Upper-Bounds for Quadratic $0-1$ Maximization[1]

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Abstract

In this paper, we generalize three different approaches to obtain upper bounds for the maximum of a quadratic pseudo-Boolean function f over $\{0,1\}^n$. The original approaches (complementation, majorization and linearization) were introduced by Hammer, Hansen and Simeone [9].

Our generalization yields three upper bounds, C_k, M_k and L_k for each integer $k \geq 2$, where $C_n = L_n = M_n$ is the maximum of f, and $C_2 = L_2 = M_2$ is the roof duality bound studied in [9]. We prove here that $C_k = M_k = L_k$ for all values of k.

1 Introduction

A *pseudo-Boolean function* is a real-valued function defined on $\{0,1\}^n$. Such a function is called *quadratic* if its unique expression as a multilinear polynomial in its variables has degree at most 2. The quadratic $0-1$ maximization problem is to find the maximum over $\{0,1\}^n$ of a quadratic pseudo-Boolean function, given in polynomial form.

In [9] three possible approaches were considered to obtain good upper-bounds on the optimal value of quadratic $0-1$ maximization problems: complementation, majorization and linearization (see below). It has been shown there that these apparently distinct approaches yield in fact the same bound.

In this paper, we propose some natural extensions of these approaches, and we study their mutual relationships. More precisely, for every $k \geq 2$, we define three upper-bounds C_k, M_k and L_k on the maximum of a quadratic pseudo-Boolean function, such that $C_{k+1} \leq C_k$, $M_{k+1} \leq M_k$ and $L_{k+1} \leq L_k$. When $k = 2$, these bounds are exactly those obtained by complementation, majorization and linearization in [9]. When $k = n$, the bounds coincide with the optimal value of f. Our main result is that $C_k = M_k = L_k$ for all $k \geq 2$.

All these bounds can, in principle, be obtained by solving some linear programming problems, but writing these LPs can be prohibitively expensive for large values of k. The original $0-1$ quadratic maximization problem itself can be written as a $0-1$ linear programming problem, over the "Boolean quadric polytope", i.e., over the convex hull of

$$\left\{ (x,y) \;\middle|\; \begin{array}{cc} y_{ij} = x_i x_j & 1 \leq i < j \leq n \\ x_i = 0 \text{ or } 1 & i = 1,...,n \end{array} \right\},$$

the usual continuous relaxation of which gives the value L_2. We present a correspondence between the facets of this polytope and the extremal elements of the cone of the nonnegative pseudo-Boolean functions.

In a companion paper [4], we study in more detail the bound obtained for $k = 3$. We show there that the LP defining L_3 is produced by adding all first order Chvátal cuts to the LP obtained when $k = 2$. It follows from this result that $C_3 = M_3 = L_3 < C_2 = M_2 = L_2$ whenever $\max_{x\in\{0,1\}^n} f(x) < C_2$.

2 Complementation

Let $V = \{x_1, x_2, ..., x_n\}$ denote a set of $0-1$ variables, and $\overline{V} = \{\overline{x}_1, \overline{x}_2, ..., \overline{x}_n\}$, where $\overline{x}_i = 1 - x_i$ is the *complement* of x_i $(i = 1, ..., n)$. The elements of $L = V \cup \overline{V}$ are called *literals.* A *posiform* is an expression of the form

$$\phi(x_1, ..., x_n, \overline{x}_1, ..., \overline{x}_n) = \sum_{T \in \Omega} a_T \prod_{u \in T} u, \tag{2.1}$$

where Ω is a collection of subsets of L, and $a_T > 0$ for all $T \in \Omega$. The *degree* of the posiform (2.1) is the maximum size of a set $T \in \Omega$.

