

Quadratic Optimization with Switching Variables: The Convex Hull for $n = 2$

Kurt M. Anstreicher* Samuel Burer†

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Abstract

We consider quadratic optimization in variables (x, y) where $0 \leq x \leq y$, and $y \in \{0, 1\}^n$. Such binary y are commonly referred to as *indicator* or *switching* variables and occur commonly in applications. One approach to such problems is based on representing or approximating the convex hull of the set $\{(x, xx^T, yy^T) : 0 \leq x \leq y \in \{0, 1\}^n\}$. A representation for the case $n = 1$ is known and has been widely used. We give an exact representation for the case $n = 2$ by starting with a disjunctive representation for the convex hull and then eliminating auxiliary variables and constraints that do not change the projection onto the original variables. An alternative derivation for this representation leads to an appealing conjecture for a simplified representation of the convex hull for $n = 2$ when the product term $y_1 y_2$ is ignored.

Keywords: Quadratic optimization, switching variables, convex hull, perspective cone, semidefinite programming.

1 Introduction

This paper concerns quadratic optimization in variables $x \in \mathbb{R}^n$ and $y \in \{0, 1\}^n$, where $0 \leq x \leq y$. The y variables are referred to as *indicator* or *switching* variables and occur frequently in applications, including electrical power production [8], constrained portfolio optimization [8, 9], nonlinear machine scheduling problems [1] and chemical pooling problems

*Department of Business Analytics, University of Iowa, Iowa City, IA, 52242-1994, USA. Email: kurt-anstreicher@uiowa.edu.

†Department of Business Analytics, University of Iowa, Iowa City, IA, 52242-1994, USA. Email: samuel-burer@uiowa.edu.

[6]. A typical feature of such problems is that the objective function is separable in x and y . In addition, many applications do not involve the cross-terms $y_i y_j$ for $i \neq j$.

One approach for such problems is to consider symmetric matrix variables X and Y that replace the rank-1 matrices xx^T and yy^T , respectively. Using such variables, an objective of the form $c^T x + x^T Q x + y^T D y$ can be replaced by the linear function $c^T x + Q \bullet X + D \bullet Y$, where (x, X, Y) should then be in the set

$$\mathcal{H} := \text{conv}\{(x, xx^T, yy^T) : 0 \leq x \leq y \in \{0, 1\}^n\}.$$

The problem is then to represent \mathcal{H} in a computable manner. Note that, because y is binary, $\text{diag}(Y)$ captures y , and in particular, when the cross-terms $y_i y_j$ are not of interest, we may consider the simpler convex hull

$$\mathcal{H}' := \text{conv}\{(x, xx^T, y) : 0 \leq x \leq y \in \{0, 1\}^n\}.$$

For general n , determining computable representations of \mathcal{H} and \mathcal{H}' is difficult. For example, even when y is fixed to e , the resulting convex hull, called QPB in [5] for “quadratic programming over the box,” is intractable. When $n = 2$, an exact representation for QPB was given in [2], but such a representation is not known for $n \geq 3$. For general n , the paper [7] studies valid inequalities for \mathcal{H}' . For the case $n = 1$, $\mathcal{H} = \mathcal{H}'$ since there are no cross-terms, and a computable representation was given in [9] based on prior work in [8]. This representation has subsequently been used in a variety of applications; see for example [10, 12]. Several authors have also studied the case when $n = 2$ but have focused on convexifying in the space of (x, y, t) , where t is a scalar associated with the epigraph of a specially structured quadratic function, e.g., a convex quadratic one; see [3] and references therein.

In Section 2, we consider the case of $n = 1$ and reprove the representation of $\mathcal{H} = \mathcal{H}'$ in a new way which incorporates standard ideas from the literature on constructing strong semidefinite programming (SDP) relaxations of quadratic programs. In particular, our proof can be viewed as establishing that \mathcal{H} for $n = 1$ is captured exactly by the relaxation which uses the standard positive semidefinite (PSD) condition along with the standard Reformulation–Linearization Technique (RLT) constraints [13].

Our main result in this paper is a representation of \mathcal{H} for $n = 2$, which we derive in several steps. Note that in this case there is only a single cross-term $y_1 y_2$, and we can write \mathcal{H} in the form

$$\mathcal{H} = \text{conv}\{(x, xx^T, y, y_1 y_2) : 0 \leq x \leq y \in \{0, 1\}^2\}.$$

First, in Section 3, we give a disjunctive representation of \mathcal{H} that involves additional variables $\alpha \in \mathbb{R}^2$, $\beta \in \mathbb{R}^2$. Then in Section 4 we project out β by replacing a single PSD constraint with four PSD constraints. The primary effort in the paper occurs in Section 5, where we show that it is in fact only necessary to impose one of these four PSD constraints in order to represent \mathcal{H} . This analysis is relatively complex due to the fact that we are attempting to characterize the projection of $(x, X, y, Y_{12}, \alpha)$ onto (x, X, y, Y_{12}) where the constraints on $(x, X, y, Y_{12}, \alpha)$ include PSD conditions. If all constraints on $(x, X, y, Y_{12}, \alpha)$ were linear, we could use standard polyhedral techniques to perform this projection. However, since our case includes PSD conditions, we are unaware of any general methodology for characterizing such a projection, and therefore our proof technique is tailored to the structure of \mathcal{H} for $n = 2$.

Finally, in Section 6, we describe an alternative derivation for the representation of \mathcal{H} obtained in Section 5. This derivation provides another interpretation for the single remaining PSD condition and also leads to a conjecture that a weaker PSD condition is sufficient to characterize \mathcal{H}' for $n = 2$. If true, this conjecture would establish that \mathcal{H}' can be represented using PSD, RLT, and simple linear conditions derived from the binary nature of y , thus generalizing the results of Section 2 for $n = 1$ as well as the representation of QPB for $n = 2$ from [2]. This conjecture is supported by extensive numerical computations but remains unproved.

Notation. We use e to denote a vector of arbitrary dimension with each component equal to one, and e_i to denote an elementary vector with all components equal to zero except for a one in component i . For symmetric matrices X and Y , $X \succeq Y$ denotes that $X - Y$ is positive semidefinite (PSD) and $X \succ Y$ denotes that $X - Y$ is positive definite. The vector whose components are those of the diagonal entries of a matrix X is denoted $\text{diag}(X)$. The convex hull of a set is denoted $\text{conv}\{\cdot\}$.

2 The convex hull for $n = 1$

In this section we consider the representation of \mathcal{H} for $n = 1$; note that $\mathcal{H} = \mathcal{H}'$ in this case. The representation given in Theorem 1 below is known, but to our knowledge the proof given here is new. We define

$$\text{PER} := \left\{ (\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R} : \begin{array}{l} \alpha^2 \leq \beta\gamma \\ 0 \leq \beta \leq \alpha \leq \gamma \end{array} \right\}$$

to be the so-called *perspective cone* in \mathbb{R}^3 . In particular, the constraint $\alpha^2 \leq \beta\gamma$ is called a *perspective constraint* in the literature [9].

Theorem 1. For $n = 1$, $\mathcal{H} = \mathcal{H}' = \{(x_1, X_{11}, y_1) \in \text{PER} : y_1 \leq 1\}$.

