$f(\lambda) = -c_i\lambda + \sum_{j\in N}(-q_{ij}\lambda + \alpha_j)^+$$

Note that (6) is equivalent to $f(\lambda^1) \leq \beta$. We break this proof into two cases:

Case 1 $\exists\lambda^1 \in (0, 1)$ such that $f(\lambda^1) < \beta$

In this case, we can use the fact that $q_{ii}\alpha^0 + \alpha_i > 0$ in a simple perturbation argument as before to show that

$$q_{ij}\alpha^0 + \alpha_j \geq 0\ \forall j \in F^+ \quad \text{and} \quad q_{ij}\alpha^0 + \alpha_j \leq 0\ \forall j \in F^-.$$

Using this, we may write (7)–(9) as

$$\alpha_i + \sum_{j\in A_q^+} q_{ij} + \sum_{j\in F^+} \alpha_j = \beta, \tag{28}$$

$$-c_i + \sum_{j\in A_0^-} (-q_{ij}) + \sum_{j\in F^-} (\alpha_j - q_{ij}) = \beta, \tag{29}$$

$$\alpha^0 c_i + \sum_{j\in A_0^-} \alpha^0 q_{ij} + \sum_{j\in A_q^+} (\alpha^0 + 1)q_{ij} + \sum_{j\in F^+} (\alpha^0 q_{ij} + \alpha_j) = \beta. \tag{30}$$

Combining (28) and (29), we obtain:

$$\alpha_i = \left(-c_i - \sum_{j\in A_0^-} q_{ij} - \sum_{j\in F^-} q_{ij} - \sum_{j\in A_q^+} q_{ij}\right) - \sum_{j\in F^+} \alpha_j + \sum_{j\in F^-} \alpha_j. \tag{31}$$

By summing (30) + $\alpha^0\times$ (29) − $(1 + \alpha^0)\times$ (28), we obtain

$$-(\alpha^0 + 1)\alpha_i + \alpha^0 \left(\sum_{j\in F^+} (q_{ij} - \alpha_j) + \sum_{j\in F^-} (\alpha_j - q_{ij})\right) = 0. \tag{32}$$

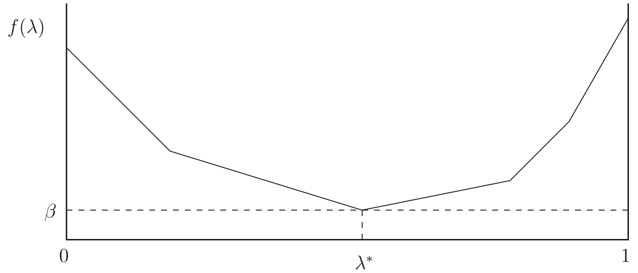

Fig. 1 Example of $f(\lambda)$

Denote

$$\epsilon_i = \sum_{j\in F^+}(q_{ij} - \alpha_j) + \sum_{j\in F^-}(\alpha_j - q_{ij}) > 0.$$

Rewriting (32), we get $(\alpha^0 + 1)\alpha_i - \alpha^0\epsilon_i = 0$. Adding and subtracting $\alpha^0 q_{ii}$, we obtain $\alpha^0(-q_{ii} + \alpha_i - \epsilon_i) + (\alpha^0 q_{ii} + \alpha_i) = 0$. By assumption, the second term is positive, and since $\alpha^0 < 0$, this implies that $-q_{ii} + \alpha_i - \epsilon_i > 0$.
From (31), we have that

$$\alpha_i - \epsilon_i = -c_i - \sum_{j\in A_0^-} q_{ij} - \sum_{j\in F^+} q_{ij} - \sum_{j\in A_q^+} q_{ij} < 0$$

Since $-q_{ii} + \alpha_i - \epsilon_i > 0$, then we get that

$$0 < \frac{-c_i - \sum_{j\in A_0^-} q_{ij} - \sum_{j\in A_q^+} q_{ij} - \sum_{j\in F^+} q_{ij}}{q_{ii}} < 1,$$

By setting x_i equal to this last quantity and setting $x_j = 1\ \forall j \in A_0^- \cup A_q^+ \cup F^+$, we get a feasible solution of PR_i that violates (12) since $\alpha_i < 0$.