Every posiform ϕ defines a unique pseudo-Boolean function, f, through the natural correspondence:

$$f(x_1, ..., x_n) = \phi(x_1, ..., x_n, \overline{x}_1, ..., \overline{x}_n) \quad \text{for all} \quad (x_1, ..., x_n) \in \{0, 1\}^n. \tag{2.2}$$

When (2.2) holds, ϕ is said to be a posiform of f. Observe that a nonnegative pseudo-Boolean function may have many distinct posiforms. A pseudo-Boolean function always has a unique polynomial form

$$f(x_1, ..., x_n) = \sum_{T \in \Lambda} q_T \prod_{x \in T} x, \tag{2.3}$$

where Λ is now a collection of subsets of V, and $q_T \neq 0$ for $T \in \Lambda$. The function f is *quadratic* if the maximum size of a set $T \in \Lambda$ is 2.

The quadratic pseudo-Boolean functions of n variables form a vector space (of dimension $1+n+\binom{n}{2}$) over the reals. For any fixed k-element subset $W \subset V$ of the variables, the set of quadratic pseudo-Boolean functions of these variables form a subspace (of dimension $1+k+\binom{k}{2}$). For $2 \leq k \leq n$, let $\mathcal{F}_k$ denote the union of these subspaces for all k element subsets of V, i.e., $\mathcal{F}_k$ is the set (and not a subspace, in general) of quadratic pseudo-Boolean functions whose polynomial expression (2.3) involves at most k variables out of $x_1, ..., x_n$. Let $\mathcal{P}_k$ be the cone generated by the nonnegative functions of $\mathcal{F}_k$. Then, $\mathcal{P}_2$ is the set of posiforms of degree two (*quadratic posiforms*), $\mathcal{P}_2 \subseteq \mathcal{P}_3 \subseteq \cdots \subseteq \mathcal{P}_n$, and $\mathcal{P}_n$ is the set of all nonnegative, quadratic pseudo-Boolean functions in n variables.

Now, let f be a (fixed) quadratic pseudo-Boolean function, and c be a real constant. Then, c is an upper bound on the maximum of f over $\{0, 1\}^n$ if and only if $\phi = c - f$ is a nonnegative pseudo-Boolean function, i.e. $\phi \in \mathcal{P}_n$. More generally, for every $k \geq 2$, we define

$$C_k \stackrel{\text{def}}{=} \min\{c \in \mathbf{R} | f + \phi = c, \quad \phi \in \mathcal{P}_k\}. \tag{2.4}$$

Then we have,

$$\max\{f(x) | x \in \{0, 1\}^n\} = C_n \leq C_{n-1} \leq \cdots \leq C_3 \leq C_2.$$

In [9], C_2 is called the *height* of f.

Example 2.1 *Consider the following quadratic pseudo-Boolean function:*

$$\begin{aligned} f(x) = \quad & -3x_1 - x_3 - 5x_4 + 3x_1x_2 - 5x_1x_3 + 5x_1x_4 + \\ & +3x_1x_5 + x_2x_3 - 3x_2x_5 + 5x_3x_4. \end{aligned}$$

Here we have,

$$\begin{aligned} C_2 = 4 = \quad & f + 3x_1\overline{x}_2 + x_1x_3 + 4\overline{x}_1\overline{x}_3 + x_1\overline{x}_4 + 4\overline{x}_1x_4 \\ & +3x_1\overline{x}_5 + \overline{x}_2x_3 + 3x_2x_5 + 4x_3\overline{x}_4 + \overline{x}_3x_4, \end{aligned}$$

and

$$C_3 = 0 = \quad f + \overline{x}_2x_3 + 3(x_1\overline{x}_2\overline{x}_5 + \overline{x}_1x_2x_5) + 5(x_1x_3\overline{x}_4 + \overline{x}_1\overline{x}_3x_4),$$

and, since $f(0) = 0$*,* $\max f = 0$ *is already implied. Here we used that*

$$\begin{aligned} x_1\overline{x}_2\overline{x}_5 + \overline{x}_1x_2x_5 \quad &= x_1 - x_1x_2 - x_1x_5 + x_2x_5, \quad \text{and} \\ x_1x_3\overline{x}_4 + \overline{x}_1\overline{x}_3x_4 \quad &= x_4 + x_1x_3 - x_1x_4 - x_3x_4, \end{aligned}$$