Proof. Let $t_1 = 1 - y_1$. Then the constraints $0 \leq x_1 \leq y_1, y_1 \in \{0, 1\}$ can be written in the form $x_1 + s_1 + t_1 = 1, x_1 \geq 0, s_1 \geq 0, t_1 \in \{0, 1\}$. By relaxing the rank-one matrix $(1, x_1, s_1, t_1)^T(1, x_1, s_1, t_1)$ we obtain a matrix

$$W = \begin{pmatrix} 1 & x_1 & s_1 & t_1 \\ x_1 & X_{11} & Z_{11} & 0 \\ s_1 & Z_{11} & S_{11} & 0 \\ t_1 & 0 & 0 & t_1 \end{pmatrix}, \quad (1)$$

where we are using the fact that, for binary t_1 , it holds that $t_1^2 = t_1$ and $x_1 t_1 = s_1 t_1 = 0$. Multiplying $x_1 + s_1 + t_1 = 1$ in turn by the variables x_1 and s_1 , we next obtain the RLT constraints $X_{11} + Z_{11} = x_1$ and $S_{11} + Z_{11} = s_1$. Let

$$\begin{aligned} \mathcal{C} &= \text{conv}\{(1, x_1, s_1, t_1)^T(1, x_1, s_1, t_1) : x_1 + s_1 + t_1 = 1, x_1 \geq 0, s_1 \geq 0, t_1 \in \{0, 1\}\}, \\ \mathcal{D} &= \{W \in \text{DNN} : x_1 + s_1 + t_1 = 1, X_{11} + Z_{11} = x_1, S_{11} + Z_{11} = s_1\}, \end{aligned}$$

where the matrix W in the definition of \mathcal{D} has the form (1), and DNN denotes the cone of doubly nonnegative matrices, that is, matrices that are both componentwise nonnegative and PSD. We claim that $\mathcal{C} = \mathcal{D}$. The inclusion $\mathcal{C} \subset \mathcal{D}$ is obvious by standard SDP-relaxation techniques. However, from [4, Corollary 2.5] we know that

$$\mathcal{C} = \{W \in \text{CP} : x_1 + s_1 + t_1 = 1, X_{11} + S_{11} + t_1 + 2Z_{11} = 1\},$$

where CP denotes the cone of completely positive matrices, that is, matrices that can be represented as a sum of nonnegative rank-one matrices. Note that $X_{11} + S_{11} + t_1 + 2Z_{11} = 1$ is the ‘‘squared’’ constraint obtained by substituting appropriate variables into the expression $(x_1 + s_1 + t_1)^2 = 1$. Then $\mathcal{C} = \mathcal{D}$ follows from the facts that since W is 4×4 , $W \in \text{CP} \iff W \in \text{DNN}$, and the constraints $x_1 + s_1 + t_1 = 1, X_{11} + Z_{11} = x_1$ and $S_{11} + Z_{11} = s_1$ together imply $X_{11} + S_{11} + t_1 + 2Z_{11} = 1$.

From $\mathcal{C} = \mathcal{D}$ we conclude that $\text{conv}\{(x_1, x_1^2, y_1) : 0 \leq x_1 \leq y_1, y_1 \in \{0, 1\}\} = \{(x_1, X_{11}, 1 - t_1) : x_1 + s_1 + t_1 = 1, X_{11} + Z_{11} = x_1, S_{11} + Z_{11} = s_1, W \in \text{DNN}\}$. To complete the proof we

will simplify the condition that $W \succeq 0$. Note that

$$W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_1 & t_1 \\ x_1 & X_{11} & 0 \\ t_1 & 0 & t_1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}.$$

Then $W \succeq 0$ if and only if

$$\begin{pmatrix} 1 & x_1 & t_1 \\ x_1 & X_{11} & 0 \\ t_1 & 0 & t_1 \end{pmatrix} \succeq 0 \Leftrightarrow \begin{pmatrix} 1 - t_1 & x_1 \\ x_1 & X_{11} \end{pmatrix} \succeq 0,$$

which using $y_1 = 1 - t_1$ is equivalent to $y_1 \geq 0$, $X_{11} \geq 0$, $y_1 X_{11} \geq x_1^2$. The conditions of the theorem thus insure that $W \in \text{DNN}$, where $t_1 = 1 - y_1 \geq 0$, $s_1 = 1 - t_1 - x_1 = y_1 - x_1 \geq 0$, $Z_{11} = x_1 - X_{11} \geq 0$ and $S_{11} = 1 + X_{11} - 2x_1 - t_1 = y_1 + X_{11} - 2x_1 \geq 0$. \square

Note that the characterization in Theorem 1 is sometimes written in terms of the lower convex envelope rather than the convex hull, in which case the condition $X_{11} \leq x_1$ is omitted.

3 The disjunctive convex hull for $n = 2$

In this section, we develop an explicit disjunctive formulation for the convex hull \mathcal{H} when $n = 2$. As described in the Introduction, we will use that fact that $\text{diag}(Y) = y$ and that there is only one cross-term $y_1 y_2$ to write (x, X, y, Y_{12}) for points in \mathcal{H} .

The representation for \mathcal{H} obtained in this section is based on the four values of $y \in \{0, 1\}^2 = \{0, e_1, e_2, e\}$. Specifically, note that $\mathcal{H} = \text{conv}(\mathcal{H}_0 \cup \mathcal{H}_{e_1} \cup \mathcal{H}_{e_2} \cup \mathcal{H}_e)$, where for each fixed y ,

$$\mathcal{H}_y := \text{conv} \left\{ (x, xx^T, y, y_1 y_2) : 0 \leq x \leq y \right\}.$$

Each such \mathcal{H}_y has a known representation. \mathcal{H}_0 is just a singleton, and for $y = e_1$ and $y = e_2$ representations based on PER are provided by Theorem 1. For $y = e$, a representation is given in [2] as follows. Define

$$\text{RLT}_x := \left\{ \begin{pmatrix} \lambda & x^T \\ x & X \end{pmatrix} : \begin{array}{l} \lambda \geq 0, 0 \leq \text{diag}(X) \leq x \\ \max\{0, x_1 + x_2 - \lambda\} \leq X_{12} \leq \min\{x_1, x_2\} \end{array} \right\},$$

which is the homogenization of those points (x, X) satisfying the standard RLT constraints

associated with $0 \leq x \leq e$. Then [2]

$$\mathcal{H}_e = \left\{ (x, X, y, Y_{12}) : \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \text{PSD} \cap \text{RLT}_x, y = e, Y_{12} = 1 \right\},$$

where PSD denotes the cone of positive semidefinite matrices. In the sequel we will also need

$$\text{RLT}_y := \left\{ (y, Y_{12}) \in \mathbb{R}^2 \times \mathbb{R} : \max\{0, y_1 + y_2 - 1\} \leq Y_{12} \leq \min\{y_1, y_2\} \right\},$$

which gives the convex hull of $(y, y_1 y_2)$ over all four $y \in \{0, 1\}^2$. Note that RLT_y is a polytope, unlike PER, RLT_x and PSD, which are convex cones.

In many applications, the product $y_1 y_2$ is not of interest, so it is also natural to consider the convex hull \mathcal{H}' that ignores this product. Based on the known representations for \mathcal{H}_{e_1} , \mathcal{H}_{e_2} and \mathcal{H}_e , \mathcal{H}' is certainly contained in the set of (x, X, y) satisfying the constraints

$$\begin{aligned} \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} &\in \text{PSD} \cap \text{RLT}_x \\ (x_j, X_{jj}, y_j) &\in \text{PER}, \quad y_j \leq 1 \quad \forall j = 1, 2. \end{aligned}$$

However it is easy to generate examples that satisfy these constraints but are not in \mathcal{H}' . In the next theorem we will focus on \mathcal{H} , but we will return to a discussion of \mathcal{H}' in Section 6.

Theorem 2. \mathcal{H} equals the projection onto (x, X, y, Y_{12}) of $(x, X, y, Y_{12}, \alpha, \beta)$ satisfying the convex constraints

$$x \leq y \tag{2a}$$

$$\begin{pmatrix} Y_{12} & (x - \alpha)^T \\ x - \alpha & X - \text{Diag}(\beta) \end{pmatrix} \in \text{PSD} \cap \text{RLT}_x \tag{2b}$$

$$(\alpha_j, \beta_j, y_j - Y_{12}) \in \text{PER} \quad \forall j = 1, 2 \tag{2c}$$

$$(y, Y_{12}) \in \text{RLT}_y \tag{2d}$$

where $\alpha \in \mathbb{R}^2$, $\beta \in \mathbb{R}^2$ are auxiliary variables.

