

Compact quadratizations for pseudo-Boolean functions

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Abstract The problem of minimizing a pseudo-Boolean function, that is, a real-valued function of 0-1 variables, arises in many applications. A quadratization is a reformulation of this nonlinear problem into a quadratic one, obtained by introducing a set of auxiliary binary variables. A desirable property for a quadratization is to introduce a small number of auxiliary variables. We present upper and lower bounds on the number of auxiliary variables required to define a quadratization for several classes of specially structured functions, such as functions with many zeros, symmetric, exact k-out-of-n, at least k-out-of-n and parity functions, and monomials with a positive coefficient, also called positive monomials. Most of these bounds are logarithmic in the number of original variables, and we prove that they are best possible for several of the classes under consideration. For positive monomials and for some other symmetric functions, a logarithmic bound represents a significant improvement with respect to the best bounds previously published, which are linear in the number of original variables. Moreover, the case of positive monomials is particularly interesting: indeed, when a pseudo-Boolean function is represented by its unique multilinear polynomial expression, a quadratization can be obtained by separately quadratizing its monomials.

Keywords nonlinear binary optimization · quadratic binary optimization · pseudo-Boolean functions · reformulation methods

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1 Introduction.

A pseudo-Boolean function is a mapping $f : \{0, 1\}^n \rightarrow \mathbb{R}$ that assigns a real value to each tuple of n binary variables (x_1, \dots, x_n) . Pseudo-Boolean functions have been extensively used and studied during the last century and especially in the last 50 years, given that they model problems in a wide range of areas such as reliability theory, computer science, statistics, economics, finance, operations research, management science, discrete mathematics, or computer vision (see [5, 7] for applications and references). In most of these applications the function f has to be optimized, therefore we are interested in the problem

$$\min_{x \in \{0, 1\}^n} f(x), \quad (1)$$

which is NP-hard even when f is expressed as a quadratic polynomial.

Several techniques have been proposed to solve problem (1), such as enumerative methods, algebraic methods, linear reformulations and quadratic reformulations, which are then solved using a linear or quadratic solver, respectively (see the books and surveys [5–8, 11–13]). It is not clear whether one of the previous techniques is generally better than the others. In fact, the performance of the different approaches seems to depend on the underlying structure of the problem, among other factors.

In this paper, we focus on *quadratizations*, that is, quadratic reformulations of problem (1). Interestingly, much progress in the understanding of quadratizations has been made in the field of computer vision, where this type of technique performs especially well for problems such as image restoration. A systematic study of quadratizations and of their properties has been initiated in Anthony et al. [3], where a quadratization is formally defined as follows.

Definition 1 Given a pseudo-Boolean function $f(x)$ on $\{0, 1\}^n$, we say that $g(x, y)$ is a *quadratization* of f if $g(x, y)$ is a quadratic polynomial depending on x and on m *auxiliary variables* y_1, \dots, y_m , such that

$$f(x) = \min_{y \in \{0, 1\}^m} g(x, y) \quad \text{for all } x \in \{0, 1\}^n. \quad (2)$$

It is known that every pseudo-Boolean function f admits a quadratization [19], and that various quadratizations can actually be computed in polynomial time. Moreover, it is clear that given a pseudo-Boolean function f and a quadratization g , minimizing f over $x \in \{0, 1\}^n$ is equivalent to minimizing g over $(x, y) \in \{0, 1\}^{n+m}$. Therefore, when a quadratization of f is available, the pseudo-Boolean minimization problem (1) can be reformulated as a quadratic one. Of course, the problem of optimizing the quadratic reformulation is still NP-hard, and under the hypothesis that $P \neq NP$, one cannot hope for much better. Rather, the quadratization approach attempts to draw benefit from numerous recent advances in the resolution of unconstrained quadratic optimization problems, both in theoretical and computational aspects (just as classical linearization techniques attempt to reduce the nonlinear problem (1) to an NP-hard, but much better understood, linear programming problem in

binary variables). Resolution techniques based on quadratizations have proven to be especially useful to solve very large-scale problems in the field of computer vision, such as image restoration or segmentation.

However, not all quadratizations perform equally well when solving the resulting quadratic problem. A desirable property of a quadratization is to have a small set of auxiliary variables, so that the size of the reformulation does not increase too much with respect to the size of the original problem (although one should keep in mind that there may be other criteria to define “good quadratizations”, such as providing tight relaxation bounds, preserving structural properties of the original function, and so forth). In this paper we focus on defining compact quadratizations, i.e., quadratizations that require a smallest possible number of auxiliary variables for some specific classes of functions.

Anthony et al. [3] established tight upper and lower bounds on the number of variables that a quadratization requires, independently of the procedure used to define the quadratization. More precisely, Anthony et al. prove that there exist pseudo-Boolean functions of n variables for which every quadratization must involve at least $\Omega(2^{\frac{n}{2}})$ auxiliary variables. They give a matching upper bound by proving that every pseudo-Boolean function of n variables has a quadratization involving at most $O(2^{\frac{n}{2}})$ variables. Furthermore, when considering functions of fixed degree d , similar results are established in [3], with a lower bound of $\Omega(n^{\frac{d}{2}})$ variables and an upper bound of $O(n^{\frac{d}{2}})$ variables. The same authors provided in [2] several upper and lower bounds concerning some of the classes of functions that we consider here. The precise bounds are given in Section 2.

