Cones of Nonnegative Quadratic Pseudo-Boolean Functions*

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Abstract

Numerous combinatorial optimization problems can be formulated as the minimization of a quadratic pseudo-Boolean function in n variables, which on its own turn is equivalent with a linear programming problem over the so called *Boolean Quadric Polytope* (BQ) in $n + \binom{2}{2}$ dimension (Padberg, 1989). This polytope is very well studied, still we know in fact very little about its structure and its facets (complete description is known only for $n \leq 6$.) It is known and easy to see that the facets of BQ are in a one to one correspondence with the extremal rays of the cone of nonnegative quadratic pseudo-Boolean functions. Consequently, subcones of this cone correspond to polyhedral relaxations of BQ. Several such relaxations were introduced in the past with several open question remaining regarding the relation of these relaxations. The aim of this short note is to fill in some of these gaps and bring more clarity to the relations between the corresponding polyhedral hierarchies. Our approach utilizes the above cited connection to the cone of nonnegative quadratic pseudo-Boolean functions and is rather algebraic.

Basic Notations and Definitions

Let n be a positive integer, $\mathbb{B} = \{0,1\}$, and $[n] = \{1,2,...,n\}$. We denote by $\mathbb{R}$ the set of reals and by $\mathbb{Z}$ the set of integers. Let us further denote by $\bar{x} = 1 - x$ the *complement* of a binary variable x, and let $\mathbb{L} = \{x_1, \bar{x}_1, ..., x_n, \bar{x}_n\}$ be the set of *literals*.

A *pseudo-Boolean function* (or PBF in short) is a real-valued mapping $f : \mathbb{B}^n \to \mathbb{R}$, represented by an algebraic formula in terms of its variables. It is known (see (Hammer and Rudeanu 1968)) that a pseudo-Boolean function f has a unique multilinear polynomial expression of the form:

$$f(x) = \sum_{S\subseteq[n]} q_S \prod_{j\in S} x_j$$

where $q_S \in \mathbb{R}$ for all $S \subseteq [n]$. When we talk about the size of such an expression, we take into consideration only the terms with nonzero q_S coefficients. The degree $\deg(f)$ of f is the size of the largest subset $S \subseteq [n]$ with $q_S \neq 0$. To simplify notation, we shall write q_0 instead of $q_\emptyset$, q_j instead of $q_{\{j\}}$, $q_{i,j}$ instead of $q_{\{i,j\}}$, etc., for low degree PBFs. We say that f is a *nonnegative PBF* if $f(x) \geq 0$ for all $x \in \mathbb{B}^n$.

A *posiform* is an expression of the form

$$\phi(x_1, ..., x_n) = \sum_{k=1}^{m} a_k \prod_{i\in I_k} x_i \prod_{j\in J_k} \bar{x}_j,$$

where $a_k > 0$, and I_k and J_k are disjoint subsets of $[n]$ for all $k = 1, \ldots, m$. The *degree* $\deg(\phi)$ of the posiform ϕ is the maximum of $|I_k \cup J_k|$, $k = 1, ..., m$. Let us note that a posiform is a multilinear polynomial in terms of the $2n$ literals, and it represents a unique (nonnegative) PBF. It is well-known that every nonnegative PBF f can be represented by a posiform ϕ such that $\deg(f) \leq \deg(\phi) \leq n$, however such posiform representations are not unique.

In our paper we shall pay special attention to low degree, and in particular, to quadratic PBFs (or QPBFs in short), that is to PBFs f for which $\deg(f) \leq 2$. Given a QPBF

$$f(x) = q_0 + \sum_{j\in[n]} q_j x_j + \sum_{i,j\in[n]:i<j} q_{ij} x_j x_j, \qquad (1)$$

the *Quadratic Unconstrained Boolean Optimization* (QUBO) is the problem of finding the minimum of $f(x)$ over $\mathbb{B}^n$. Many hard combinatorial optimization problems arise naturally or can be formulated easily as QUBO problems. Numerous papers addressed this problem and proposed various techniques to deal with it, see e.g., (Hammer and Rudeanu 1968; Hammer, Hansen, and Simeone 1984; De Simone 1990; Padberg 1989; Boros, Crama, and Hammer 1990; Boros and Hammer 2002). Among the many approaches, a number of papers proposed various polyhedral descriptions and approximations to QUBO. Our focus is to consider the various different polyhedra (and polyhedral hierarchies) and establish containment relations between them.