Proof. We first argue that (2) is a relaxation of \mathcal{H} in the lifted space that includes α and β . It suffices to show that each “rank-1” solution $(x, x x^T, y, y_1 y_2)$ for $y \in \{0, 1\}^2$ can be extended in (α, β) to a feasible solution of (2), and we handle the four cases for $y \in \{0, 1\}^2$ separately. We clearly always have $x \leq y$ and $(y, Y_{12}) \in \text{RLT}_y$, so it remains to check that (2b) and (2c) hold in each case.

We introduce the notation

$$Z := \begin{pmatrix} Y_{12} & (x - \alpha)^T \\ x - \alpha & X - \text{Diag}(\beta) \end{pmatrix}.$$

First, let $y = 0 \Rightarrow x = 0$. Then $(x, xx^T, y, y_1 y_2) = (0, 0, 0, 0)$, and we choose $(\alpha, \beta) = (0, 0)$. Since all variables are zero, it is straightforward to check that (2b) and (2c) are satisfied. Second, let $y = e \Rightarrow 0 \leq x \leq e$. Then $(x, xx^T, y, y_1 y_2) = (x, xx^T, e, 1)$, and we choose $(\alpha, \beta) = (0, 0)$ for this case also, which yields $(\alpha_j, \beta_j, y_j - Y_{12}) = (0, 0, 0) \in \text{PER}$ for $j = 1, 2$. Moreover,

$$Z = \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} = \begin{pmatrix} 1 & x^T \\ x & xx^T \end{pmatrix} \in \text{PSD} \cap \text{RLT}_x,$$

as desired.

Next we consider the case $y = e_1$, which implies $x_1 \leq 1$ and $x_2 = 0$. Then $(x, xx^T, y, y_1 y_2) = (x_1 e_1, x_1^2 e_1 e_1^T, e_1, 0)$, and we choose $(\alpha, \beta) = (x_1 e_1, x_1^2 e_1)$. Hence,

$$Z = \begin{pmatrix} 0 & (x - x_1 e_1)^T \\ x - x_1 e_1 & X - x_1^2 e_1 e_1^T \end{pmatrix} = 0 \in \text{PSD} \cap \text{RLT}_x,$$

satisfying (2b). Moreover, $(\alpha_1, \beta_1, y_1 - y_1 y_2) = (x_1, x_1^2, 1) \in \text{PER}$ and $(\alpha_2, \beta_2, y_2 - y_1 y_2) = (0, 0, 0) \in \text{PER}$, so that (2c) is satisfied. The final case $y = e_2$ is similar. We have thus shown that (2) is a relaxation of \mathcal{H} .

To complete the proof, we show the reverse containment, i.e., that any $(x, X, y, Y_{12}, \alpha, \beta)$ satisfying (2) is also a member of \mathcal{H} . Define the four scalars

$$\lambda_0 := 1 - y_1 - y_2 + Y_{12}, \quad \lambda_{e_1} := y_1 - Y_{12}, \quad \lambda_{e_2} := y_1 - Y_{12}, \quad \lambda_e := Y_{12}, \quad (3)$$

and note that $(y, Y_{12}) \in \text{RLT}_y$ implies $\lambda_0 + \lambda_{e_1} + \lambda_{e_2} + \lambda_e = 1$ with each term nonnegative, i.e., $(\lambda_0, \lambda_{e_1}, \lambda_{e_2}, \lambda_e)$ is a convex combination. Next, letting $0/0 := 0$, define

$$\begin{aligned} Z_0 &:= \lambda_0^{-1} \begin{pmatrix} \lambda_0 & 0^T \\ 0 & 0 \end{pmatrix} & Z_{e_2} &:= \lambda_{e_2}^{-1} \begin{pmatrix} \lambda_{e_2} & \alpha_2 e_2^T \\ \alpha_2 e_2 & \beta_2 e_2 e_2^T \end{pmatrix} \\ Z_{e_1} &:= \lambda_{e_1}^{-1} \begin{pmatrix} \lambda_{e_1} & \alpha_1 e_1^T \\ \alpha_1 e_1 & \beta_1 e_1 e_1^T \end{pmatrix} & Z_e &:= \lambda_e^{-1} \begin{pmatrix} \lambda_e & (x - \alpha)^T \\ x - \alpha & X - \text{Diag}(\beta) \end{pmatrix}. \end{aligned}$$

Note that $Z_y \in \mathcal{H}_y$ for each $y \in \{0, 1\}^2$; for $y = e_1$ and $y = e_2$ we use the representation from Theorem 1, and for $y = e$ we use the result from [2] stated above this theorem. Hence,

the easily verified equations $(y, Y_{12}) = \lambda_0(0, 0) + \lambda_{e_1}(e_1, 0) + \lambda_{e_2}(e_2, 0) + \lambda_e(e, 1)$ and

$$\begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} = \lambda_0 Z_0 + \lambda_{e_1} Z_{e_1} + \lambda_{e_2} Z_{e_2} + \lambda_e Z_e,$$

establish that $(x, X, y, Y_{12}) \in \mathcal{H}$. □

4 Eliminating β

System (2) captures \mathcal{H} by projection from a lifted space, which includes the additional variables $\alpha \in \mathbb{R}^2$, $\beta \in \mathbb{R}^2$. In this section, we eliminate the β variables from (2), but the price we pay is to replace the semidefinite constraint in (2b) with PSD conditions on four matrices. In Section 5 we will show that, in order to obtain a characterization of \mathcal{H} , it is in fact only necessary to impose one of these four PSD conditions.

We begin by introducing some notation. First, define the matrix function $M : \mathbb{R}^2 \times \mathbb{S}^2 \times \mathbb{R} \times \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{S}^3$ by

$$M(\beta) := M(x, X, Y_{12}, \alpha, \beta) := \begin{pmatrix} Y_{12} & (x - \alpha)^T \\ x - \alpha & X - \text{Diag}(\beta) \end{pmatrix}. \quad (4)$$

The simplified notation $M(\beta)$ will be convenient because instances of M will only differ in the values of β ; note also that M does not depend on y . We also define four different functions $\beta_{pq} : \mathbb{R}^2 \times \mathbb{R} \times \mathbb{R}^2 \rightarrow \mathbb{R}^2$ depending on (y, Y_{12}, α) for the indices $(p, q) \in \{1, 2\}^2$, where $0/0 := 0$:

$$\begin{aligned} \beta_{11} &:= \beta_{11}(y, Y_{12}, \alpha) := (X_{11} - x_1 + \alpha_1, X_{22} - x_2 + \alpha_2) \\ \beta_{21} &:= \beta_{21}(y, Y_{12}, \alpha) := ((y_1 - Y_{12})^{-1} \alpha_1^2, X_{22} - x_2 + \alpha_2) \\ \beta_{12} &:= \beta_{12}(y, Y_{12}, \alpha) := (X_{11} - x_1 + \alpha_1, (y_2 - Y_{12})^{-1} \alpha_2^2) \\ \beta_{22} &:= \beta_{22}(y, Y_{12}, \alpha) := ((y_1 - Y_{12})^{-1} \alpha_1^2, (y_2 - Y_{12})^{-1} \alpha_2^2). \end{aligned}$$

As with $M(\beta)$, the shorter notation β_{pq} will prove more convenient. Note also that p and q are only index labels to designate the four functions. The result below replaces the PSD condition in (2b) with the four conditions $M(\beta_{pq}) \succeq 0$, $p, q \in \{1, 2\}$.