Case 2 $\min_{\lambda\in[0,1]} f(\lambda) = \beta$

It is not difficult to see that $f(\lambda)$ is a convex piece-wise linear function, where the breakpoints occur when $-\lambda q_{ij} + \alpha_j$ changes sign for some $j \in F \cup i$. We will denote a point at which the minimum is attained as λ^*. Figure 1 depicts an example of one such $f(\lambda)$.

Note that we may assume that λ^* is a breakpoint of $f(\cdot)$. Furthermore, we must have that $\lambda^* > -\alpha^0$. Since $q_{ii}\alpha^0 + \alpha_i > 0$ implies that $q_{ii} < 0$, we may also conclude that $-q_{ii}\lambda^* + \alpha_i > 0$. Choose some $\epsilon > 0$ small enough so that there are no breakpoints of f between $\lambda^* - \epsilon$ and ϵ. Since λ^* is a minimizer of $f(\cdot)$, we must have that the slope of f at $\lambda^* - \epsilon$ must be nonpositive, i.e., $f'(\lambda^* - \epsilon) \le 0$. Define $X^\epsilon = \{j \in F : -q_{ij}(\lambda^* - \epsilon) + \alpha_j > 0\}$. It is easy to see that

$$f'(\lambda^* - \epsilon) = -c_i - q_{ii} - \sum_{j\in A_0^-} q_{ij} - \sum_{j\in A_q^+} q_{ij} - \sum_{j\in X^\epsilon} q_{ij} \le 0$$

By setting $y_i^1 = -f'(\lambda^* - \epsilon)$ and $x_j = 1\ \forall j \in A_0^- \cup A_q^+ \cup X^\epsilon \cup i$, we have feasible a point in PR_i. This point must satisfy (12) and hence we have

$$\alpha_i + \sum_{j\in A_q^+} q_{ij} + \sum_{j\in X^\epsilon} \alpha_j \le \beta \tag{33}$$

Furthermore, $f(\lambda^*) = \beta$ implies that

$$-\lambda^* c_i - \lambda^* q_{ii} + \alpha_i - \sum_{j\in A_0^-} \lambda^* q_{ij} + \sum_{j\in A_q^+} (1-\lambda^*) q_{ij} + \sum_{j\in X^\epsilon} (\alpha_j - \lambda^* q_{ij}) = \beta \tag{34}$$

Subtracting (34) from (33), we find that $-\lambda^* f'(\lambda^* - \epsilon) \leq 0$, which implies that $f'(\lambda^* - \epsilon) = 0$. This means that the breakpoint to the left of λ^*, say $\bar{\lambda}$, also satisfies $f(\bar{\lambda}) = \beta$. If $-\bar{\lambda} q_{ii} + \alpha_i > 0$, we can repeat the argument and move left again. However, we have that $-\lambda q_{ii} + \alpha_i > 0 \ \forall \lambda \geq -\alpha^0$, which implies that the slope of each line segment of f between $-\alpha^0$ and λ^* is zero. Therefore, $f(-\alpha^0) = \beta$, a contradiction. □

Lemmas 16–18 show that if $\alpha_i < 0$, then we may assume that if (12) defines a nontrivial facet, it is of the form

$$z_i - y_i^0 + \sum_{j\in N} \alpha_j x_j \leq \beta. \tag{35}$$

In the remainder of this section, we would like to characterize these inequalities to be exactly a class of inequalities defined by Vandenbussche and Nemhauser [30] for $R_i|_{y_i^0=0}$. We begin by showing

Proposition 19 *If inequality (35) is a nontrivial facet with $\alpha_i < 0$, then we must have that $-q_{ii} + \alpha_i \leq 0$.*