Given a pseudo-Boolean function f , there are many different methods to construct a quadratization. In particular, *termwise quadratizations* have attracted much interest in the literature. This type of procedure assumes that a pseudo-Boolean function f is represented by its unique multilinear polynomial expression. This assumption relies in turn on the well-known fact that a pseudo-Boolean function f can be represented uniquely as a multilinear polynomial of the form

$$f(x_1, \dots, x_n) = \sum_{S \in 2^{[n]}} a_S \prod_{i \in S} x_i, \quad (3)$$

where $2^{[n]}$ is the set of subsets of $\{1, \dots, n\}$ (see [10, 11]). We denote by $\deg(f)$ the degree of the polynomial representation of f . Observe that if $g_S(x, y_S)$ is a quadratization of the monomial $a_S \prod_{i \in S} x_i$, where the vectors of auxiliary variables y_S are distinct for all monomials, then $g(x, y) = \sum_{S \in 2^{[n]}} g_S(x, y_S)$ is a quadratization of f . In order to construct small termwise quadratizations in this manner, it is necessary to understand quadratizations of positive monomials ($a_S > 0$) and of negative monomials ($a_S < 0$).

The case of negative monomials, or monomials with a negative coefficient, is well understood. A simple expression to quadratize cubic negative monomials was introduced by Kolmogorov and Zabih [16]. This expression was later

extended to higher degrees by Freedman and Drineas [9], who observed that a quadratization for the degree- n negative monomial $N_n(x) = -\prod_{i=1}^n x_i$ is derived from the identity

$$N_n(x) = \min_{y \in \{0,1\}} (n-1)y - \sum_{i=1}^n x_i y. \quad (4)$$

This quadratization uses a single auxiliary variable, which is the best that one can expect for $n \geq 3$.

Surprisingly, the case of monomials with a positive coefficient is much less understood. Rosenberg [19] provided a quadratization procedure which can be applied to any pseudo-Boolean function (given in polynomial form), and which consists in recursively selecting a product of two variables $x_i x_j$ and substituting this product by a new variable y_{ij} . The fact that y_{ij} should be equal to the product $x_i x_j$ is imposed by adding a quadratic penalty term to the function. Defining a quadratization for the degree- n positive monomial $P_n(x) = \prod_{i=1}^n x_i$ using Rosenberg's procedure requires the introduction of $n-2$ auxiliary variables. More recently, Ishikawa [14,15] defined the following quadratization for $P_n(x)$:

$$P_n(x) = \min_{y \in \{0,1\}^m} \sum_{i=1}^m y_i (c_{i,n}(-|x| + 2i) - 1) + \frac{|x|(|x| - 1)}{2}, \quad (5)$$

where $|x| = \sum_{i=1}^n x_i$, $m = \lfloor \frac{n-1}{2} \rfloor$ and

$$c_{i,n} = \begin{cases} 1, & \text{if } n \text{ is odd and } i = m, \\ 2, & \text{otherwise.} \end{cases}$$

Quadratization (5) uses $\lfloor \frac{n-1}{2} \rfloor$ auxiliary variables, and this is currently the best published upper bound on the number of variables required to define a quadratization for the positive monomial. Anthony et al. [2] gave an independent proof of the upper bound $\lfloor \frac{n-1}{2} \rfloor$, based on a representation result for arbitrary discrete functions. Interestingly, the quadratization of the positive monomial defined in [2] is identical to Ishikawa's for even values of n , but it is slightly different for odd values.

In this paper we provide a quadratization for the positive monomial using only $m = \lceil \log(n) \rceil - 1$ auxiliary variables, which is a significant improvement with respect to Ishikawa's quadratization and which reduces the upper bound on the number of auxiliary variables by orders of magnitude. Moreover, we prove that one cannot quadratize the positive monomial using less than $m = \lceil \log(n) \rceil - 1$ variables, thus providing a lower bound that exactly matches the upper bound.

Our quadratization of the POSITIVE MONOMIAL is presented as a direct consequence of two more general results that define quadratizations for EXACT k -OUT-OF- n and AT LEAST k -OUT-OF- n functions. Moreover, lower bounds on the number of variables required to quadratize EXACT k -OUT-OF- n and AT

LEAST k -OUT-OF- n functions, and hence the POSITIVE MONOMIAL, are derived from a lower bound for an even more general class of functions, that we call ZERO UNTIL k functions.

In this paper, we also define a quadratization for SYMMETRIC functions using $O(\sqrt{n}) = 2\lceil\sqrt{n+1}\rceil$ variables, which matches the lower bound of $\Omega(\sqrt{n})$ variables given in [2]. We also establish lower and upper bounds for a particular symmetric function, the PARITY function.

Section 2 formally defines the functions considered in this paper, illustrates their relations and provides a summary of the bounds. The precise statements for lower and upper bounds are presented in Section 3 and in Section 4, respectively. Finally, Section 5 establishes some additional lower bounds which are derived from a generalization of some of functions considered in the first sections. These last bounds are weaker than the bounds presented in Sections 3 and 4, but might nevertheless be useful in other situations.