Theorem 3. \mathcal{H} equals the projection onto (x, X, y, Y_{12}) of $(x, X, y, Y_{12}, \alpha)$ satisfying the

convex constraints

$$\text{diag}(X) \leq x \leq y \tag{5a}$$

$$\max\{0, x_1 - \alpha_1 + x_2 - \alpha_2 - Y_{12}\} \leq X_{12} \leq \min\{x_1 - \alpha_1, x_2 - \alpha_2\} \tag{5b}$$

$$0 \leq \alpha_j \leq y_j - Y_{12} \quad \forall j = 1, 2 \tag{5c}$$

$$(y, Y_{12}) \in \text{RLT}_y \tag{5d}$$

$$M(\beta_{11}) \succeq 0 \tag{5e}$$

$$M(\beta_{12}) \succeq 0 \tag{5f}$$

$$M(\beta_{21}) \succeq 0 \tag{5g}$$

$$M(\beta_{22}) \succeq 0. \tag{5h}$$

Proof. The proof is based on reformulating (2), which using $M(\beta)$ can be restated as

$$\begin{aligned} x &\leq y \\ M(\beta) &\in \text{PSD} \cap \text{RLT}_x \\ (\alpha_j, \beta_j, y_j - Y_{12}) &\in \text{PER} \quad \forall j = 1, 2 \\ (y, Y_{12}) &\in \text{RLT}_y. \end{aligned}$$

In particular, considering $(x, X, y, Y_{12}, \alpha)$ fixed, the above system includes four linear conditions on β :

$$\beta_j \geq \max\{(y_j - Y_{12})^{-1}\alpha_j^2, X_{jj} - x_j + \alpha_j\} \quad \forall j = 1, 2.$$

Moreover, since decreasing β_1 and β_2 while holding all other variables constant does not violate $M(\beta) \succeq 0$, we may define β_1 and β_2 by

$$\beta_j(x, X, y, Y_{12}, \alpha) := \max\{(y_j - Y_{12})^{-1}\alpha_j^2, X_{jj} - x_j + \alpha_j\} \quad \forall j = 1, 2$$

without affecting the projection onto (x, X, y, Y_{12}) . It follows that values $(x, X, y, Y_{12}, \alpha)$, which are feasible for (5a)–(5d), are feasible for the constraints (2) if and only if $M(\beta_{pq}) \succeq 0$, $(p, q) \in \{1, 2\}^2$. \square

In Section 5, we will show that in order to obtain an exact representation of \mathcal{H} only the condition $M(\beta_{22}) \succeq 0$ is required. For clarity in the exposition it is helpful to write out the

conditions $M(\beta_{pq}) \succeq 0$ explicitly. In particular, (5e) can be written

$$\begin{pmatrix} Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ x_1 - \alpha_1 & x_1 - \alpha_1 & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} \succeq 0. \quad (5e')$$

In the remaining cases we can utilize the well-known Schur complement condition to conclude that (5f) is equivalent to

$$\begin{pmatrix} y_1 - Y_{12} & 0 & \alpha_1 & 0 \\ 0 & Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ \alpha_1 & x_1 - \alpha_1 & X_{11} & X_{12} \\ 0 & x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} \succeq 0, \quad (5f')$$

(5g) is equivalent to

$$\begin{pmatrix} y_2 - Y_{12} & 0 & 0 & \alpha_2 \\ 0 & Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ 0 & x_1 - \alpha_1 & x_1 - \alpha_1 & X_{12} \\ \alpha_2 & x_2 - \alpha_2 & X_{12} & X_{22} \end{pmatrix} \succeq 0, \quad (5g')$$

and (5h) is equivalent to

$$\begin{pmatrix} y_1 - Y_{12} & 0 & 0 & \alpha_1 & 0 \\ 0 & y_2 - Y_{12} & 0 & 0 & \alpha_2 \\ 0 & 0 & Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ \alpha_1 & 0 & x_1 - \alpha_1 & X_{11} & X_{12} \\ 0 & \alpha_2 & x_2 - \alpha_2 & X_{12} & X_{22} \end{pmatrix} \succeq 0. \quad (5h')$$

In the statement of results in the sequel we will always refer to the conditions (5e)–(5h), but these statements may be easier to understand if the reader refers to (5e')–(5h').

5 Reducing to a single semidefinite condition

Theorem 3 establishes that \mathcal{H} is described in part by the four PSD conditions (5e)–(5h)—one of size 3×3 , two of size 4×4 , and one of size 5×5 . In this section, we show that Theorem 3 holds even if (5e)–(5g) are not enforced. We show this in several steps. First, we prove that (5e) is redundant.

5.1 Condition (5e) is redundant

Lemma 1. *If $(x, X, y, Y_{12}, \alpha)$ satisfies (5a)–(5d), then it satisfies (5e).*

Proof. Consider the linear conditions (5a)–(5d) of (5). In terms of the remaining variables, the constraints on X_{12} are simple bounds:

$$l := \max\{0, x_1 - \alpha_1 + x_2 - \alpha_2 - Y_{12}\} \leq X_{12} \leq \min\{x_1 - \alpha_1, x_2 - \alpha_2\} =: u.$$

We claim that (5e) is satisfied at both endpoints $X_{12} = l$ and $X_{12} = u$, which will prove the theorem since the determinant of every principal submatrix of $M(\beta_{11})$ that includes X_{12} is a concave quadratic function of X_{12} .

So we need $M(\beta_{11}) \succeq 0$ at both $X_{12} = l$ and $X_{12} = u$, i.e.,

$$\begin{pmatrix} Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ x_1 - \alpha_1 & x_1 - \alpha_1 & l \\ x_2 - \alpha_2 & l & x_2 - \alpha_2 \end{pmatrix} \succeq 0 \quad \text{and} \quad \begin{pmatrix} Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ x_1 - \alpha_1 & x_1 - \alpha_1 & u \\ x_2 - \alpha_2 & u & x_2 - \alpha_2 \end{pmatrix} \succeq 0.$$

The two matrices above share several properties necessary for positive semidefiniteness. Both have nonnegative diagonals, and all 2×2 principal minors are nonnegative:

- For each, the $\{1, 2\}$ principal minor is nonnegative if and only if $Y_{12}(x_1 - \alpha_1) - (x_1 - \alpha_1)^2 \geq 0$. This follows from (5b):

$$Y_{12} \geq (x_1 - \alpha_1) + (x_2 - \alpha_2 - X_{12}) \geq (x_1 - \alpha_1) + 0 = x_1 - \alpha_1, \quad (6)$$

which implies $Y_{12}(x_1 - \alpha_1) \geq (x_1 - \alpha_1)^2$.

- For each, the $\{1, 3\}$ principal minor is similarly nonnegative.
- The respective $\{2, 3\}$ minors are nonnegative if $(x_1 - \alpha_1)(x_2 - \alpha_2) - l^2 \geq 0$ and $(x_1 - \alpha_1)(x_2 - \alpha_2) - u^2 \geq 0$, which hold because $0 \leq l \leq u \leq x_1 - \alpha_1$ and $0 \leq l \leq u \leq x_2 - \alpha_2$.