Proof A similar result is shown by Vandenbussche and Nemhauser [30] for inequalities $z_i + \sum_j \alpha_j x_j \leq \beta$ valid for the set $R_i|_{y_i^0=0}$. The authors assume that $q_{ii} < \alpha_i < 0$ and show, for an exhaustive list of cases, that $z_i + \sum_j \alpha_j x_j \leq \beta$ is a convex combination of two inequalities $z_i + \sum_j \alpha_j^\ell x_j \leq \beta^\ell$ for $\ell = 1, 2$. While the choice of these two inequalities varies case by case, they all satisfy $\sum_{j\in N\setminus i}(-q_{ij} + \alpha_j^\ell) = \beta^\ell + c_i$. Because of this, it is easy to see that $z_i - y_i^0 + \sum_j \alpha_j^\ell x_j \leq \beta^\ell$ is valid for R_i and hence the result follows. □

Using the equality $y_i^1 + y_i^0 - z_i - \sum_j q_{ij} x_j = c_i$ and defining $\tilde{\alpha}_j = \alpha_j - q_{ij} \ \forall j \in N$ and $\tilde{\beta} = \beta + c_i$, we can rewrite inequality (35) as

$$y_i + \sum_{j\in N} \alpha_j x_j \leq \tilde{\beta} \tag{36}$$

such that $\alpha_i \leq 0$, $0 \leq \alpha_j \leq -q_{ij} \ \forall j \in N_i^-$, and $-q_{ij} \leq \alpha_j \leq 0 \ \forall j \in N_i^+$. Since the inequality is a nontrivial facet, we can satisfy (7)–(9) by setting $\lambda^2 = 1$ and $\lambda^3 = \lambda^4 = 0$. By proposition 19, $\alpha_i \leq 0$, and hence we can satisfy (6) by setting $\lambda^1 = 0$. Hence, from these four inequalities, we now have just two distinct ones:

$$c_i + (q_{ii} + \alpha_i) + \sum_{j\in N_i^+} (q_{ij} + \alpha_j) = \tilde{\beta}$$

$$\sum_{j\in N_i^-} \alpha_j = \tilde{\beta}$$

Substituting out $\tilde{\beta}$, we find that we must have

$$\alpha \in \left\{ \alpha \in \mathbb{R}^n | \begin{array}{c} \sum_{j \in N_i^-} \alpha_j - \sum_{j \in N_i^+} \alpha_j - \alpha_i = \bar{y}_i^1 \\ 0 \leq \alpha_j \leq -q_{ij} \ \forall j \in N_i^- \\ -q_{ij} \leq \alpha_j \leq 0 \ \forall j \in N_i^+ \end{array} \right\} := SEP^1$$

Vandenbussche and Nemhauser [30] showed that if α is a vertex of SEP^1, then if either

(**A**) $\alpha_j \in \{0, -q_{ij}\} \ \forall j \in N \setminus i$, or
(**B**) $\alpha_k \notin \{0, -q_{ik}\}$ for some $k \in N \setminus i$, $q_{ii} < 0$, and

$$c_i + \sum_{j \in N_i^- : \alpha_j > 0} q_{ij} + \sum_{j \in N_i^+ : \alpha_j = 0} q_{ij} > 0, \tag{37}$$

then (36) is a facet of $R_i|_{y_i^0=0}$.

They also showed that if either of these conditions are not met, then the inequality does not induce a facet. Using a simple lifting argument, we show that if we maximally lift the coefficient of y_i^0 for either of these cases, we get a coefficient of 0 and hence (36) is also facet-defining for PR_i in those cases. This will prove Theorem 4, which we restate here.

Theorem 4 *Suppose α is a vertex of SEP^1 and suppose either* (**A**) *or* (**B**) *holds, then* (36) *is a facet of PR_i.*