Let us next introduce new variables $y_{ij} = x_i x_j$ for all $1 \leq i < j \leq n$, substitute in f the quadratic terms by these new variables, and denote the obtained linear function by

$$L_f(x, y) = q_0 + \sum_{j\in[n]} q_j x_j + \sum_{i,j\in[n]:i<j} q_{ij} y_{ij}.$$

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It was noted (see e.g., (Fortet 1960)) that if $x \in \mathbb{B}^n$ and $y \in \mathbb{R}^{\binom{n}{2}}$ are satisfying the inequalities

$$\begin{array}{rrrcl} x_i & & -y_{ij} & \geq & 0 \\ & x_j & -y_{ij} & \geq & 0 \\ & & y_{ij} & \geq & 0 \\ -x_i & -x_j & +y_{ij} & \geq & -1 \end{array} \quad 1 \leq i < j \leq n, \qquad (2)$$

then the equalities $y_{ij} = x_i x_j$ must also hold for all pairs of indices. Consequently, the minimization of f over $\mathbb{B}^n$ can equivalently be formulated as the mixed integer linear program (MILP) of minimizing $L_f(x, y)$ subject to the constraints of (2) and requiring that x takes only binary values. The so called *standard linearization* $\mathbf{SL}$ of QUBO is the LP relaxation of this MILP, in which we drop the integrality of x, and require instead $0 \leq x \leq 1$.

The *Boolean Quadric Polytope* is the corresponding convex hull of the integral feasible solutions of $\mathbf{SL}$ in $N = n + \binom{n}{2}$ dimensions, introduced by (Padberg 1989):

$$\mathbf{BQ} = \text{conv}\left\{(x, y) \in \mathbb{R}^N \;\middle|\; \begin{array}{c} x \in \mathbb{B}^n,\ y_{ij} = x_i x_j \\ \text{for all } 1 \leq i < j \leq n \end{array}\right\}.$$

Consequently, QUBO is equivalent to the problem of minimizing $L_f(x, y)$ over $\mathbf{BQ}$.

Cones and Polyhedral Hierarchies

In this section we define several different hierarchies of polyhedral relaxations of the Boolean Quadric Polytope. Two of these relaxations are based on hierarchies of cones of nonnegative quadratic pseudo-Boolean functions, while the other two are based on a lift and project procedure applied to $\mathbf{SL}$.

In the sequel we will view quadratic pseudo-Boolean functions in n variables as vectors of their coefficients in $\mathbb{R}^{N+1}$. Note that inequalities in $\mathbb{R}^N$ also have $N+1$ coefficients, and in fact any linear inequality in $\mathbb{R}^N$ can be viewed as $L_g(x, y) \geq 0$ for the naturally corresponding quadratic pseudo-Boolean function g. Let us also recall that $L_f(x, y) \geq 0$ is a valid inequality for $\mathbf{BQ}$ if and only if the corresponding quadratic pseudo-Boolean function $f(x)$ is nonnegative for every $x \in \mathbb{B}^n$. Furthermore, all facet defining inequalities of $\mathbf{BQ}$ correspond to extremal rays of the cone of nonnegative quadratic pseudo-Boolean functions and viceversa. (See e.g., (Boros and Hammer 1993) for a short proof.)

In order to avoid confusion, in our notation, we will use bold capital letters to denote polyhedra and calligraphic capital letters to denote the corresponding cones of quadratic pseudo-Boolean functions.