2 Definitions, notations and summary of contributions.

Let us first define some notations. We assume throughout the paper that $n \geq 1$. Let $x = (x_1, \dots, x_n) \in \{0, 1\}^n$ and let $[n] = \{1, \dots, n\}$. The *Hamming weight* of x is $|x| = \sum_{i=1}^n x_i$, that is, the number of ones in x . We denote the *complement* of x by $\bar{x} = (\bar{x}_1, \dots, \bar{x}_n) = (1 - x_1, \dots, 1 - x_n)$. Notice that $|\bar{x}| = \sum_{i=1}^n \bar{x}_i = n - |x|$.

The original variables of the considered functions will be denoted by x , while auxiliary variables of quadratizations will be denoted by y and in some cases z .

Definition 2 Zero until k functions. Let $0 \leq k \leq n$ be an integer. A ZERO UNTIL k function $f : \{0, 1\}^n \rightarrow \mathbb{R}$ is a pseudo-Boolean function such that $f(x) = 0$ if $|x| < k$, and such that there exists a point $x^* \in \{0, 1\}^n$ with $|x^*| = k$ and $f(x^*) > 0$.

It is easy to check that f is a ZERO UNTIL k function if and only if, in its unique multilinear representation (3), all terms of degree smaller than k have coefficient zero, and there is one term of degree k with a positive coefficient. In fact, when this is the case, $a_S = f(x^S)$ for all $|S| \leq k$, where $x^S \in \{0, 1\}^n$ is the characteristic vector of S , with components $x_i^S = 1$ for $i \in S$ and $x_i^S = 0$ for $i \notin S$.

Definition 3 Symmetric functions. A pseudo-Boolean function $f : \{0, 1\}^n \rightarrow \mathbb{R}$ is SYMMETRIC if its value only depends on $|x|$, that is, if there exists a function $r : \{0, \dots, n\} \rightarrow \mathbb{R}$ such that $f(x) = r(|x|)$.

Definition 4 The Exact k -out-of- n function. Let $0 \leq k \leq n$ be an integer. The EXACT k -OUT-OF- n function is defined as

$$f_{=k}(x) = \begin{cases} 1, & \text{if } |x| = k \\ 0, & \text{otherwise.} \end{cases} \quad (6)$$

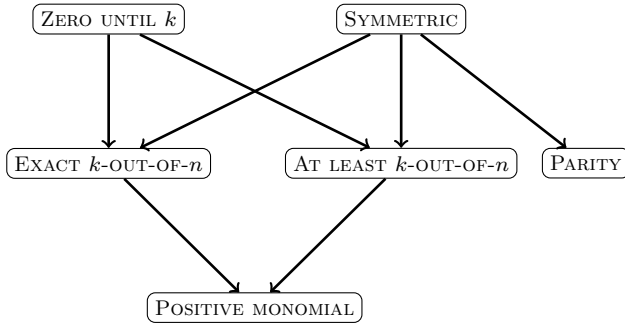


Fig. 1 Relation between the considered classes of functions.

Definition 5 The **At least k -out-of- n function**. Let $0 \leq k \leq n$ be an integer. The AT LEAST k -OUT-OF- n function is defined as

$$f_{\geq k}(x) = \begin{cases} 1, & \text{if } |x| \geq k \\ 0, & \text{otherwise.} \end{cases} \quad (7)$$

Definition 6 The **Positive monomial**. When $k = n$, the EXACT n -OUT-OF- n function is equal to the AT LEAST n -OUT-OF- n function. We call this function POSITIVE MONOMIAL and denote it $P_n(x)$. Its polynomial expression is

$$P_n(x) = \prod_{i=1}^n x_i \quad (8)$$

Definition 7 The **Parity function**. The PARITY function $\pi_n(x)$ is defined as follows:

$$\pi_n(x) = \begin{cases} 1, & \text{if } |x| \text{ is even,} \\ 0, & \text{otherwise.} \end{cases} \quad (9)$$

Observe that ZERO UNTIL k and SYMMETRIC functions refer to *classes* of functions satisfying certain properties, while EXACT k -OUT-OF- n , AT LEAST k -OUT-OF- n , POSITIVE MONOMIAL and PARITY refer to *uniquely defined* functions, for a given n and a given k .

Figure 1 schematizes the relations between the previously defined classes of functions. Classes on top of the figure are more general, and an arrow indicates whether a function is a particular case of another one.

Table 1 presents a summary of the values of the lower and upper bounds described in Section 3 and Section 4. (Here, and everywhere in the paper we use the convention that $\log(0) = -\infty$.)

It should be noted that the meaning of the lower and upper bounds presented in Table 1 for the class of SYMMETRIC functions, and the $\Omega(2^{\frac{n}{2}})$ bound for ZERO UNTIL k functions are different from the rest. For example, for the EXACT k -OUT-OF- n function, the lower bound means that *we cannot quadratize the EXACT k -OUT-OF- n function with fewer than $\max\{\lceil \log(k) \rceil, \lceil \log(n -$*

Table 1 Summary of lower and upper bounds.