thus both expressions are in $\mathcal{P}_3 \subset \mathcal{F}_3$*.*

To see that C_k can be expressed as the optimum of a linear programming problem, notice again that $\mathcal{P}_k$ is a cone in the vector space of all quadratic pseudo-Boolean functions. Since the nonnegative elements of $\mathcal{F}_k$ are characterized by a finite ($\binom{n}{k}2^k$) system of linear inequalities, to be satisfied by the coefficients of their polynomial expression, it follows that $\mathcal{F}_k$ has a finite set of extremal directions, consequently $\mathcal{P}_k$ has a finite basis, say $\mathcal{B}(\mathcal{P}_k) = \{\psi_1, ..., \psi_m\}$, such that every $\phi \in \mathcal{P}_k$ can be expressed as $\phi = \sum_{i=1}^m \lambda_i\psi_i$ for some reals $\lambda_i \geq 0$ $(i = 1, ..., m)$, and every basis element $b \in \mathcal{B}(\mathcal{P}_k)$ is a function of at most k variables. So, C_k can be expressed as

$$C_k = \min \quad c \tag{2.5}$$

$$\text{s.t.} \quad c - \sum_{\psi \in \mathcal{B}(\mathcal{P}_k)} \lambda_\psi \psi \quad \equiv f \tag{2.6}$$

$$\lambda_\psi \quad \geq 0 \quad \psi \in \mathcal{B}(\mathcal{P}_k). \tag{2.7}$$

Since the multilinear polynomial expression of a pseudo-Boolean function is unique, the identity (2.6) can in turn be rewritten as a set of linear equations in the variables c, λ_ψ, $(\psi \in \mathcal{B}(\mathcal{P}_k))$, where each equation expresses the equality of a coefficient of f with the corresponding coefficient of $c - \sum_{\psi \in \mathcal{B}(\mathcal{P}_k)} \lambda_\psi \psi$.

For each fixed k, this transformation can in principle be used to turn (2.5)–(2.7) into a linear programming problem with $O(n^k)$ variables and $O(n^2)$ constraints. When $k = 2$, the resulting LP is given by [9]. For $k = 3$, it is explicitly described in [4].

Finally, the following result provides an alternative characterization of the bound C_k:

Lemma 2.1 *For $2 \le k \le n$,*

$$C_k = \min_{\substack{\phi \in \mathcal{P}_k \\ f + \phi = l \text{ is linear}}} \max_{x \in \{0,1\}^n} l(x). \tag{2.8}$$

Proof. Since a constant c is itself a linear function, the minimum value in the lemma is not larger then C_k. To show the equality, assume that l and ϕ achieve the minimum in the right-hand side of (2.8). Let $l(x) = l_0 + \sum_{i=1}^n l_i x_i$. Then $\max_{x \in \{0,1\}^n} l(x) = l_0 + \sum_{l_i > 0} l_i$. On the other hand, defining $\psi = \phi + \sum_{l_i>0} l_i \overline{x}_i + \sum_{l_i<0}(-l_i)x_i$, we have $f + \psi = l_0 + \sum_{l_i>0} l_i$. Here $\psi \in \mathcal{P}_k$, thus $C_k \le l_0 + \sum_{l_i>0} l_i$ by the definition of C_k.

□

3 Majorization

In this section, we introduce a class of linear functions, all majorizing the quadratic pseudo-Boolean function f over $\{0,1\}^n$, and we obtain an upper bound of f by finding the "best" among these linear functions. A similar approach was already taken in [9] and, for the constrained case, in [2, 3].