It remains to show that the both determinants of both matrices are nonnegative. Let us first examine the case for $X_{12} = l$, which itself breaks into two subcases: (i) $x_1 - \alpha_1 + x_2 - \alpha_2 - Y_{12} \leq 0 = l$; (ii) $0 \leq x_1 - \alpha_1 + x_2 - \alpha_2 - Y_{12} = l$. For subcase (i), the determinant equals $(x_1 - \alpha_1)(x_2 - \alpha_2)(Y_{12} - x_1 + \alpha_1 - x_2 + \alpha_2)$, which is the product of three nonnegative terms. For subcase (ii), the determinant equals

$$(Y_{12} - x_2 + \alpha_2)(Y_{12} - x_1 + \alpha_1)(x_1 - \alpha_1 + x_2 - \alpha_2 - Y_{12})$$

which is also the product of three nonnegative terms; in particular, see (6). The case for $X_{12} = u$ similarly breaks down into two subcases, which mirror (i) and (ii) above. \square

5.2 Reduction to $\alpha_1 = 0$

In order to prove that Theorem 3 holds even without (5f) and (5g), we will first reduce to the case $\alpha_1 = 0$. In fact if (5a)–(5d) and (5h) hold, then at most one of (5f) and (5g) can be violated. This is because, if both were violated, then we would have $X_{11} - \alpha_1^2/(y_1 - Y_{12}) > x_1 - \alpha_1$ and $X_{22} - \alpha_2^2/(y_2 - Y_{12}) > x_2 - \alpha_2$; otherwise, by comparing diagonal elements (5h) would not hold. However, these two strict inequalities then imply that (5e) \Rightarrow (5f)–(5h), which is a contradiction. So we assume without loss of generality that (5f) is violated while (5g) holds, and use the following terminology regarding system (5): we say that a point $(x, X, y, Y_{12}, \alpha)$ *lacks only* (5f) when the point satisfies all conditions in (5) except that it violates (5f).

Lemma 2. *Suppose that $(x, X, y, Y_{12}, \alpha)$ lacks only (5f), and suppose $\alpha_1 > 0$. Then $y_1 - Y_{12} > 0$ and $(\bar{x}, \bar{X}, y, Y_{12}, \bar{\alpha})$ lacks only (5f), where*

$$\bar{x} := \begin{pmatrix} x_1 - \alpha_1 \\ x_2 \end{pmatrix}, \quad \bar{X} := \begin{pmatrix} X_{11} - \alpha_1^2/(y_1 - Y_{12}) & X_{12} \\ X_{12} & X_{22} \end{pmatrix}, \quad \bar{\alpha} := \begin{pmatrix} 0 \\ \alpha_2 \end{pmatrix}.$$

Proof. If $\alpha_1 > 0$ then (5h) implies that $y_1 - Y_{12} > 0$. For notational convenience, define $v := (x, X, y, Y_{12}, \alpha)$ and $\bar{v} := (\bar{x}, \bar{X}, y, Y_{12}, \bar{\alpha})$. We need to check that \bar{v} satisfies all conditions in (5) except (5f). Since only \bar{x}_1 , \bar{X}_{11} , and $\bar{\alpha}_1$ differ between v and \bar{v} , and since $\bar{x}_1 - \bar{\alpha}_1 = x_1 - \alpha_1$, we need to verify $\bar{X}_{11} \leq \bar{x}_1 \leq y_1$, $0 \leq \bar{\alpha}_1 \leq y_1 - Y_{12}$, and (5h) at \bar{v} , and we need to show (5f) does *not* hold at \bar{v} . Clearly $0 \leq \bar{\alpha}_1 \leq y_1 - Y_{12}$ because $\bar{\alpha}_1 = 0$, and $\bar{x}_1 \leq x_1 \leq y_1$.

With $\bar{\alpha}_1 = 0$ and $\bar{x}_1 = x_1 - \alpha_1$, conditions (5e) and (5f) at \bar{v} are respectively equivalent to

$$\begin{pmatrix} Y_{12} & \bar{x}_1 & x_2 - \alpha_2 \\ \bar{x}_1 & \bar{x}_1 & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} = \begin{pmatrix} Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ x_1 - \alpha_1 & x_1 - \alpha_1 & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} \succeq 0,$$

and

$$\begin{pmatrix} Y_{12} & \bar{x}_1 & x_2 - \alpha_2 \\ \bar{x}_1 & \bar{X}_{11} & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} = \begin{pmatrix} Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ x_1 - \alpha_1 & X_{11} - \alpha_1^2/(y_1 - Y_{12}) & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} \succeq 0.$$

These conditions both match the conditions of (5e) and (5f) at v , showing that (5e) holds

at v if and only if (5e) holds at \bar{v} , and similarly for (5f). In particular, this implies \bar{v} does not satisfy (5f), as desired. In addition, we conclude $\bar{X}_{11} \leq \bar{x}_1$ because, if \bar{X}_{11} were greater than \bar{x}_1 , then (5e) holding at v would imply (5f) holds at v by just comparing the diagonal elements above, but this would violate our assumptions.

Finally, using again the relationship between \bar{v} and v , (5h) holds at \bar{v} if and only if

$$\begin{pmatrix} y_2 - Y_{12} & 0 & 0 & \alpha_2 \\ 0 & Y_{12} & x_1 - \alpha_1 & x_2 - \alpha_2 \\ 0 & x_1 - \alpha_1 & X_{11} - \alpha_1^2/(y_1 - Y_{12}) & X_{12} \\ \alpha_2 & x_2 - \alpha_2 & X_{12} & X_{22} \end{pmatrix} \succeq 0,$$

which is true by applying the Schur complement, using the fact that (5h) holds at v . \square

5.3 Characterizing (5f) and (5h) in terms of α_2

Given $(x, X, y, Y_{12}, \alpha)$ with $\alpha_1 = 0$ that lacks only (5f), in Section 5.4 our goal will be to modify α_2 to a new value $\hat{\alpha}_2$ so as to satisfy all the constraints of (5). To facilitate this analysis, we now carefully examine how conditions (5f) and (5h) depend on α_2 .

Because $y_1 - Y_{12} \geq 0$ and $\alpha_1 = 0$, (5f) is equivalent to

$$V := \begin{pmatrix} Y_{12} & x_1 & x_2 - \alpha_2 \\ x_1 & X_{11} & X_{12} \\ x_2 - \alpha_2 & X_{12} & x_2 - \alpha_2 \end{pmatrix} \succeq 0. \quad (7)$$

Now letting $\bar{x}_2 := x_2 - \alpha_2$, we have $\det(V) = -X_{11}\bar{x}_2^2 + (2X_{12}x_1 + Y_{12}X_{11} - x_1^2)\bar{x}_2 - Y_{12}X_{12}^2$. As a function of \bar{x}_2 , this is a strictly concave quadratic assuming that $X_{11} > 0$. Moreover, the discriminant for this quadratic is

$$\begin{aligned} & (Y_{12}X_{11} - x_1^2 + 2x_1X_{12})^2 - 4Y_{12}X_{11}X_{12}^2 \\ &= (Y_{12}X_{11} - x_1^2)^2 + 4x_1X_{12}(Y_{12}X_{11} - x_1^2) + 4x_1^2X_{12}^2 - 4Y_{12}X_{11}X_{12}^2 \\ &= (Y_{12}X_{11} - x_1^2)^2 + 4x_1^2X_{12}(X_{12} - x_1) + 4Y_{12}X_{11}X_{12}(x_1 - X_{12}) \\ &= (Y_{12}X_{11} - x_1^2)^2 + 4X_{12}(x_1 - X_{12})(Y_{12}X_{11} - x_1^2) \\ &= \theta(\theta + 4X_{12}(x_1 - X_{12})), \end{aligned}$$

where $\theta := Y_{12}X_{11} - x_1^2 \geq 0$. It follows that $\det(V) \geq 0$ if and only if \bar{x}_2 is contained in the

interval bounded by the roots

$$\frac{X_{12}x_1}{X_{11}} + \frac{\theta \pm \sqrt{\theta(\theta + 4X_{12}(x_1 - X_{12}))}}{2X_{11}},$$

or equivalently, if and only if $\alpha_2 \in [\alpha_2^-, \alpha_2^+]$, where

$$\alpha_2^- := x_2 - \frac{X_{12}x_1}{X_{11}} - \frac{\theta + \sqrt{\theta(\theta + 4X_{12}(x_1 - X_{12}))}}{2X_{11}} \leq x_2 - \frac{X_{12}x_1}{X_{11}} - \frac{\theta}{X_{11}} \quad (8a)$$

$$\alpha_2^+ := x_2 - \frac{X_{12}x_1}{X_{11}} - \frac{\theta - \sqrt{\theta(\theta + 4X_{12}(x_1 - X_{12}))}}{2X_{11}} \geq x_2 - \frac{X_{12}x_1}{X_{11}}. \quad (8b)$$

From the above, if $(x, X, y, Y_{12}, \alpha)$ lacks only (5f), where $\alpha_1 = 0$ and $X_{11} > 0$ then to have $(x, X, y, Y_{12}, \hat{\alpha})$ satisfy (5f) with $\hat{\alpha}_1 = 0$ we certainly require that $\hat{\alpha}_2 \in [\alpha_2^-, \alpha_2^+]$. In the next lemma we show that in fact this condition is necessary and sufficient.