Function	Lower Bound	Upper Bound
ZERO UNTIL k	$\Omega(2^{\frac{n}{2}})$ for some function (see [3]) $\lceil \log(k) \rceil - 1$ for all functions	$O(2^{\frac{n}{2}})$ (see [3])
SYMMETRIC	$\Omega(\sqrt{n})$ for some function (see [2])	$O(\sqrt{n}) = 2\lceil \sqrt{n+1} \rceil$
EXACT k -OUT-OF- n	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil) - 1$	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil)$
AT LEAST k -OUT-OF- n	$\lceil \log(k) \rceil - 1$	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil)$
POSITIVE MONOMIAL	$\lceil \log(n) \rceil - 1$	$\lceil \log(n) \rceil - 1$
PARITY	$\lceil \log(n) \rceil - 1$	$\lceil \log(n) \rceil - 1$

$k) \rceil - 1$ variables and the upper bound means that *we have defined a precise quadratization for the EXACT k -OUT-OF- n function using $\max\{\lceil \log(k) \rceil, \lceil \log(n-k) \rceil\}$ variables.* For SYMMETRIC functions, the lower bound means that *there exists at least one symmetric function requiring $\Omega(\sqrt{n})$ variables*, while the upper bound means that *all symmetric functions can be quadratized using $O(\sqrt{n})$ variables.* See Section 3.1 and Section 4.1 for precise statements.

Anthony et al. established in [2] an upper bound of $\lceil \frac{n}{2} \rceil$ variables for the AT LEAST k -OUT-OF- n function, and an upper bound of $\lfloor \frac{n}{2} \rfloor$ variables for the EXACT k -OUT-OF- n function. These bounds are significantly improved in this paper, where we define tight upper and lower bounds that are logarithmic in n .

The lower bound for SYMMETRIC functions presented in Table 1 is given in [2]. In the same paper, a lower bound of $\Omega(\sqrt{n})$ variables is also proved for quadratizations of the PARITY function that are linear in the y variables (so called y -linear quadratizations), and an upper bound of $\lfloor \frac{n}{2} \rfloor$ variables is provided for the PARITY function. These earlier results for PARITY are also improved here, firstly because we do not restrict ourselves to y -linear quadratizations, and secondly because the number of necessary auxiliary variables is reduced from linear to logarithmic in the upper bound; the resulting lower and upper bounds are exactly equal.

For ZERO UNTIL k functions, we present two different lower bounds. The lower bound $\lceil \log(k) \rceil - 1$ is valid for *all* ZERO UNTIL k functions, while the lower bound $\Omega(2^{\frac{n}{2}})$ is valid for *almost all* ZERO UNTIL k functions. The corresponding result states that there exist ZERO UNTIL k functions requiring $\Omega(2^{\frac{n}{2}})$ auxiliary variables in any quadratization. The upper bound for ZERO UNTIL k functions is the same as for general pseudo-Boolean functions (see [3]). Indeed, the lower bound $\Omega(2^{\frac{n}{2}})$ implies that the order of magnitude of the upper bound cannot be less than this value; this is actually a rather natural observation, since for small values of k , most pseudo-Boolean functions are ZERO UNTIL k functions.

3 Lower bounds.

This section formally states and proves the lower bounds on the number of auxiliary variables summarized in Table 1.

3.1 SYMMETRIC functions.

A lower bound for the number of variables required to quadratize symmetric functions was established by Anthony et al. [2]. We state their theorem for completeness.

Theorem 1 (Theorem 5.3 in [2]) *There exist SYMMETRIC functions of n variables for which any quadratization must involve at least $\Omega(\sqrt{n})$ auxiliary variables.*

3.2 ZERO UNTIL k functions, EXACT k -OUT-OF- n , AT LEAST k -OUT-OF- n functions, and the POSITIVE MONOMIAL.

We start this section with a lower bound for ZERO UNTIL k functions which is a direct extension of a result due to Anthony et al. [3].

Theorem 2 *For every fixed integer k , there exist ZERO UNTIL k functions of n variables for which every quadratization must involve at least $\Omega(2^{\frac{n}{2}})$ auxiliary variables.*

Proof The proof is analogous to the proof of Theorem 1 in [3], and we only briefly sketch it here. For any m , let V_m be the set of pseudo-Boolean functions of n variables which can be quadratized using at most m auxiliary variables. It was observed in [3] that V_m , viewed as a subset of the vector space of all pseudo-Boolean functions, is contained in a finite union of subspaces, each of dimension $\ell(n, m) = O(nm + n^2 + m^2)$. On the other hand, for any fixed k , the set of ZERO UNTIL k pseudo-Boolean functions of n variables contains a subspace of dimension $2^n - O(n^k) = \Omega(2^n)$, namely, the subspace spanned by the monomials $\prod_{i \in S} x_i$ with $|S| > k$. It follows that, if m auxiliary variables are sufficient to quadratize every ZERO UNTIL k function, then $\ell(n, m) = \Omega(2^n)$, and $m = \Omega(2^{\frac{n}{2}})$. \square

Observe that, as was the case for general pseudo-Boolean functions in [3], the bound in Theorem 2 actually holds for *almost all* ZERO UNTIL k functions, in the sense that the set of ZERO UNTIL k functions that require less than $\Omega(2^{\frac{n}{2}})$ auxiliary variables has Lebesgue measure zero, when compared to the whole space of ZERO UNTIL k functions.