Proof By our previous observations, we know that such an inequality defines a facet of $R_i|_{y_i^0=0}$. We now show that maximally lifting y_i^0 yields a coefficient of 0. For convenience, define $A^+ = \{j \in N_i^- : \alpha_j > 0\}$, $A^0 = \{j \in N \setminus i : \alpha_j = 0\}$, and $A^- = \{j \in N_i^+ : \alpha_j < 0\}$. The lifting problem reads

$$\begin{aligned} \alpha^0 &= \min \left\{ \frac{\sum_{j \in N_i^-} \alpha_j - \sum_j \alpha_j x_j - y_i^1}{y_i^0} \mid (y_i^0, y_i^1, z_i, x) \in R_i, y_i^0 > 0 \right\} \\ &= \min \left\{ \frac{\sum_{j \in N_i^-} \alpha_j - \sum_{j \in N \setminus i} \alpha_j x_j}{y_i^0} \mid (y_i^0, 0, 0, x) \in R_i, y_i^0 > 0 \right\} \\ &= \min \left\{ \frac{\sum_{j \in A^+} \alpha_j (1 - x_j) - \sum_{j \in A^-} \alpha_j x_j}{y_i^0} \mid (y_i^0, 0, 0, x) \in R_i, y_i^0 > 0 \right\}. \end{aligned} \tag{38}$$

It is easy to see that the numerator in (38) is nonnegative. Hence, any solution that makes the numerator 0 and has $y_i^0 > 0$ will be optimal for (38). To do this, we must set $x_j = 1 \ \forall j \in A^+$ and $x_j = 0 \ \forall j \in A^-$. Note that we must also have $x_i = 0$ since $y_i^0 > 0$. In order to make y_i^0 as large as possible, we set $x_j = 0 \ \forall j \in N_i^- \cap A^0$ and $x_j = 1 \ \forall j \in N_i^+ \cap A^0$. This implies that we have $y_i^0 = c_i + \sum_{j \in A^+} q_{ij} + \sum_{j \in N_i^+ \cap A^0} q_{ij}$. Note that if (**B**) holds, then $y_i^0 > 0$ and hence the optimal value of the lifting problem is $\alpha^0 = 0$.

We now show that $y_i^0 > 0$ when (**A**) holds. We have that $\alpha_j \in \{0, -q_{ij}\} \ \forall j \in N \setminus i$. Since $\alpha \in SEP^1$, we have that $\sum_{j \in N} |\alpha_j| = \bar{y}_i^1$, which in this case implies

$$-\alpha_i - \sum_{j \in A^+} q_{ij} + \sum_{j \in A^-} q_{ij} = \sum_{j \in N_i^+} q_{ij} + q_{ii} + c_i.$$

Rearranging, we get

$$y_i^0 = c_i + \sum_{j \in A^+} q_{ij} + \sum_{j \in N_i^+ \cap A^0} q_{ij} = -(\alpha_i + q_{ii}).$$

However, observe that $\alpha_i + q_{ii} < 0$ since $\alpha_i = \alpha_i - q_{ii}$ and we have assumed $\alpha_i < 0$.

We have now shown that the optimal value of the lifting problem is $\alpha^0 = 0$ when either sufficient condition holds, and hence (36) is a facet of PR_i under these circumstances. □

What remains is to show that if neither of the sufficient conditions above hold, then inequality (36) cannot define a facet.

Proposition 20 *Suppose that α is a vertex of SEP^1 and assume that $\alpha_k \notin \{0, -q_{ik}\}$ for some $k \in N \setminus i$. If either $q_{ii} \geq 0$ or (37) does not hold, then (36) cannot define a facet.*

Proof Much as in the proof of proposition 19, we observe that we can use proofs of equivalent results for $R_i|_{y_i^0=0}$ (see propositions 15 and 19 in Ref. [30]). Again, those proofs find two inequalities valid for $R_i|_{y_i^0=0}$ such that (36) is a convex combination of these two. It is easy to see that in this case, these inequalities are also valid for PR_i and hence the same result holds here. □

7 Inequalities with $\alpha^z = 0$

In this section, we characterize all nontrivial facets (11) of PR_i that have $\alpha^z = 0$. From Proposition 9, we know that $\alpha^0 > 0$ and $\alpha_i = 0$ in this case and hence such inequalities may be written as

$$y_i^0 + \sum_{j \in N \setminus i} \alpha_j x_j \leq \beta. \tag{39}$$

Proposition 21 *Suppose that (39) is a nontrivial facet of PR_i, then*

- $\sum_{j \in N \setminus i} |\alpha_j| = \bar{y}_i^0$
- $0 \leq \alpha_j \leq -q_{ij} \quad \forall j \in N_i^-$
- $-q_{ij} \leq \alpha_j \leq 0 \quad \forall j \in N_i^+$
- $\beta = \sum_{i \in N_i^-} \alpha_j$