Functions in k variables

For a given subset $K \subseteq [n]$, let $\mathcal{F}[K] \subseteq \mathbb{R}^{N+1}$ be the set of nonnegative quadratic pseudo-Boolean functions depending only on variables x_j $j \in K$ and, for each $k = 2, \ldots, n$, consider the cone in $\mathbb{R}^{N+1}$ defined by

$$\mathcal{F}_k = \text{cone}\left\{\mathcal{F}[K] \mid K \subseteq [n], |K| \leq k\right\}.$$

Based on these cones (Boros, Crama, and Hammer 1990) introduced the following polyhedral relaxations of $\mathbf{BQ}$:

$$\mathbf{P}_k = \left\{(x, y) \in R^N \mid L_f(x, y) \geq 0, \forall f \in \mathcal{F}_k\right\}$$

for $k = 2, 3, ..., n$. The following relations were shown in (Boros, Crama, and Hammer 1990):

$$\mathbf{SL} = \mathbf{P}_2 \supsetneq \mathbf{P}_3 \supsetneq \ldots \supsetneq \mathbf{P}_n = \mathbf{BQ}, \qquad (3)$$

where all of the above inclusions are strict. Note also that, for a fixed k, $\mathcal{F}_k$ can be polynomially generated by a system of $\binom{n}{2}2^k$ linear inequalities which must be satisfied by the coefficients of the multilinear expressions of its elements.

Degree k posiforms

The second hierarchy is based on the fact that every pseudo-Boolean function can be represented by a posiform. For $k = 2, \ldots, n$, let $\mathcal{G}_k$ be the cone of nonnegative quadratic pseudo-Boolean functions having a degree k posiform representation.

Analogously to the above, we can introduce the following polyhedral relaxations of $\mathbf{BQ}$, corresponding to cones $\mathcal{G}_k$:

$$\mathbf{Q}_k = \left\{(x, y) \in R^N \mid L_f(x, y) \geq 0, \forall f \in \mathcal{G}_k\right\}$$

for $k = 2, 3, ..., n$. It is again easy to see that, the following relations must hold:

$$\mathbf{SL} = \mathbf{Q}_2 \supseteq \mathbf{Q}_3 \supseteq \ldots \supseteq \mathbf{Q}_n = \mathbf{BQ}. \qquad (4)$$

Unlike for the previous hierarchy, it is however not known whether, for any fixed k, $\mathcal{G}_k$ and hence $\mathbf{Q}_k$ can be polynomially generated.

Lift and Project Hierarchies

The remaining hierarchies we consider are motivated by integer programming techniques. As we remarked in the introduction, $\mathbf{BQ}$ is the integral core of $\mathbf{SL}$, and while $\mathbf{SL}$ has a "small" (polynomial) polyhedral description, and thus we can optimize a linear objective over it, the polyhedron $\mathbf{BQ}$ does have exponentially many different facets. The so called lift and project (L&P) type methods developed recently provide a constructive way to describe polyhedra $\mathbf{BQ} \subseteq \mathbf{R} \subset \mathbf{SL}$ such that we can still solve a linear program over $\mathbf{R}$ efficiently, and $\mathbf{R}$ is a tighter description of $\mathbf{BQ}$ than $\mathbf{SL}$ (see e.g., (Balas, Ceria, and Cornuéjols 1993; Lovász and Schrijver 1991; Sherali and Adams 1990).)

For this, let us first recall the L&P procedure, when applied to a mixed integer programming problem. We shall follow the method essentially as introduced in (Lovász and Schrijver 1991). To allow us to simplify our notation and the whole procedure we assume that the considered polyhedral region is within $\mathbf{SL}$:

$$F = \left\{(x, y) \in \mathbb{R}^N \mid Ax + By \leq b\right\} \subseteq \mathbf{SL} \qquad (5)$$

where $b \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{m \times \binom{n}{2}}$ for some positive integers n and m. As in all previous cases, we also assume that components of x denote binary variables, while components of y are continuous. Then the integer core of F is the polytope

$$F_I = \operatorname{conv}\left\{(x,y) \in \mathbb{R}^N \;\middle|\; \begin{array}{c} Ax + By \le b, \\ x \in \mathbb{B}^n \end{array}\right\} \subseteq \mathbf{BQ}. \tag{6}$$

Clearly, $F_I \subseteq F$; the polyhedral representation of F_I may involve an exponentially large family of inequalities, in general.