Furthermore, Theorem 2 implies that it is not possible to find an upper bound on the number of auxiliary variables to define a quadratization for ZERO UNTIL k that is smaller than exponential in n – see Table 1. This also makes sense intuitively, since for a fixed k , the proportion of ZERO UNTIL k

functions among all pseudo-Boolean functions tends to 1 as n goes to infinity, and therefore, the same lower and upper bounds apply to ZERO UNTIL k functions as to general pseudo-Boolean functions.

We next present another lower bound for ZERO UNTIL k functions.

Theorem 3 *Assume that f is a ZERO UNTIL k function with $k \geq 1$ and that $g(x, y)$ is a quadratization of f with m auxiliary variables. Then,*

$$m \geq \lceil \log(k) \rceil - 1.$$

Proof Let us define

$$r(x) = \prod_{y \in \{0,1\}^m} g(x, y). \quad (10)$$

For every point $x \in \{0,1\}^n$ with $|x| < k$, $f(x) = 0$ by definition of ZERO UNTIL k functions. Also, since $g(x, y)$ is a quadratization of $f(x)$, there exists $y \in \{0,1\}^m$ such that $g(x, y) = 0$, which implies that $r(x) = 0$ for all points x with $|x| < k$.

Moreover, since f is a ZERO UNTIL k function we know that there exists a point $x^* \in \{0,1\}^n$ such that $|x^*| = k$ and $f(x^*) > 0$, which implies that $g(x^*, y) > 0$ for all $y \in \{0,1\}^m$, and hence $r(x^*) > 0$. Let $S^* = \{i \in [n] \mid x_i^* = 1\}$ with $|S^*| = k$.

In view of the observations following Definition 2, the unique multilinear expression of r can be written as

$$r(x) = \sum_{\substack{S \subseteq [n] \\ |S| \geq k}} a_S \prod_{i \in S} x_i \quad (11)$$

where $a_{S^*} = r(x^*) > 0$. Thus,

$$\deg(r) \geq k. \quad (12)$$

Now, the right-hand-side of (10) is a product of 2^m functions of degree two, meaning that

$$\deg(r) \leq 2^{m+1}, \quad (13)$$

which together with (12) implies that $m + 1 \geq \lceil \log(k) \rceil$. \square

Notice the difference, of orders of magnitude, between the bounds given in Theorem 2, which is valid for almost all functions, and in Theorem 3, which is valid for all functions. The lower bound $\lceil \log(k) \rceil - 1$ given in Theorem 3 is rather weak for low values of k . However, for the particular case of the POSITIVE MONOMIAL it leads to a lower bound that exactly matches the upper bound that we provide in Section 4.

Corollary 1 *The POSITIVE MONOMIAL $P_n(x)$ is a ZERO UNTIL n function, and therefore it cannot be quadratized using less than $\lceil \log(n) \rceil - 1$ auxiliary variables.*

For AT LEAST k -OUT-OF- n and EXACT k -OUT-OF- n functions, the lower bound of Theorem 3 remains weak for small values of k .

Corollary 2 *For every fixed $k \geq 1$, the AT LEAST k -OUT-OF- n function is a ZERO UNTIL k function, and therefore it cannot be quadratized using less than $\lceil \log(k) \rceil - 1$ auxiliary variables.*

Corollary 3 *For every fixed $k \geq 1$, the EXACT k -OUT-OF- n function is a ZERO UNTIL k function, and therefore it cannot be quadratized using less than $\lceil \log(k) \rceil - 1$ auxiliary variables.*

However, for EXACT k -OUT-OF- n functions we can derive a tighter lower bound on the number of auxiliary variables, with a difference of only one unit with respect to the upper bound that will be defined in Section 4.2, by relying on the following property:

Remark 1 The EXACT k -OUT-OF- n function is such that

$$f_{=k}(x_1, \dots, x_n) = f_{=n-k}(\bar{x}_1, \dots, \bar{x}_n).$$

Theorem 4 *Let $k \geq 1$ and assume that $g(x, y)$ is a quadratization of the EXACT k -OUT-OF- n function $f_{=k}$ with m auxiliary variables. Then,*

$$m \geq \max(\lceil \log(k) \rceil, \lceil \log(n - k) \rceil) - 1.$$

Proof By Corollary 3, $m \geq \lceil \log(k) \rceil - 1$. By Remark 1, $f_{=k}(x_1, \dots, x_n) = f_{=n-k}(\bar{x}_1, \dots, \bar{x}_n)$, thus, by changing the names of the x variables we see that $h(x, y) = g(\bar{x}, y)$, viewed as a function of (x, y) , is a quadratization of $f_{=n-k}(x_1, \dots, x_n)$ using m auxiliary variables. Corollary 3 implies that any quadratization of $f_{=n-k}(x_1, \dots, x_n)$ uses at least $\lceil \log(n - k) \rceil - 1$ auxiliary variables, thus $m \geq \lceil \log(n - k) \rceil - 1$, which completes the proof. \square

Remark 2 Observe that $\max(\lceil \log(k) \rceil, \lceil \log(n - k) \rceil) - 1$ is not a valid lower bound for all ZERO UNTIL k functions. Indeed, consider for example a POSITIVE MONOMIAL of degree k , seen as a function f of n variables: $f(x_1, \dots, x_n) = \prod_{i=1}^k x_j$, where n is such that $\lceil \log(n - k) \rceil > \lceil \log(k) \rceil$. This is a ZERO UNTIL k function. In Theorem 9 hereunder, we define a quadratization for this POSITIVE MONOMIAL that uses $\lceil \log(k) \rceil - 1$ auxiliary variables. This shows that $\lceil \log(n - k) \rceil - 1$ cannot be a lower bound on the number of auxiliary variables for all ZERO UNTIL k functions.