For a *purely quadratic* function h (i.e. for which $h(0,...,0) = h(1,0,...,0) = \cdots = h(0,...,0,1) = 0$) of k variables, let

$$\mathcal{M}(h) \stackrel{\text{def}}{=} \{l | l \text{ linear};\ h(x) \le l(x) \text{ for all } x \in \{0,1\}^k\} \tag{3.1}$$

denote the set of linear majorants of h over the Boolean vectors.

Now let f be a quadratic pseudo-Boolean function, k be a (possibly small) integer, and let us consider a representation of f in the form

$$f = l + \sum_{j \in J} f_j, \tag{3.2}$$

where l is linear, and $f_j \in \mathcal{F}_k$ are purely quadratic functions of at most k variables. Then the linear functions of the form

$$p = l + \sum_{j \in J} l_j, \tag{3.3}$$

with $l_j \in \mathcal{M}(f_j)$ for $j \in J$, are linear majorants of f. Let $\mathcal{M}^k(f)$ denote the set of all linear majorants of f obtained in this way, varying (3.2) over all possible representations. Then, by definition,

$$\mathcal{M}(f) = \mathcal{M}^n(f) \supseteq \mathcal{M}^{n-1}(f) \supseteq \cdots \supseteq \mathcal{M}^3(f) \supseteq \mathcal{M}^2(f).$$

Defining

$$M_k \stackrel{\text{def}}{=} \min_{p \in \mathcal{M}^k(f)} \max_{x \in \{0,1\}^n} p(x), \tag{3.4}$$

we have

$$\max_{x \in \{0,1\}^n} f(x) = M_n \leq M_{n-1} \leq \cdots \leq M_3 \leq M_2.$$

The elements of $\mathcal{M}^2(f)$ were called paved upper planes in [9]. It was also shown there that the bound R_2, obtained by taking the minimum in (3.4) over certain "minimal" elements $p(x)$ of $\mathcal{M}^2(f)$, rather than over all of $\mathcal{M}^2(f)$, is always equal to C_2. As a consequence, $M_2 \leq C_2$. Later, in [12] it has been proved that $C_2 = M_2$ (see also [11, 1, 6]). Here we extend these results, and show that

Theorem 3.1 *$C_k = M_k$ for $2 \leq k \leq n$.*

For the proof of this theorem, we need first an easy observation.

For a quadratic pseudo-Boolean function f, let l_f and q_f be the linear and the purely quadratic functions, respectively, defined (uniquely) by the equation $f = l_f - q_f$.

Remark 3.2 *For any quadratic pseudo-Boolean function f, $l_f \in \mathcal{M}(q_f)$ if and only if f is nonnegative.*

Proof of Theorem 3.1. Let us use Lemma 2.1, and let ϕ denote an optimal complement of f, i.e., $\phi \in \mathcal{P}_k$, $l = f + \phi$ is linear and $\max_{x \in \{0,1\}^n} l(x) = C_k$. Since $\mathcal{P}_k$ is generated by $\mathcal{B}(\mathcal{P}_k)$, we can write

$$\phi = \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b b, \quad \alpha_b \geq 0,\ b \in \mathcal{B}(\mathcal{P}_k).$$

Thus we have

$$\begin{aligned} f &= l - \phi = l - \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b (l_b - q_b) = \\ &= (l - \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b l_b) + \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b q_b, \end{aligned}$$

where $l_b \in \mathcal{M}(q_b)$ by Remark 3.2. Since $\mathcal{B}(\mathcal{P}_k)$ contains nonnegative subfunctions of at most k variables, $l = (l - \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b l_b) + \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b l_b$ belongs to $\mathcal{M}^k(f)$, implying $M_k \le C_k$.

Conversely, let $p = l + \sum l_i$ be an optimal linear function for the majorization problem, i.e., $f = l + \sum q_i$, $l_i \in \mathcal{M}(q_i)$, and $M_k = \max_{x \in \{0,1\}^n} p(x)$. Then $l_i - q_i$ are nonnegative functions, belonging to $\mathcal{P}_k$, by Remark 3.2; thus, with $\phi \stackrel{\text{def}}{=} \sum (l_i - q_i)$, we get $\phi \in \mathcal{P}_k$ and $l = f + \phi$ is linear. Together with Lemma 2.1, this implies that $C_k \le M_k$.