L&P involves three main steps. In the **first step** we multiply each of the m inequalities describing F by both x_i and separately by $\overline{x}_i = 1 - x_i$ for all indices $i = 1, ..., n$. We obtain in this way $2mn$ nonlinear inequalities, involving variables x, y and products of these variables of the form $x_i x_j$ and $x_i y_{jk}$ for indices $i, j, k \in [n]$.

In the **second step** of L&P we linearize these nonlinear products. Namely we introduce the following substitutions:

$$\begin{array}{rcll} x_i &=& x_i^2 & \text{for all } i \in [n], \\ Y_{ij} &=& x_i x_j & \text{for all } i,j \in [n],\ i < j, \\ Z_{i(jk)} &=& x_i y_{jk} & \text{for all } i,j,k \in [n],\ j < k. \end{array} \tag{7}$$

Note that the first substitution is valid for all binary values of variables x_i, $i \in [n]$, while the other two groups of substitutions are simply introductions of new variables in place of the products in the expressions. In this way we obtain $2mn$ linear inequalities in $n + 2\binom{n}{2} + n\binom{n}{2}$ variables x, y, Y, and Z:

$$\widehat{A}x + \widehat{B}y + \widehat{C}Y + \widehat{D}Z \le \widehat{b}. \tag{8}$$

We denote by $M(F)$ the polyhedral set of feasible solutions to this system of inequalities in $\mathbb{R}^{n+(n+2)\binom{n}{2}}$. It is both well-known and easy to see that if $(x, y, Y, Z) \in M(F)$, then we have $(x, y) \in F$; furthermore, for every $(x, y) \in F$, $x \in \mathbb{B}^n$ there exists vectors Y and Z such that $(x, y, Y, Z) \in M(F)$.

Let us next recall a useful statement from (Minoux and Ouzia 2010).

Lemma 1 *If $F \subseteq \mathbf{SL}$, then we have the following equalities for all feasible vectors $(x, y, Y, Z) \in M(F)$:*

$$Y_{ij} = Z_{i(ij)} = Z_{j(ij)} = y_{ij} \quad \textit{for all } 1 \le i < j \le n.$$

□

Due to the above lemma, we can eliminate variables Y, and rewrite the representation of $M(F)$ equivalently as:

$$\widetilde{A}x + \widetilde{B}y + \widetilde{C}Z \le \widetilde{b}, \tag{9}$$

where $\widetilde{b} \in \mathbb{R}^{2mn}$, $\widetilde{A} \in \mathbb{R}^{2mn\times n}$, $\widetilde{B} \in \mathbb{R}^{2mn\times\binom{n}{2}}$ and $\widetilde{C} \in \mathbb{R}^{2mn\times(n-2)\binom{n}{2}}$.

Since $F \subseteq \mathbf{SL}$, for $(x, y) \in F$, x binary we have y binary, and consequently for all $i, j, k \in [n], i < j, k \ne i, j$ the equalities

$$x_k y_{ij} = x_i y_{ik} = x_j y_{jk}$$

are implied. We could as well add the constraints $Z_{i(jk)} = Z_{j(ik)} = Z_{k(ij)}$ and obtain another polyhedron in the variables (x, y, Z) that is contained in $M(F)$. By introducing new variables $z_{ijk} = Z_{i(jk)} = Z_{j(ik)} = Z_{k(ij)}$ for all $1 \le i < j < k \le n$, we can rewrite the inequalities defining $M(F)$ as

$$\overline{A}x + \overline{B}y + \overline{C}z \le \overline{b}, \tag{10}$$

and denote by $\overline{M}(F)$ the corresponding polyhedral set of feasible solutions. Note that here we have $\overline{b} \in \mathbb{R}^{2mn}$, $\overline{A} \in \mathbb{R}^{2mn\times n}$, $\overline{B} \in \mathbb{R}^{2mn\times\binom{n}{2}}$ and $\overline{C} \in \mathbb{R}^{2mn\times\binom{n}{3}}$.