Lemma 3. *Suppose $(x, X, y, Y_{12}, \alpha)$ lacks only (5f), where $\alpha_1 = 0$, and let $\hat{\alpha} := (0, \hat{\alpha}_2)$. Then $X_{11} > 0$, $y_2 - Y_{12} > 0$, and $(x, X, y, Y_{12}, \hat{\alpha})$ satisfies (5f) if and only if $\hat{\alpha}_2 \in [\alpha_2^-, \alpha_2^+]$.*

Proof. Note that if $(x, X, y, Y_{12}, \alpha)$ with $\alpha_1 = 0$ satisfies (5h), then $X_{11} = 0$ implies that $x_1 = X_{12} = 0$. In this case (5f) follows immediately from (5b). In addition, if $y_2 - Y_{12} = 0$ then (5h) implies that $\alpha_2 = 0$, in which case (5f) would follow immediately from $X_{22} \leq x_2$. Thus if $(x, X, y, Y_{12}, \alpha)$ with $\alpha_1 = 0$ lacks only (5f) we must have $X_{11} > 0$ and $y_2 - Y_{12} > 0$.

We consider V defined in (7) with $\hat{\alpha}_2$ substituted for α_2 ; we wish to show $V \succeq 0$ if and only if $\hat{\alpha}_2 \in [\alpha_2^-, \alpha_2^+]$. As discussed before the lemma, $\det(V) \geq 0$ for such $\hat{\alpha}_2$, but it could happen that $V \not\succeq 0$ even when $\det(V) \geq 0$. Note that, since $(x, X, y, Y_{12}, \alpha)$ satisfies (5h) by assumption, then by the eigenvalue interlacing theorem (see, for example, Theorem 4.3.8 of Horn and Johnson [11]), V has at most one negative eigenvalue.

We consider two cases based on whether $\theta \geq 0$ is positive or zero. If $\theta > 0$, then by the determinant and discriminant formulas above we have $\det(V) > 0 \Rightarrow V \succ 0$ for $\hat{\alpha}_2 \in (\alpha_2^-, \alpha_2^+)$, and $V \succeq 0$ with $\det(V) = 0$ when $\hat{\alpha}_2 = \alpha_2^-$ or $\hat{\alpha}_2 = \alpha_2^+$. The latter follows, for example, by continuity of the determinants of all principal submatrices. On the other hand, if $\theta = 0$, then: $\alpha_2^- = \alpha_2^+ = x_2 - X_{12}x_1/X_{11}$; $\det(V) = 0$ when $\hat{\alpha}_2 = x_2 - X_{12}x_1/X_{11}$; and $\det(V) < 0$ for any other value of $\hat{\alpha}_2$. Focusing then on $\hat{\alpha}_2 = x_2 - X_{12}x_1/X_{11}$, we have

$$V = \begin{pmatrix} Y_{12} & x_1 & X_{12}x_1/X_{11} \\ x_1 & X_{11} & X_{12} \\ X_{12}x_1/X_{11} & X_{12} & X_{12}x_1/X_{11} \end{pmatrix}.$$

In this case $\text{diag}(V) \geq 0$ and $\det(V) = 0$, so to demonstrate $V \succeq 0$, we need to show that

the 2×2 principal submatrices are positive semidefinite or equivalently have nonnegative determinants. The $\{1, 2\}$ submatrix is positive semidefinite since (5h) is satisfied; the determinant of the $\{1, 3\}$ submatrix is nonnegative because $Y_{12}X_{11} \geq x_1^2 \geq X_{12}x_1$; and the determinant of the $\{2, 3\}$ submatrix is nonnegative because $x_1 \geq X_{12}$. \square

It will also be important that we understand how (5h) depends on α_2 . When $\alpha_1 = 0$ and $(x, X, y, Y_{12}, \alpha)$ satisfies (5h), we certainly have

$$\begin{vmatrix} y_2 - Y_{12} & 0 & 0 & \alpha_2 \\ 0 & Y_{12} & x_1 & x_2 - \alpha_2 \\ 0 & x_1 & X_{11} & X_{12} \\ \alpha_2 & x_2 - \alpha_2 & X_{12} & X_{22} \end{vmatrix} \geq 0. \quad (9)$$

Assuming that $X_{11} > 0$ and $y_2 - Y_{12} > 0$, the left side of (9) is a strictly concave quadratic function of α_2 , and it is straightforward to compute that the maximizer of this determinant is

$$\alpha_2^* := \frac{(y_2 - Y_{12})(x_2 X_{11} - x_1 X_{12})}{y_2 X_{11} - x_1^2} = \left(x_2 - \frac{X_{12}x_1}{X_{11}} \right) \frac{y_2 - Y_{12}}{y_2 - x_1^2/X_{11}} \leq x_2 - \frac{X_{12}x_1}{X_{11}}. \quad (10)$$

In (10) the denominator $y_2 X_{11} - x_1^2$ is strictly positive since $Y_{12}X_{11} \geq x_1^2$ and $y_2 > Y_{12}$, and then the inequality follows from the fact that $Y_{12}X_{11} \geq x_1^2$.

Finally, for $\alpha_1 = 0$ the lemma below considers conditions under which (5f) \Rightarrow (5h), and (5h) \Rightarrow (5f).

Lemma 4. *Let $(x, X, y, Y_{12}, \alpha)$ be given with $\alpha_1 = 0$, $y_2 - Y_{12} > 0$ and $0 \leq x_2 - X_{22} \leq \frac{1}{4}(y_2 - Y_{12})$. Define $\rho := \sqrt{1 - 4(x_2 - X_{22})/(y_2 - Y_{12})} \leq 1$. Also define*

$$\lambda^- := \frac{1}{2}(1 - \rho)(y_2 - Y_{12}) \leq \frac{1}{2}(1 + \rho)(y_2 - Y_{12}) =: \lambda^+.$$

Then $\lambda^- \leq \alpha_2 \leq \lambda^+$ ensures (5f) \Rightarrow (5h), and $\alpha_2 \leq \lambda^-$ or $\lambda^+ \leq \alpha_2$ ensures (5h) \Rightarrow (5f).

Proof. By exploiting $\alpha_1 = 0$, using the Schur complement theorem, and comparing diagonal elements, we see that: (i) (5f) \Rightarrow (5h) is ensured when $x_2 - \alpha_2 \leq X_{22} - \alpha_2^2/(y_2 - Y_{12})$; and (ii) (5h) \Rightarrow (5f) is ensured when the reverse inequality $x_2 - \alpha_2 \geq X_{22} - \alpha_2^2/(y_2 - Y_{12})$ holds. Note that λ^- and λ^+ are the roots of the quadratic equation $x_2 - \alpha_2 = X_{22} - \alpha_2^2/(y_2 - Y_{12})$ in α_2 . In particular, the assumption $0 \leq x_2 - X_{22} \leq \frac{1}{4}(y_2 - Y_{12})$ guarantees that the discriminant is nonnegative and that $x_2 - \alpha_2 \leq X_{22} - \alpha_2^2/(y_2 - Y_{12})$ is satisfied at the midpoint $\frac{1}{2}(y_2 - Y_{12})$ of λ^- and λ^+ . Then the final statement of the lemma is just the restatement of (i) and (ii). \square

5.4 Adjusting α_2 when $\alpha_1 = 0$

Assume that $(x, X, y, Y_{12}, \alpha)$ lacks only (5f) with $\alpha_1 = 0$. Then by Lemma 3 either $\alpha_2 < \alpha_2^-$ or $\alpha_2 > \alpha_2^+$; see (8) for the definitions of α_2^- and α_2^+ . The next two lemmas show that $(x, X, y, Y_{12}, \hat{\alpha})$ then satisfies (5), where in the first case $\hat{\alpha} = (0, \alpha_2^-)$ and in the second case $\hat{\alpha} = (0, \alpha_2^+)$.