□

As a corollary of this theorem, we can obtain a computationally simpler form of Problem (3.4).

Using again the notation $b = l_b - q_b$ for $b \in \mathcal{B}(\mathcal{P}_k)$, where l_b denotes the linear part of b, and q_b is purely quadratic, we get

$$M_k = \min_{\substack{l \text{ is linear}, \ \alpha_b \ge 0 \\ f = l + \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b q_b}} \ \max_{x \in \{0,1\}^n} \left[l + \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b l_b \right]. \tag{3.5}$$

4 Linearization

A standard technique to linearize the quadratic $0-1$ maximization problem is as follows (see the survey [10]).

Let us introduce new variables y_{ij} and impose the identities $y_{ij} = x_i x_j$, for $1 \le i < j \le n$. This can be done by prescribing the conditions

$$\begin{array}{rrrcr} & & y_{ij} & \ge & 0 \\ x_i & & -y_{ij} & \ge & 0 \\ & x_j & -y_{ij} & \ge & 0 \\ -x_i & -x_j & +y_{ij} & \ge & -1 \end{array} \quad 1 \le i < j \le n, \tag{4.1}$$

$$x_i \in \{0,1\}, \quad i = 1, ..., n. \tag{4.2}$$

In this way, we have a natural one-to-one correspondence between the quadratic pseudo-Boolean functions over $\{0,1\}^n$

$$f(x) \stackrel{\text{def}}{=} q_0 + \sum_{i=1}^{n} q_i x_i + \sum_{1 \le i < j \le n} q_{ij} x_i x_j$$

and the linear functions over $\mathbf{R}^{n+\binom{n}{2}}$, given by:

$$\mathbf{L}_f(x,y) \stackrel{\text{def}}{=} q_0 + \sum_{i=1}^{n} q_i x_i + \sum_{1 \le i < j \le n} q_{ij} y_{ij},$$

where (x,y) denotes the vector $(x_1, ..., x_n, y_{12}, ..., y_{n-1,n}) \in \mathbf{R}^{n+\binom{n}{2}}$.

The maximization of $f(x)$ over $\{0,1\}^n$ can be reformulated as a linear programming problem

$$\max \mathbf{L}_f(x,y) \quad \text{s.t.} \quad (x,y) \in \mathbf{QP}, \tag{4.3}$$

where $\mathbf{QP}$ denotes the Boolean Quadric polytope, introduced in [13], as the convex hull of the points $(x,y) \in \mathbf{R}^{n+\binom{n}{2}}$ satisfying (4.1) – (4.2). Equivalently,

$$\mathbf{QP} \stackrel{\text{def}}{=} \text{conv} \left\{ (x,y) \,\middle|\, \begin{array}{c} y_{ij} = x_i x_j \ 1 \le i < j \le n; \\ x_i \in \{0,1\}, \ i = 1, ..., n \end{array} \right\}. \tag{4.4}$$

Omitting the integrality constraints (4.2), introducing the polyhedron $\mathbf{SL}$ as the set of vectors satisfying (4.1), and defining

$$L_2 \stackrel{\text{def}}{=} \max \mathbf{L}_f(x,y) \quad \text{s.t.} \quad (x,y) \in \mathbf{SL}, \tag{4.5}$$

we get the *standard linearization* of the maximization problem for f. Clearly, $\mathbf{QP} \subseteq \mathbf{SL}$, hence L_2 is an upper bound on the maximum of f over $\{0,1\}^n$. This bound was introduced in [9], where it was shown that $C_2 = L_2$.

We shall describe here a hierarchical way of adding new constraints to $\mathbf{SL}$, and thus, improving L_2.