In the **third and last step** of L&P we project $M(F)$ or $\overline{M}(F)$ back to the (x, y) space, and denote by $\mathcal{L}(F)$ and $\bar{\mathcal{L}}(F)$ the obtained polyedra:

$$\mathcal{L}(F) = \left\{(x,y) \;\middle|\; \begin{array}{l} u^T\widetilde{A}x + u^T\widetilde{B}y \le u^T\widetilde{b} \\ \text{for all } u \ge 0,\ u^T\widetilde{C} = 0 \end{array}\right\} \tag{11}$$

$$\bar{\mathcal{L}}(F) = \left\{(x,y) \;\middle|\; \begin{array}{l} u^T\overline{A}x + u^T\overline{B}y \le u^T\overline{b} \\ \text{for all } u \ge 0,\ u^T\overline{C} = 0 \end{array}\right\} \tag{12}$$

Note that by the above procedure we have

$$F_I \subseteq \bar{\mathcal{L}}(F) \subseteq \mathcal{L}(F) \subseteq F.$$

By applying the two L&P variations defined above to **SL** we obtain two hierarchies of polyhedra. To be consistent with our previous notations, we shall denote by $\mathbf{R}_2 = \overline{\mathbf{R}} = \mathbf{SL}$ the starting polyhedron, and define $\mathbf{R}_{k+1} = \mathcal{L}(\mathbf{R}_k)$, and $\overline{\mathbf{R}}_{k+1} = \bar{\mathcal{L}}(\overline{\mathbf{R}}_k)$ for $k = 2, 3, ...$ Then we have the following hierarchies:

$$\mathbf{SL} = \mathbf{R}_2 \supseteq \mathbf{R}_3 \supseteq \cdots \supseteq \mathbf{R}_n = \mathbf{BQ}. \tag{13}$$

$$\mathbf{SL} = \overline{\mathbf{R}}_2 \supseteq \overline{\mathbf{R}}_3 \supseteq \cdots \supseteq \overline{\mathbf{R}}_n = \mathbf{BQ}. \tag{14}$$

We remark that $\mathbf{R}_k \supseteq \bar{\mathbf{R}}_k$ holds for all $k = 2, 3, ..., n$.

Relations among the polyhedral hierarchies

In this section we will investigate the connections between the above defined polyhedral hierarchies. First of all we recall that any quadratic pseudo-Boolean function in k variables can be represented as a degree k posiform in the same set of k variables. It follows that $\mathcal{G}_k \supseteq \mathcal{F}_k$ for all $k = 2, \ldots, n$ and hence we have

$$\mathbf{Q}_k \subseteq \mathbf{P}_k \text{ for all } k = 2, \ldots, n.$$

Let us point out that, without giving detailed proof in this short version and describing only in loose terms the approach, viewing the inequalities for variables (x, y) as nonnegative quadratic pseudo-Boolean functions (or more specifically, as posiforms) the first two steps of L&P tells that we can view the inequalities defining $M(.)$ as inequalities in terms of some linearizations of cubic pseudo-Boolean functions. The last step then considers nonnegative linear combinations such that the cubic terms cancel out, and hence we obtain again a nonnegative quadratic function.

Our first claim, derived in a simple way along the above lines is as follows:

Theorem 2

$$\mathbf{Q}_k \subseteq \bar{\mathbf{R}}_k \subseteq \mathbf{R}_k$$

and

$$\mathbf{Q}_{k+1} \subseteq \bar{\mathcal{L}}(\mathbf{Q}_k) \subseteq \mathcal{L}(\mathbf{Q}_k)$$

for all $k = 2, 3, ..., n$.