Lemma 5. *Assume that $(x, X, y, Y_{12}, \alpha)$ lacks only (5f) with $\alpha_1 = 0$, and $\alpha_2 < \alpha_2^-$. Then $(x, X, y, Y_{12}, \hat{\alpha})$ satisfies (5) with $\hat{\alpha} = (0, \alpha_2^-)$.*

Proof. From Lemma 3 we know that $X_{11} > 0$, $y_2 - Y_{12} > 0$ and $(x, X, y, Y_{12}, \hat{\alpha})$ satisfies (5f). Since (5a)–(5d) \Rightarrow (5e) by Proposition 1 and (5h) \Rightarrow (5g) when $\alpha_1 = 0$ by inspection, we need to establish just (5a)–(5d) and (5h). Since $(x, X, y, Y_{12}, \alpha)$ satisfies (5a)–(5d) and we have increased α_2 to α_2^- to form $\hat{\alpha}$, we need only show $\alpha_2^- \leq x_2 - X_{12}$ and $\alpha_2^- \leq y_2 - Y_{12}$ to establish that (5a)–(5d) hold for $(x, X, y, Y_{12}, \hat{\alpha})$. In fact, we will show $\alpha_2^- \leq x_2 - X_{12}$ as well as the stronger inequality $\alpha_2^- \leq \lambda^+$, where $\lambda^+ = \frac{1}{2}(1 + \rho)(y_2 - Y_{12})$ and $0 \leq \rho \leq 1$ are defined in Lemma 4. Indeed, the conditions of Lemma 4 hold here because, as (5h) is satisfied but (5f) is violated at α_2 , we have $x_2 - \alpha_2 \leq X_{22} - \alpha_2^2/(y_2 - Y_{12})$, which ensures $0 \leq x_2 - X_{22} \leq \frac{1}{4}(y_2 - Y_{12})$ and $\alpha_2 \leq \lambda^+$. Hence, proving $\alpha_2^- \leq \lambda^+$ will ensure (5f) \Rightarrow (5h).

To prove $\alpha_2^- \leq x_2 - X_{12}$, we note that (8a) and $x_1 \geq X_{11}$ imply

$$\alpha_2^- \leq x_2 - \frac{X_{12}x_1}{X_{11}} \leq x_2 - X_{12}.$$

Next, to prove $\alpha_2^- \leq \lambda^+$, assume for contradiction that $\alpha_2 \leq \lambda^+ < \alpha_2^-$. Consider α_2^* as defined in (10). We claim $\lambda^+ < \alpha_2^*$, which from (10) is equivalent to

$$x_2 - \frac{X_{12}x_1}{X_{11}} > \frac{1}{2}(1 + \rho) \left(y_2 - \frac{x_1^2}{X_{11}} \right).$$

From (8a), the definition of θ , and the assumption that $\lambda^+ < \alpha_2^-$, we then have

$$\begin{aligned} x_2 - \frac{X_{12}x_1}{X_{11}} &\geq \alpha_2^- + \frac{\theta}{X_{11}} \\ &> \frac{1}{2}(1 + \rho)(y_2 - Y_{12}) + \left(Y_{12} - \frac{x_1^2}{X_{11}} \right) \\ &\geq \frac{1}{2}(1 + \rho)(y_2 - Y_{12}) + \frac{1}{2}(1 + \rho) \left(Y_{12} - \frac{x_1^2}{X_{11}} \right) \\ &= \frac{1}{2}(1 + \rho) \left(y_2 - \frac{x_1^2}{X_{11}} \right), \end{aligned}$$

as required. Since (9) holds at $\alpha_2 \leq \lambda^+$ and $\alpha_2^* > \lambda^+$, the determinant in (9) must be strictly positive at λ^+ ; recall that this determinant is a strictly concave function of α_2 . Then (5h) holds with α_2 replaced by λ^+ , since eigenvalue interlacing implies that the matrix in (5h) can have at most one negative eigenvalue as α_2 is varied. However Lemma 4 then implies that (5f) also then holds with α_2 replaced by λ^+ , and therefore $\alpha_2^- \leq \lambda^+$ from Lemma 3. This is the desired contradiction of $\lambda^+ < \alpha_2^-$. We must therefore have $\alpha_2^- \leq \lambda^+$, which completes the proof. \square

Lemma 6. *Assume $(x, X, y, Y_{12}, \alpha)$ lacks only (5f) with $\alpha_1 = 0$, and $\alpha_2 > \alpha_2^+$. Then $(x, X, y, Y_{12}, \hat{\alpha})$ satisfies (5) with $\hat{\alpha} = (0, \alpha_2^+)$.*

Proof. We follow a similar proof as for the preceding lemma. In this case, however, since we are decreasing α_2 to α_2^+ , we need to show $\alpha_2^+ \geq x_1 + x_2 - X_{12} - Y_{12}$ and $\alpha_2^+ \geq \lambda^-$, where $\lambda^- = \frac{1}{2}(1 - \rho)(y_2 - Y_{12})$ as defined in Lemma 4. Note that $\alpha_2 \geq \lambda^-$ because $(x, X, y, Y_{12}, \alpha)$ lacks only (5f), just as in the preceding lemma.

For the first inequality, from (8b) it suffices to show

$$x_2 - \frac{X_{12}x_1}{X_{11}} \geq x_1 + x_2 - X_{12} - Y_{12}$$

which is equivalent to

$$X_{12}x_1 + X_{11}x_1 - X_{11}X_{12} \leq X_{11}Y_{12}.$$

Since $\theta = Y_{12}X_{11} - x_1^2 \geq 0$, it thus suffices to show

$$\begin{aligned} X_{12}x_1 + X_{11}x_1 - X_{11}X_{12} &\leq x_1^2 \\ X_{12}(x_1 - X_{11}) &\leq x_1(x_1 - X_{11}), \end{aligned}$$

which certainly holds because $X_{12} \leq x_1$ and $X_{11} \leq x_1$.

For the second inequality, assume by contradiction that $\alpha_2^+ < \lambda^-$. We claim $\alpha_2^* < \lambda^-$, which by (10) is equivalent to

$$x_2 - \frac{X_{12}x_1}{X_{11}} < \frac{1}{2}(1 - \rho) \left(y_2 - \frac{x_1^2}{X_{11}} \right).$$

From (8b), the assumption $\alpha_2^+ < \lambda^-$, and the inequality $Y_{12}X_{11} \geq x_1^2$, we have

$$x_2 - \frac{X_{12}x_1}{X_{11}} \leq \alpha_2^+ < \lambda^- = \frac{1}{2}(1 - \rho)(y_2 - Y_{12}) \leq \frac{1}{2}(1 - \rho) \left(y_2 - \frac{x_1^2}{X_{11}} \right),$$

as desired. Since (9) holds at $\alpha_2 \geq \lambda^-$ and $\alpha_2^* < \lambda^-$, the determinant in (9) is strictly positive

at λ^- , which implies that (5h) holds with α_2 replaced by λ^- ; the logic is identical to that for λ^+ in the proof of Lemma 5. Then Lemma 4 implies that (5f) holds with α_2 replaced by λ^- , contradicting the assumption that $\alpha_2^+ < \lambda^-$, so in fact $\alpha_2^+ \geq \lambda^-$. \square

5.5 Removing (5f) and (5g) does not affect the projection

We can now prove the following streamlined version of Theorem 3, which requires only one of the four PSD conditions (5e)–(5h).