We say that a linear function

$$l(x,y) = l_0 + \sum_{i=1}^{n} l_i x_i + \sum_{1 \le i < j \le n} l_{ij} y_{ij}$$

induces a valid inequality for $\mathbf{QP}$ if

$$\forall (x,y) \in \mathbf{QP} : \quad l(x,y) \ge 0.$$

The following observation is immediate, using the bijection $f \leftrightarrow \mathbf{L}_f$.

Remark 4.1 *A quadratic function f is nonnegative, (i.e., $f \in \mathcal{P}_n$)if and only if $\mathbf{L}_f$ induces a valid inequality for* **QP**. *Moreover, $f \in \mathcal{B}(\mathcal{P}_n)$ if and only if $\mathbf{L}_f$ induces a facet for* **QP**.

Let us define the polyhedron $\mathbf{SL}^{[k]}$ as the set of vectors (x, y) satisfying the conditions

$$\mathbf{L}_g(x, y) \geq 0 \quad \forall\, g \in \mathcal{B}(\mathcal{P}_k), \tag{4.6}$$

and let

$$L_k \stackrel{\text{def}}{=} \max \mathbf{L}_f(x, y) \quad \text{s.t.} \quad (x, y) \in \mathbf{SL}^{[k]}, \tag{4.7}$$

for $k = 2, ..., n$. Obviously, $\mathbf{SL} \equiv \mathbf{SL}^{[2]}$, $\mathbf{SL}^{[n]} \equiv \mathbf{QP}$ and $L_{k+1} \leq L_k$, $k = 2, ..., n-1$.

Theorem 4.2 *$L_k = C_k$ for $2 \leq k \leq n$.*

Proof. If $f + \phi = C_k$ for some $\phi \in \mathcal{P}_k$, then there are nonnegative reals α_b such that $\phi = \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b b$. Therefore $\mathbf{L}_{C_k - f} = \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \alpha_b \mathbf{L}_b$, and hence $C_k \geq \mathbf{L}_f$ is a linear consequence of (4.6), implying $L_k \leq C_k$.

Conversely, since the system of inequalities in (4.6) has full rank ($\mathcal{B}(\mathcal{P}_2) \subset \mathcal{B}(\mathcal{P}_k)$ for any $k \geq 2$, and $\mathcal{B}(\mathcal{P}_2)$ clearly has full rank), the inequality $L_k \geq \mathbf{L}_f$ is a linear consequence of (4.6) by linear programming duality. That means, there are nonnegative reals β_b such that $L_k - \mathbf{L}_f = \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \beta_b \mathbf{L}_b$. Therefore $L_k = f + \sum_{b \in \mathcal{B}(\mathcal{P}_k)} \beta_b b$ implying $C_k \leq L_k$.

□

In [7, 13] some classes of facets of **QP** have been described. We shall give a unified description of those using the above relation between facets of **QP** and extremal elements of $\mathcal{P}_n$.

Let $U \subset L$ be an arbitrary subset of literals, and let α be an arbitrary integer. The function, $b_{U,\alpha}$ defined by

$$b_{U,\alpha} = \binom{\sum_{u \in U} u - \alpha}{2}$$

is clearly a nonnegative quadratic pseudo-Boolean function. ($\binom{a}{2} = \frac{a(a-1)}{2}$, hence $\binom{a}{2} > 0$ for any integer a, except for $a = 0$ or $a = 1$, when it is 0.) It is also clear that if $\overline{U} = \{\overline{u}\,|u \in U\}$, then $b_{U,\alpha} \equiv b_{\overline{U},|U|-\alpha-1}$.