Proof By setting $\lambda^1 = 0$, $\lambda^2 = 0$, and $\lambda^3 = 0$ and since $\alpha_i = 0$, (6), (7), and (8) can be written as

$$\sum_{j \in N \setminus i} \alpha_j^+ = \beta. \tag{40}$$

By setting $\lambda^4 = 1$, (9) becomes

$$c_i + \sum_{j \in N \setminus i} (q_{ij} + \alpha_j)^+ = \beta. \tag{41}$$

Suppose that $\alpha_j > 0$ for some $j \in N_i^+$, then one can decrease both α_j and β and (40) and (41) would still be satisfied. But then the original inequality is a nonnegative combination of this new inequality and the bound inequality $x_j \leq 1$. Hence, in any nontrivial facet, we must have $\alpha_j \leq 0 \; \forall j \in N_i^+$. If $\alpha_j < -q_{ij}$ for some $j \in N_i^+$, then index j does not contribute to the left hand side of (40) and (41). Hence we can increase this coefficient and maintain validity, which implies the inequality could not be a facet. From this we may conclude that $\alpha_j \geq -q_{ij}\ \forall j \in N_i^+$. Similarly, one can show that $0 \leq \alpha_j \leq -q_{ij}\ \forall j \in N_i^-$. By equating (40) and (41), the rest of the proposition follows. □

Because of Proposition 21, we are led to define

$$SEP^0 = \left\{ \alpha \in \mathbb{R}^n | \begin{array}{c} \sum_{j\in N_i^-} \alpha_j - \sum_{j\in N_i^+} \alpha_j = \bar{y}_i^0 \\ 0 \leq \alpha_j \leq -q_{ij}\ \forall j \in N_i^- \\ -q_{ij} \leq \alpha_j \leq 0\ \forall j \in N_i^+ \\ \alpha_i = 0 \end{array} \right\}$$

Clearly, any facet of the form (39) must be such that α is a vertex of SEP^0. Furthermore, in order to have a point with $y_i^1 > 0$ that lies on the facet, we must have

$$K^0 := c_i + q_{ii} + \sum_{j\in N_i^+\cap A^0} q_{ij} + \sum_{j\in A^+} q_{ij} > 0, \tag{42}$$

where $A^0 = \{j \in N \setminus i : \alpha_j = 0\}$, $A^+ = \{j \in N \setminus i : \alpha_j > 0\}$. Theorem 5 states that the above conditions are sufficient for (39) to define a facet of PR_i, we repeat it here.

Theorem 5 *Suppose that α is a vertex of SEP^0 and that* (42) *holds, then* (39) *is a facet of PR_i.*

Proof The proof of this result requires the construction of a number of points that lie on the face defined by (39). Since the proof proceeds in much the same way as that of Theorem 2, we again refer the reader to Ref. [15] for details. □

8 Computational results

To demonstrate the use of the facets described in the previous sections, we have implemented a branch-and-cut algorithm using the MINTO framework [17]. Although intended for solving mixed integer programs, this framework allows one to implement LP-based branch-and-bound algorithms that branch on other entities (such as complementarity constraints) as well. The framework requires an LP solver to solve the nodes of the branch-and-bound tree, for this we used CPLEX 9.1 [14]. The runs were executed on a Linux PC with a 2.4 GHz Intel Xeon processor and 1 Gb of RAM.

We briefly describe the cuts that were used and how they were separated. Recall that the sets SEP^0, SEP^z, and SEP^1 are all continuous knapsack sets, that is, they have one equality constraint and otherwise contain only bound constraints. Consequently, optimizing over them can be done very quickly with a sorting algorithm, see [31] for similar separation problems. Note that by using these separation techniques, we may add inequalities that are valid but do not define facets of PR_i. Given the ease with which the separation can be carried out, we add these inequalities nonetheless. We have not yet developed a way to choose B appropriately to separate cuts that can be derived from SEP^B. We leave the separation of these inequalities to future work. Some initial computations indicated that using MINTO's separation routines for standard IP inequalities such as flow covers was not effective, so we turned off all standard MINTO cut generation.