Let us now compare the hierarchy based on k-variables functions with the one based on degree k posiforms. It is easy to see that

$$\mathbf{P}_2 = \mathbf{Q}_2 = \mathbf{SL}$$

and

$$\mathbf{P}_n = \mathbf{Q}_n = \mathbf{BQ}.$$

Furthermore, (Boros, Crama, and Hammer 1992) proved that

Theorem 3 *(Boros, Crama, and Hammer 1992) The set of posiform representations of extremal rays of $\mathcal{G}_2$ and $\mathcal{F}_2$ is $\{uv|u, v \in \mathbb{L}\}$. The set of posiform representations of extremal rays of $\mathcal{G}_3 \backslash \mathcal{G}_2$ is $\{uvw + \bar{u}\bar{v}\bar{w}|u, v, w \in \mathbb{L}\}$.*

From the above theorem it follows that any extremal ray of $\mathcal{G}_3$ is a function of at most 3 variables and then belongs also to $\mathcal{F}_3$. Hence

$$\mathbf{P}_3 = \mathbf{Q}_3. \tag{15}$$

By the above results one might conjecture that $\mathbf{Q}_k = \mathbf{P}_k$, for all $k = 2, \ldots, n$. However, this is not the case.

Theorem 4 *For all $n \geq 6$ there is a QPBF $f^0 \in (\mathcal{G}_4 \cap \mathcal{F}_6) \setminus \mathcal{F}_5$ implying that*

$$\mathbf{Q}_4 \subset \mathbf{P}_4$$

and there is a QPBF $f^1 \in (\mathcal{G}_5 \cap \mathcal{F}_6) \setminus \mathcal{F}_5$, implying that

$$\mathbf{Q}_5 \subset \mathbf{P}_5.$$

Proof. For instance the quadratic function

$$\begin{aligned} f^0(x) &= 2 + x_1 + x_2 - x_3 - x_4 - x_5 - 2x_6 \\ &\quad -x_1x_2 - x_1x_4 + x_1x_5 - x_2x_3 + x_2x_4 \\ &\quad -x_2x_5 + x_3x_5 + x_3x_6 + x_4x_6 + x_5x_6 \end{aligned}$$

is an extreme ray of $\mathcal{F}_6$, not belonging to $\mathcal{F}_5$ that can be represented by a posiform of degree 4

$$\begin{aligned} f^0(x) = \;& \overline{x}_3\overline{x}_5\overline{x}_6 + x_2x_4x_5x_6 + x_2\overline{x}_4\overline{x}_5\overline{x}_6 + x_2\overline{x}_3\overline{x}_6 \\ & +x_2\overline{x}_3\overline{x}_5x_6 + \overline{x}_2\overline{x}_4\overline{x}_6 + \overline{x}_2x_3x_5x_6 + x_1\overline{x}_4x_5 \\ & +x_1\overline{x}_2x_4x_5 + x_1\overline{x}_2\overline{x}_4 + \overline{x}_1x_2x_4\overline{x}_5. \end{aligned}$$

The following quadratic function

$$\begin{aligned} f^1(x) = \;& 6 - 3\sum_{i=1}^{5} x_i - 5x_6 \\ & + \sum_{i=1}^{4}\sum_{j=i+1}^{5} x_ix_j + 2\sum_{i=1}^{5} x_ix_6 \\ = \;& (\sum_{i=1}^{5} x_i + 2x_6 - 3)(\sum_{i=1}^{5} x_i + 2x_6 - 4)/2. \end{aligned}$$

is another extreme ray of $\mathcal{F}_6$ not belonging to $\mathcal{F}_5$, and it can be can be represented as a posiform of degree 5