3.3 The PARITY function.

In this section we prove that $\lceil \log(n) \rceil - 1$ is a lower bound on the number of variables required to define a quadratization for the PARITY function.

Theorem 5 *Assume that $g(x, y)$ is a quadratization of the PARITY function $\pi_n(x)$ with m auxiliary variables. Then,*

$$m \geq \lceil \log(n) \rceil - 1.$$

Proof Let us define

$$r(x) = \prod_{y \in \{0,1\}^m} g(x, y). \quad (14)$$

Note that $\deg(r) \leq 2^{m+1}$, since $g(x, y)$ is quadratic.

Note also that $r(x) \geq 1$ whenever $|x|$ is even and $r(x) = 0$ whenever $|x|$ is odd. Therefore we can write

$$r(x) = \sum_{\substack{z \in \{0,1\}^n \\ |z| \text{ even}}} r(z) \prod_{i: z_i=1} x_i \prod_{i: z_i=0} (1 - x_i).$$

The sign of the coefficient of $\prod_{i=1}^n x_i$ in each of the above terms is $(-1)^n$. Thus, in the unique multilinear representation of $r(x)$, $\prod_{i=1}^n x_i$ has coefficient

$$(-1)^n \sum_{\substack{z \in \{0,1\}^n \\ |z| \text{ is even}}} r(z) \neq 0,$$

and consequently, $\deg(r) = n$. The inequality

$$n = \deg(r) \leq 2^{m+1}$$

follows, implying the claim. \square

4 Upper bounds.

This section defines the quadratizations for SYMMETRIC pseudo-Boolean functions, for the EXACT k -OUT-OF- n and AT LEAST k -OUT-OF- n functions, and for the POSITIVE MONOMIAL and the PARITY function that lead to the upper bounds displayed in Table 1.

4.1 SYMMETRIC functions.

Let \mathbb{N} be the set of nonnegative integers and $Z = \{0, 1, \dots, n\}$. Theorem 6 defines a quadratization of SYMMETRIC functions using $2\lceil\sqrt{n+1}\rceil$ auxiliary variables.

Theorem 6 *Let $f(x_1, \dots, x_n)$ be a SYMMETRIC pseudo-Boolean function such that $f(x) = r(|x|)$, with $r : \mathbb{N} \rightarrow \mathbb{R}$ and $r(k) = 0$ for $k > n$, by convention. Let $l = \lceil\sqrt{n+1}\rceil$, and choose $M \in \mathbb{R}$ such that $M > |r(k)|$ for all $k \in Z$.*

Then,

$$\begin{aligned}
g(x, y, z) &= \sum_{i=0}^{l-1} \sum_{j=0}^{l-1} r(il + j) y_i z_j \\
&+ 2M \left(1 - \sum_{i=0}^{l-1} y_i \right)^2 + 2M \left(1 - \sum_{j=0}^{l-1} z_j \right)^2 \\
&+ 2M \left(|x| - \left(l \sum_{i=0}^{l-1} i y_i + \sum_{j=0}^{l-1} j z_j \right) \right)^2
\end{aligned} \tag{15}$$

is a quadratization of f using $2\lceil\sqrt{n+1}\rceil = O(\sqrt{n})$ auxiliary variables y_i, z_i , $i = 0, \dots, l-1$.

Proof Observe first that every integer $k \in Z$ has a unique representation $k = il + j$ with $0 \leq i, j \leq l-1$. So, for every $x \in \{0, 1\}^n$, let us define integers $i(x)$ and $j(x)$ such that $|x| = i(x)l + j(x)$, $0 \leq i(x) \leq l-1$ and $0 \leq j(x) \leq l-1$ hold.

Let us then define auxiliary vectors $y^*, z^* \in \{0, 1\}^l$ (with components indexed from 0 to $l-1$), such that

$$\begin{aligned}
y_i^* &= \begin{cases} 1 & \text{if } i = i(x), \\ 0 & \text{otherwise,} \end{cases} \\
z_j^* &= \begin{cases} 1 & \text{if } j = j(x), \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

Let us observe next that due to the three terms involving M in (15), $g(x, y, z) < M$ if and only if $y = y^*$ and $z = z^*$. Due to the definition of the first term of g , in this case $g(x, y^*, z^*) = r(|x|) = f(x)$. \square

The upper bound in Theorem 6 matches the order of magnitude of the lower bound given in Theorem 1. Interestingly, in combination with Lemma 5.1 of [2], it also implies that *every* pseudo-Boolean function can be quadratized using $O(2^{n/2})$ auxiliary variables, a result proved by another approach in [3].