After some experimentation, we found that branching on violated integrality constraints first, before branching on complementarity constraints yielded reasonably good results.

Hence after solving an LP at a node, the algorithm checks to see if any binary variable is fractional and, if so, branches on it. Otherwise it uses a *maximum-violation* strategy to select a complementarity constraint on which to branch. For example, given an LP solution $(\tilde{y}^1, \tilde{y}^0, \tilde{z}, \tilde{x})$, we compute $\mathrm{argmax}_{i \in N}\{\tilde{z}_i \tilde{x}_i / \bar{z}_i\}$ to find the maximally violated complementarity constraint $z_i x_i = 0$. We carry out similar computations for the other complementarity constraints and branch on the most violated constraint. For instance, if branching on the constraint $y_i^0 x_i = 0$, then the branching dichotomy is

$$\left(y_i^0 = 0\right) \bigvee \left(x_i = 0, y_i^1 = 0, z_i = 0\right).$$

Note that we include $z_i = 0$ in the second branch since we can assume that $y_i^0 z_i = 0$.

From a result by Rosenberg [26], it is easy to see that if $q_{ii} \geq 0$ for some $i \in N$, then there exists an optimal solution that has $x_i \in \{0, 1\}$. Our branching rules reflect this by defining the branching dichotomy for an index i with $q_{ii} \geq 0$ as

$$\left(x_i = 0, y_i^1 = 0\right) \bigvee \left(x_i = 1, y_i^0 = 0, z_i = 0\right).$$

Cuts are added at every node, using as many rounds as necessary to exhaust all violated inequalities. Since these cuts are very easy to generate, we also deactivate rows very aggressively, removing a cut from the active LP if the corresponding dual variable has been zero in more than two consecutive LP solutions.

To initialize the LP relaxation, we include the following valid inequalities:

$$y_i^1 \leq \bar{y}_i^1 x_i, \;\; z_i + \bar{z}_i x_i \leq \bar{z}_i, \;\; y_i^0 + \bar{y}_i^0 x_i \leq \bar{y}_i^0 \;\forall i \in N$$

These inequalities follow immediately from complementarity and are included in the initial LP and are not subject to the row deactivation scheme.

We also initialized the branch-and-bound algorithm with an initial feasible solution. We obtained this solution by finding a locally optimal solution of the QP

$$\max \;\frac{1}{2} x^T Q x + (c - f)^T x \text{ subject to } 0 \leq x \leq e,$$

and using this x to construct a feasible solution (x, δ) to FCQP. We use MATLAB's optimization toolbox to find a locally optimal solution. We only used this primal heuristic once, at the root node of the search tree.

We randomly generated a set of 39 instances with different sizes and densities for the matrix Q. The nonzero entries of Q and c are random integers in the range $[-50, 50]$ while the fixed costs f are random integers in the range $[0, 50]$. Instances are labeled as $n - d - s$, where n is the size, d is the density, and s is the seed used to generate the instance. We solved the instances with and without generating cuts. For the purposes of comparison, we also solved these instances using BARON 7.5 [28] with a 0.001% relative optimality tolerance. The default optimality tolerance in MINTO is 0.0001 %. All runs were given a 4000 second time limit. Due to memory limitations, we limited the branch-and-bound runs to 1 million nodes. The results are reported in Table 1. For those instances that did not terminate within the time limit, we list the relative optimality gap as a percentage in the CPU column, marked with a $(\star)$. Similarly, for instances that reached the node limit, we list the gap marked with a $(\dagger)$. Note that CPU times were rounded to the nearest integer.