$$\begin{aligned} f^1(x) = \;& x_3x_4x_5x_6 + \overline{x}_3\overline{x}_4\overline{x}_5\overline{x}_6 + x_2x_3x_5x_6 \\ & +x_2x_3x_4\overline{x}_5x_6 + \overline{x}_2\overline{x}_4\overline{x}_5\overline{x}_6 + \overline{x}_2\overline{x}_3\overline{x}_4x_5\overline{x}_6 \\ & +x_1x_4x_5x_6 + x_1x_3x_5x_6 + x_1x_3x_4\overline{x}_5x_6 \\ & +x_1x_2x_3x_6 + x_1x_2x_3x_4x_5 + x_1x_2\overline{x}_3x_5x_6 \\ & +x_1x_2\overline{x}_3x_4x_6 + x_1\overline{x}_2\overline{x}_3\overline{x}_5\overline{x}_6 + \overline{x}_1x_3\overline{x}_4\overline{x}_5\overline{x}_6 \\ & +\overline{x}_1\overline{x}_3\overline{x}_5\overline{x}_6 + \overline{x}_1x_2x_4x_5x_6 + \overline{x}_1x_2\overline{x}_3\overline{x}_4\overline{x}_6 \\ & +\overline{x}_1\overline{x}_2\overline{x}_5\overline{x}_6 + \overline{x}_1\overline{x}_2\overline{x}_4x_5\overline{x}_6 + \overline{x}_1\overline{x}_2\overline{x}_3\overline{x}_6 \\ & +\overline{x}_1\overline{x}_2\overline{x}_3\overline{x}_4\overline{x}_5. \end{aligned} \tag{16}$$

□

The following theorem is a consequence of Theorem 3.

Theorem 5 $\mathcal{L}(\mathbf{Q}_2) = \mathbf{Q}_3$. □

Since, as we have seen before, $\mathbf{Q}_{k+1} \subseteq \bar{\mathcal{L}}(\mathbf{Q}_k) \subseteq \mathcal{L}(\mathbf{Q}_k)$ for all $k = 2, \ldots, n-1$, by the above theorem we can state the following result.

Corollary 6 $\bar{\mathcal{L}}(\mathbf{Q}_2) = \mathbf{Q}_3$.

Lemma 7 *Let $g \in \mathcal{G}_4 \backslash \mathcal{G}_3$. There exists a posiform representation of g*

$$\phi = \phi^4 + \phi^3$$

where ϕ^4 contains the terms of degree 4 of ϕ and ϕ^3 is a degree 3 posiform and

$$\phi^4 = \sum_{(p,q) \in H} \gamma_{(p,q)}(p+q) \tag{17}$$

where H is a set of unordered pairs (p, q) of degree 4 terms such that q is obtained from p by negating three literals.

The above then will imply the equality:

Theorem 8 $\bar{\mathcal{L}}(\mathbf{Q}_3) = \mathbf{Q}_4$.

From the above Theorem and from the connections between $\mathbf{P_k}$ and $\mathbf{Q_k}$ found in the previous section, we obtain the following Corollary.

Corollary 9 $\bar{\mathcal{L}}(\mathbf{P}_3) \subset \mathbf{P}_4$.

Let us turn to relations between the degree k posiform hierarchy and the ones based on the L&P procedure. The following Lemma will be useful for obtaining results with the posiform based hierarchy.

Lemma 10 *The inequality $L_f(x, y) \geq 0$ is valid for $\bar{\mathcal{L}}(\mathbf{Q}_k)$ if and only if there exist $\lambda_i, \mu_i \geq 0$ and $g_i, h_i \in \mathcal{G}_k$, $i = 1, \ldots, n$, such that*

$$f(x) = \sum_{i=1}^{n} \lambda_i x_i g_i(x) + \sum_{i=1}^{n} \mu_i \overline{x}_i h_i(x).$$

□

Claim 11 *Suppose $n \geq 5$. The quadratic pseudo-Boolean functions of 5 variables*

$$f^2(x) = 1 - \sum_{i=1}^{5} x_i + \sum_{i=1}^{4}\sum_{i=j+1}^{5} x_ix_j$$

and

$$f^3(x) = 3 - 2\sum_{i=1}^{4} x_i - 3x_5 + \sum_{i=1}^{3}\sum_{i=j+1}^{4} x_ix_j + 2\sum_{i=1}^{4} x_ix_5$$

are extremal rays of $\mathcal{G}_5 \backslash \mathcal{G}_4$.