Finally, observe that Theorem 6 can be generalized to a more general class of pseudo-Boolean functions, for which the value of a given $x \in \{0, 1\}^n$ is determined by a weighted sum of the values of the components x_i instead of the the Hamming weight $|x| = \sum_{i=1}^n x_i$ of x . More precisely, given a linear function $L : \{0, 1\}^n \rightarrow \{0, 1, \dots, R\}$ and a function $r : \mathbb{N} \rightarrow \mathbb{R}$ with $r(k) = 0$ for $k > R$, consider the pseudo-Boolean function $f(x) = r(L(x))$. Theorem 6 holds for f by considering $l = \lceil\sqrt{R+1}\rceil$ and substituting $|x|$ by $L(x)$ in equation (15).

4.2 EXACT k -OUT-OF- n and AT LEAST k -OUT-OF- n functions.

Theorem 7 and Theorem 8 are the main results of this section. They define, respectively, a quadratization for the EXACT k -OUT-OF- n function and a quadratization for the AT LEAST k -OUT-OF- n function using at most $\lceil \log(n) \rceil$ variables. The following observations will be useful in the proofs of Theorems 7 and 8.

Let us define the following sets

$$I_{\text{even}}^l = \{0, 2, \dots, 2^l - 2\}, \quad (16)$$

and

$$I_{\text{odd}}^l = \{1, 3, \dots, 2^l - 1\}. \quad (17)$$

Remark 3 Observe that for all $l \geq 2$,

$$I_{\text{even}}^l = \left\{ \sum_{i=1}^{l-1} 2^i y_i \mid (y_1, \dots, y_{l-1}) \in \{0, 1\}^{l-1} \right\}, \quad (18)$$

and

$$I_{\text{odd}}^l = \left\{ 1 + \sum_{i=1}^{l-1} 2^i y_i \mid (y_1, \dots, y_{l-1}) \in \{0, 1\}^{l-1} \right\}. \quad (19)$$

Remark 4 Given integers $0 \leq |x| \leq n$, $0 \leq k \leq n$ and $l = \max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil)$, observe that

$$0 \leq |x| - k + 2^l \leq 2^l - 1, \text{ for } |x| < k, \quad (20)$$

and

$$0 \leq |x| - k - 1 \leq 2^l - 1, \text{ for } |x| > k. \quad (21)$$

Proof Note first that, by definition of l , $2^l \geq k$ and $2^l \geq n - k$ are satisfied for all k . The first inequality of (20) holds because $|x| \geq 0$ and $2^l \geq k$, and the second one holds because $|x| < k$. The first inequality of (21) holds because $k < |x|$, and the second one holds because $|x| - k \leq n - k \leq 2^l$. \square

Let us define

$$A_k(x, y, z) = |x| - (k - 2^l)z - (k + 1)(1 - z) - \sum_{i=1}^{l-1} 2^i y_i,$$

where $l = \max(\lceil \log(k) \rceil, \lceil \log(n - k) \rceil)$, $z \in \{0, 1\}$ and $y = (y_1, \dots, y_{l-1}) \in \{0, 1\}^{l-1}$.

Theorem 7 For each integer $0 \leq k \leq n$, the function

$$G_k(x, y, z) = \frac{1}{2} A_k(x, y, z) (A_k(x, y, z) - 1) \quad (22)$$

is a quadratization of the EXACT k -OUT-OF- n function $f_{=k}$ using

$$l = \max(\lceil \log(k) \rceil, \lceil \log(n - k) \rceil) \leq \lceil \log(n) \rceil$$

auxiliary variables $y \in \{0, 1\}^{l-1}$ and $z \in \{0, 1\}$.

Proof Note first that $G_k(x, y, z) \geq 0$ for all (x, y, z) and for all k , since it is the half-product of two consecutive integers. Therefore, when $|x| \neq k$ we only have to show that there exists (y, z) such that $G_k(x, y, z) = f_{=k}(x) = 0$.

We consider three cases:

1. If $0 \leq |x| < k$, set $z = 1$ so that $A_k(x, y, 1) = |x| - k + 2^l - \sum_{i=1}^{l-1} 2^i y_i$. By Remark 4, $0 \leq |x| - k + 2^l \leq 2^l - 1$. Hence, using Remark 3 if $|x| - k + 2^l \in I_{odd}^l$, one can choose y such that $A_k(x, y, 1) - 1 = 0$, and if $|x| - k + 2^l \in I_{even}^l$, one can choose y such that $A_k(x, y, 1) = 0$.
2. If $k < |x| \leq n$, set $z = 0$ so that $A_k(x, y, 0) = |x| - k - 1 - \sum_{i=1}^{l-1} 2^i y_i$. By Remark 4, $0 \leq |x| - k - 1 \leq 2^l - 1$. Hence, using Remark 3 if $|x| - k - 1 \in I_{odd}^l$, one can choose y such that $A_k(x, y, 0) - 1 = 0$, and if $|x| - k - 1 \in I_{even}^l$, one can choose y such that $A_k(x, y, 0) = 0$.
3. Consider finally the case where $|x| = k$. When $z = 1$, we obtain $A_k(x, y, 1) = 2^l - \sum_{i=1}^{l-1} 2^i y_i \geq 2$, and hence $G_k(x, y, 1) \geq 1$. When $z = 0$, $A_k(x, y, 0) = -1 - \sum_{i=1}^{l-1} 2^i y_i \leq -1$, and hence again $G_k(x, y, 0) \geq 1$. The minimum value $G_k(x, y, z) = 1$ is obtained by setting either $z = y_i = 1$, or $z = y_i = 0$, for $i = 1, \dots, l - 1$. \square