Theorem 4. \mathcal{H} equals the projection onto (x, X, y, Y_{12}) of $(x, X, y, Y_{12}, \alpha)$ satisfying the convex constraints (5a)–(5d) and (5h).

Proof. We must show that if $(x, X, y, Y_{12}, \alpha)$ satisfies (5a)–(5d) and (5h), then $(x, X, y, Y_{12}) \in \mathcal{H}$. By Theorem 3 this is equivalent to showing that there is an α' so that $(x, X, y, Y_{12}, \alpha')$ satisfies all of the constraints in (5).

If (5a)–(5d) are satisfied, then (5e) is redundant by Proposition 1. Moreover, as described above Lemma 2, if (5h) also holds then at most one of (5f)–(5g) can fail to hold. If both (5f)–(5g) hold then there is nothing to show, so we assume without loss of generality that (5f) fails to hold; that is, $(x, X, y, Y_{12}, \alpha)$ lacks only (5f).

Assume first that $\alpha_1 = 0$. If $\alpha_2 < \alpha_2^-$, then by Lemma 5 we know that $(x, X, y, Y_{12}, \hat{\alpha})$ satisfies (5), where $\hat{\alpha} = (0, \alpha_2^-)$. Similarly, if $\alpha_2 > \alpha_2^+$, then by Lemma 6 we have the same conclusion using $\hat{\alpha} = (0, \alpha_2^+)$. Therefore $(x, X, y, Y_{12}) \in \mathcal{H}$.

If $\alpha_1 > 0$ we apply the transformation in Lemma 2 to obtain $(\bar{x}, \bar{X}, y, Y_{12}, \bar{\alpha})$, with $\bar{\alpha} = (0, \alpha_2)$, that lacks only (5f). We then apply either Lemma 5 or Lemma 6 to obtain $\hat{\alpha} = (0, \hat{\alpha}_2)$ so that $(\bar{x}, \bar{X}, y, Y_{12}, \hat{\alpha})$ satisfies (5). Let $\alpha' = (\alpha_1, \hat{\alpha}_2)$. We claim that $(x, X, y, Y_{12}, \alpha')$ satisfies (5) as well. For the linear conditions (5a)–(5d) this is immediate from the facts that both $(x, X, y, Y_{12}, \alpha)$ and $(\bar{x}, \bar{X}, y, Y_{12}, \hat{\alpha})$ satisfy (5a)–(5d), and $\bar{x}_1 - \bar{\alpha}_1 = x_1 - \alpha_1$. Therefore (5e) is also satisfied at $(x, X, y, Y_{12}, \alpha')$. The fact that the remaining PSD conditions (5f)–(5h) are satisfied at $(x, X, y, Y_{12}, \alpha')$ follows from the facts that these conditions are satisfied at $(\bar{x}, \bar{X}, y, Y_{12}, \hat{\alpha})$, $\bar{x}_1 - \bar{\alpha}_1 = x_1 - \alpha_1$, the definition of \bar{X}_{11} and the Schur complement condition. \square

6 Another interpretation

The representation for \mathcal{H} in Theorem 4 was obtained by starting with the representation in Theorem 3 and then arguing that only the single semidefiniteness constraint (5h) was necessary. In this section we describe an alternative derivation for the representation in

Theorem 4. This derivation provides another interpretation for the conditions of Theorem 4 and also leads to a simple conjecture for a representation of \mathcal{H}' as defined in the Introduction.

The alternative derivation is based on replacing the variables y with $t = e - y$, as was done for the case $n = 1$ in the proof of Theorem 1. Note that each y_i is binary if and only if t_i is binary, and $(y, Y_{12}) \in \text{RLT}_y$ if and only if $(t, T_{12}) \in \text{RLT}_y$ where $T_{12} = 1 + Y_{12} - y_1 - y_2$. In fact the linear constraints (5a)–(5d) can be obtained by considering the equations $x_i + s_i + t_i = 1$, $i = 1, 2$, generating RLT constraints by multiplying each equation in turn by the variables (x_j, s_j, t_j) , $i = 1, 2$, and then projecting onto the variables $(x, X, t, T_{12}, \alpha)$, where $\alpha_1 \approx x_1 t_2 = x_1(1 - y_2)$, $\alpha_2 \approx x_2 t_1 = x_2(1 - y_1)$, $T_{12} = 1 + Y_{12} - y_1 - y_2 \approx t_1 t_2$. Substituting variables and applying a symmetric transformation that preserves semidefiniteness, the PSD condition (5h') can be written in the form

$$\begin{pmatrix} 1 - T_{12} & x_1 & x_2 & t_1 - T_{12} & t_2 - T_{12} \\ x_1 & X_{11} & X_{12} & 0 & \alpha_1 \\ x_2 & X_{12} & X_{22} & \alpha_2 & 0 \\ t_1 - T_{12} & 0 & \alpha_2 & t_1 - T_{12} & 0 \\ t_2 - T_{12} & \alpha_1 & 0 & 0 & t_2 - T_{12} \end{pmatrix} \succeq 0. \quad (11)$$

The PSD constraint (11) has a simple interpretation as a strengthening of the natural PSD condition

$$\begin{pmatrix} 1 & x_1 & x_2 & t_1 & t_2 \\ x_1 & X_{11} & X_{12} & 0 & \alpha_1 \\ x_2 & X_{12} & X_{22} & \alpha_2 & 0 \\ t_1 & 0 & \alpha_2 & t_1 & T_{12} \\ t_2 & \alpha_1 & 0 & T_{12} & t_2 \end{pmatrix} \succeq 0. \quad (12)$$

The matrix in (11) is obtained from the matrix in (12) by subtracting $T_{12}uu^T$, where $u = (1, 0, 0, 1, 1)^T$. This can be interpreted as removing the portion of the matrix corresponding to $t = e$, or equivalently $y = 0$, if the matrix in (12) is decomposed into a convex combination of four matrices corresponding to $t \in \{0, e_1, e_2, e\}$, similar to the decomposition of \mathcal{H} into a convex combination of \mathcal{H}_y , $y \in \{0, e_1, e_2, e\}$ in Section 3. Note in particular that $T_{12} = \lambda_0$, as defined in (3).

We know that to obtain a representation of \mathcal{H} the condition (11) cannot be replaced by (12); there are solutions $(x, X, y, Y_{12}, \alpha)$ that are feasible with the weaker PSD condition but where $(x, X, y, Y_{12}) \notin \mathcal{H}$. However it appears that the condition (12) is sufficient to obtain a representation of \mathcal{H}' . The following conjecture regarding \mathcal{H}' is supported by extensive numerical computations, but remains unproved.

Conjecture 1. \mathcal{H}' equals the projection onto (x, X, y) of $(x, X, y, Y_{12}, \alpha)$ satisfying the constraints (5a)–(5d) and (12), where $t_1 = 1 - y_1$, $t_2 = 1 - y_2$ and $T_{12} = 1 + Y_{12} - y_1 - y_2$.

Note that (5a)–(5d) and (12) amount to the relaxation of (x, xx^T, y) , which enforces PSD and RLT in the (x, X, y, Y_{12}) space and also exploits the binary nature of y . In other words, the standard approach for creating a strong SDP relaxation would be sufficient to capture the convex hull of (x, X, y) in this case, similar to the case of $n = 1$ as shown in the proof of Theorem 1, as well as the characterization of QPB for $n = 2$ from [2].

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