Theorem 12 *If $n \geq 6$ then $\bar{\mathcal{L}}(\mathbf{Q}_4) \supset \mathbf{Q}_5$.*

Proof. Let us consider the extreme ray of $\mathcal{F}_6$ introduced in the previous section:

$$f^1(x) = (\sum_{i=1}^{5} x_i + 2x_6 - 3)(\sum_{i=1}^{5} x_i + 2x_6 - 4)/2. \quad (18)$$

Our proof first argues that f^1 is in $\mathcal{G}_5$ but not in $\mathcal{G}_4$. Next we show that f^1 is not in $\bar{\mathcal{L}}(\mathbf{Q}_4)$. This is a long and technical argument using Claim 11 and Lemma 10. The above then will imply $\bar{\mathcal{L}}(\mathbf{Q}_4) \supset \mathbf{Q}_5$, as claimed. □

From the above result we can argue that

$$\mathbf{R}_5 \supseteq \bar{\mathbf{R}}_5 \supset \mathbf{Q}_5.$$

By Corollary 9 we already know that $\bar{\mathcal{L}}(\mathbf{P}_3) \subset \mathbf{P}_4$. We will see now, by an example, that also $\mathcal{L}(\mathbf{P}_3) \subset \mathbf{P}_4$.

Suppose $n = 5$ and apply Lift&Project to $\mathbf{P}_3$ by summing the following lifted inequalities.

$$\begin{array}{rl}
(1-x_1)(1-x_2-x_5+y_{25}) & \geq 0 \\
(1-x_1)(1-x_3-x_5+y_{35}) & \geq 0 \\
x_1(1-x_2-x_3-x_5+y_{23}+y_{25}+y_{35}) & \geq 0 \\
x_1(y_{24}) & \geq 0 \\
x_1(y_{34}) & \geq 0 \\
(1-x_1)(1-x_2-x_3-x_4+y_{23}+y_{24}+y_{34}) & \geq 0.
\end{array} \quad (19)$$

By substituting the non linear terms as in (7) and taking into account Lemma 1, we obtain the inequality

$$3 - 2x_1 - 2x_2 - 2x_3 - x_4 - 2x_5 + y_{12} + y_{13} + y_{14} + y_{15} + y_{23} + y_{24} + y_{25} + y_{34} + y_{35} \geq 0$$

which cuts off the following vertex of $\mathbf{P}_4$[1].

$$\begin{array}{l}
x_1 = x_2 = x_3 = 0.5, x_4 = 0.25, x_5 = 0.75, \\
y_{12} = y_{13} = y_{15} = y_{23} = y_{25} = y_{35} = y_{45} = 0.25, \\
y_{14} = y_{24} = y_{25} = y_{34} = 0.
\end{array} \quad (20)$$

Hence we can conclude that, for $n \geq 5$, $\mathcal{L}(\mathbf{P}_3) \subset \mathbf{P}_4$ and $\mathbf{R}_4 \subset \mathbf{P}_4$.

Summarizing the obtained results we have:

$$\begin{array}{lllllll}
\mathbf{P}_2 & = & \mathbf{Q}_2 & & & & \\
\mathbf{P}_3 & = & \mathcal{L}(\mathbf{Q}_2) & = & \bar{\mathcal{L}}(\mathbf{Q}_2) & = & \mathbf{Q}_3 \\
\mathbf{P}_4 & \supset & \mathcal{L}(\mathbf{Q}_3) & \supseteq & \bar{\mathcal{L}}(\mathbf{Q}_3) & = & \mathbf{Q}_4 \\
\mathbf{P}_5 & \supset & \mathbf{Q}_5 & & \bar{\mathcal{L}}(\mathbf{Q}_4) & \supset & \mathbf{Q}_5
\end{array}$$

and, for all $k = 3, \ldots, n$,

$$\mathbf{P}_k \supseteq \mathbf{R}_k \supseteq \bar{\mathbf{R}}_k \supseteq \bar{\mathcal{L}}(\mathbf{Q}_{k-1}) \supseteq \mathbf{Q}_k.$$

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[1]We obtained this vertex by computer.