Example 4.1 *Using the fact that for* $0-1$ *variables* $x^2 = x$ *we can obtain a simple form of such a function, e.g., if* $U = \{x, \overline{y}\}$ *and* $\alpha = 1$, *then*

$$\begin{aligned} b_{\{x,\overline{y}\},1} &= \tfrac{(x+\overline{y}-1)(x+\overline{y}-2)}{2} \\ &= \tfrac{x^2+\overline{y}^2+2x\overline{y}-3(x+\overline{y})+2}{2} \\ &= x\overline{y} - x - \overline{y} + 1 \\ &= \overline{x}\, y. \end{aligned}$$

Remark 4.3 *If* $U \subset L$ *is a subset of the literals, not containing a complemented pair,* α *is an integer,* $1 \le \alpha \le |U| - 2$ *for* $|U| \ge 3$ *or* $\alpha = 1$ *for* $|U| = 2$, *then* $b_{U,\alpha} \in \mathcal{B}(\mathcal{P}_k)$ *for* $k \ge |U|$.

This remark is easy to check, and also is a consequence of [13]. These functions provide a simpler description of the facet classes of **QP** described in [13].

5 Sharpness of the bounds

For a given quadratic pseudo-Boolean function $f(x)$, the bounds C_k ($k = 2, ..., n$) approach the maximum of $f(x)$ when k approaches n. Moreover, for every fixed k, C_k can (in principle) be computed in polynomial time, as the optimum of some associated linear programming problem. But clearly, the computational burden of computing C_k grows exponentially with k.

These observations raise the problem of finding a reasonable stopping point in the computation of the sequence C_2, C_3, ..., C_n. More specifically, one would like to be able to answer questions like: (i) is C_k *sharp*, i.e., is $C_k = \max_{x \in \{0,1\}^n} f(x)$? (ii) if not, does C_{k+1} improve on C_k?

For $k = 2$, these two questions were previously answered as follows. The paper [9] presented an $O(n^2)$ algorithm to decide the sharpness of C_2. In case C_2 is not sharp, [5] showed how to compute efficiently another bound U on the maximum of $f(x)$ such that $U < C_2$. It is very easy to see from their result that $C_3 \le U$ (but one may have $C_3 < U$). In [4], we give a direct proof that $C_3 < C_2$ when C_2 is not sharp.

Thus, we may say that C_3 is "worth" computing if C_2 is not sharp.

By contrast, [5] showed that checking the sharpness of U is an NP-complete problem. A similar proof shows that deciding the sharpness of C_3 is also NP-complete. For the sake of completeness, we repeat here the argument:

Theorem 5.1 *Deciding whether* $C_3 = \max_{x\in\{0,1\}^n} f(x)$ *is NP-complete.*

Proof. The problem is clearly in NP. Consider now the NP-complete problem NOT-ALL-EQUAL 3SAT (see [8]), defined by:
INSTANCE: set V of variables, collection of clauses $E_1, ..., E_m$, $E_i \subseteq V \cup \overline{V}$, $|E_i| = 3$ $(i = 1, ..., m)$.
QUESTION: is there a truth assignment such that each clause E_i has at least one true literal and at least one false literal?

Given an instance I of NOT-ALL-EQUAL 3SAT, we define the quadratic pseudo-Boolean function:

$$f(x) = -\sum_{i=1}^{m}\left(\prod_{u\in E_i} u + \prod_{u\in E_i} \overline{u}\right).$$

It is easy to see that I is a yes-instance if and only if $\max_{x\in\{0,1\}^n} f(x) = 0$. Moreover, since $\phi(x) = -f(x)$ is a cubic posiform, and $f(x) + \phi(x) = 0$, we have $C_3 \leq 0$.

Now, if $C_3 < 0$, then I is a no-instance. If $C_3 = 0$, then we have transformed the problem of deciding whether I is a yes-instance to the problem of deciding whether C_3 is sharp.

□

From Theorem 5.1, and from the fact that computing C_4 is polynomial, we conclude that there must exist quadratic pseudo-Boolean functions f for which $\max f < C_3 = C_4$ (unless P=NP). For such functions, computing C_4 would prove a wasted effort.

More properties of the bound C_3 are studied in the companion paper [4].

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