The results clearly indicate the strength of the inequalities and their ability to solve the same instances in significantly less time compared to plain branch-and-bound or BARON. While branch-and-cut finished all but four instances in the allotted time, branch-and-bound did not prove optimality for 21 instances. BARON was not able to complete 23 of the 39

Table 1 Computational results with baron, branch-and-bound (B&B), and branch-and-cut (B&C)

Name	Objective value			CPU (s) or Gap (%)		
	Baron	B & B	B & C	Baron	B & B	B & C
20-080-1	550.50	550.50	550.50	2	0	0
20-080-2	198.50	198.50	198.50	5	0	0
20-080-3	489.56	489.56	489.56	5	1	0
20-090-1	445.50	445.50	445.50	33	3	1
20-090-2	201.00	201.00	201.00	41	2	1
20-090-3	246.50	246.50	246.50	12	1	1
20-100-1	479.50	479.50	479.50	112	3	1
20-100-2	309.50	309.50	309.50	62	6	1
20-100-3	403.00	403.00	403.00	98	4	1
30-060-1	606.00	606.00	606.00	3,173	286	8
30-060-2	269.50	269.50	269.50	2,864	24	4
30-060-3	829.00	829.00	829.00	55	3	1
30-070-1	766.50	766.50	766.50	⋆ 18.39	38	8
30-070-2	431.78	431.78	431.78	⋆ 40.98	220	19
30-070-3	885.00	885.00	885.00	478	⋆ 4.65	4
30-080-1	897.00	886.50	897.00	⋆ 19.17	⋆ 4.88	8
30-080-2	319.00	319.00	319.00	⋆ 49.62	80	13
30-080-3	1134.50	1134.50	1134.50	114	3	2
30-090-1	802.50	796.50	802.50	⋆ 39.71	⋆ 15.96	28
30-090-2	555.50	555.50	555.50	⋆ 46.33	3,479	23
30-090-3	754.00	746.85	754.00	⋆ 38.98	⋆ 30.82	36
30-100-1	476.50	435.56	476.50	⋆ 67.40	⋆ 87.16	867
30-100-2	484.50	414.33	484.50	⋆ 60.78	⋆ 110.98	128
30-100-3	1193.00	1193.00	1193.00	⋆ 33.16	⋆ 18.74	38
40-060-1	898.50	860.45	898.50	⋆ 48.81	† 19.25	423
40-060-2	611.50	611.50	611.50	⋆ 47.66	606	73
40-060-3	1217.00	1217.00	1217.00	⋆ 34.39	† 4.61	107
40-070-1	929.50	921.50	929.50	⋆ 56.17	† 31.93	1,084
40-070-2	706.00	706.00	706.00	⋆ 58.09	⋆ 17.07	261
40-070-3	1436.50	1390.73	1436.50	⋆ 40.74	† 13.82	257
40-080-1	1202.50	1201.50	1202.50	⋆ 51.12	⋆ 34.00	936
40-080-2	630.00	612.86	630.00	⋆ 64.83	⋆ 55.72	474
40-080-3	1116.50	1075.15	1116.50	⋆ 53.42	⋆ 48.30	964
40-090-1	1720.00	1708.00	1720.00	⋆ 45.78	⋆ 22.84	575
40-090-2	661.00	638.00	638.00	⋆ 73.04	⋆ 134.01	⋆ 46.15
40-090-3	896.50	749.50	749.50	⋆ 66.55	⋆ 157.91	⋆ 67.59
40-100-1	2091.00	2088.00	2091.00	⋆ 44.24	† 21.67	1,261
40-100-2	1350.00	1350.00	1350.00	⋆ 56.29	⋆ 77.42	⋆ 23.82
40-100-3	1345.50	1342.50	1342.50	⋆ 58.87	⋆ 63.19	⋆ 20.95

instances within the time limit. It is important to point out however that BARON is a general purpose global optimization solver while our approach is clearly specialized to this problem type. Regardless, these results indicate the merit of studying particular structures within mixed-integer nonlinear programming, as we have done here. In particular, one can see that the development of appropriate polyhedral results can have a significant impact on the global optimization of difficult nonlinear programming instances.

It remains to be seen how the results in this paper can be extended to handle general constraints such as those in GenQP. Furthermore, the valid inequalities in this paper do not account for the integer variables. Cutting planes that attempt to approximate both the integrality and complementarity constraints are currently not available and require further polyhedral study. We hope to develop these in future work.

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