As announced earlier, the upper bound established in Theorem 7 almost perfectly matches the lower bound given in Theorem 4. Moreover, Theorem 7 provides as a corollary an upper bound on the number of variables required to obtain a quadratization of SYMMETRIC functions.

Corollary 4 *If $f : \{0, 1\}^n \rightarrow \mathbb{R}$ is a SYMMETRIC function, the value of which is strictly above its minimum value for at most d different Hamming weights $|x|$, then f can be quadratized with at most $d(\lceil \log(n) \rceil)$ variables.*

Proof Let $r : \{0, 1, \dots, n\} \rightarrow \mathbb{R}$ be such that $f(x) = r(|x|)$. Let α be the minimum value of f (and of r), and let k_1, \dots, k_d be the values of $|x|$ such that $f(x)$ (and $r(|x|)$) is larger than α . The result follows from Theorem 7 by observing that f can be expressed as

$$f(x) = \alpha + \sum_{i=1}^d (r(k_i) - \alpha) f_{=k_i}(x). \quad \square$$

Let us now turn to the case of AT LEAST k -OUT-OF- n functions.

Theorem 8 *For each integer $0 \leq k \leq n$, the function*

$$G_k(x, y, z) = \frac{1}{2} (A_k(x, y, z)) (A_k(x, y, z) - 1) + (1 - z) \quad (23)$$

is a quadratization of the AT LEAST k -OUT-OF- n function $f_{\geq k}$ using

$$l = \max(\lceil \log(k) \rceil, \lceil \log(n - k) \rceil) \leq \lceil \log(n) \rceil$$

auxiliary variables $y \in \{0, 1\}^{l-1}$ and $z \in \{0, 1\}$.

Proof Note again that $G_k(x, y, z) \geq 0$ for all (x, y, z) , because its first term is the half-product of two consecutive integers and $1 - z \geq 0$. Therefore, when $|x| < k$ we only have to show that there exists (y, z) such that $G_k(x, y, z) = f_{\geq k}(x) = 0$.

1. If $0 \leq |x| < k$, set $z = 1$. We obtain exactly the same expression as in the proof of Theorem 7 and the same argument holds.
2. If $|x| = k$ and $z = 1$, we obtain $A_k(x, y, 1) = 2^l - \sum_{i=1}^{l-1} 2^i y_i \geq 2$, and hence $G_k(x, y, 1) \geq 1$. If $z = 0$, we have that $G_k(x, y, 0) \geq 2$. As in the proof of Theorem 7, we attain the minimum value $G_k(x, y, z) = 1$ by setting $z = y_i = 1$, for $i = 1, \dots, l-1$.
3. Finally, let $|x| > k$. For $z = 1$,

$$G_k(x, y, 1) = \frac{1}{2} \left(|x| - k + 2^l - \sum_{i=1}^{l-1} 2^i y_i \right) \left(|x| - k + 2^l - \sum_{i=1}^{l-1} 2^i y_i - 1 \right).$$

Now, $\left(|x| - k + 2^l - \sum_{i=1}^{l-1} 2^i y_i \right) \geq 2$ because $2^l - \sum_{i=1}^{l-1} 2^i y_i \geq 2$ and $|x| - k$ is strictly positive. Hence, $G_k(x, y, 1) \geq 1$.

For $z = 0$,

$$G_k(x, y, 0) = \frac{1}{2} \left(|x| - k - 1 - \sum_{i=1}^{l-1} 2^i y_i \right) \left(|x| - k - 1 - \sum_{i=1}^{l-1} 2^i y_i - 1 \right) + 1.$$

By Remark 4, $0 \leq |x| - k - 1 \leq 2^l - 1$. Hence, using Remark 3 if $|x| - k - 1 \in I_{\text{odd}}^l$, one can choose y such that $A_k(x, y, 0) - 1 = 0$, and if $|x| - k - 1 \in I_{\text{even}}^l$, one can choose y such that $A_k(x, y, 0) = 0$, thus achieving $G_k(x, y, 0) = f_{\geq k}(x) = 1$ in both cases. \square

The upper bound in Theorem 8 is larger than the lower bound given in Corollary 2 when $k < \frac{n}{2}$, but the bounds are equal, up to one unit, for larger values of k .

4.3 The POSITIVE MONOMIAL.

In this section we define a quadratization using $\lceil \log(n) \rceil - 1$ auxiliary variables for the POSITIVE MONOMIAL. Since the POSITIVE MONOMIAL is a particular case of the EXACT k -OUT-OF- n function and of the AT LEAST k -OUT-OF- n function (with $k = n$), Theorem 7 and Theorem 8 imply a slightly weaker upper bound. Nevertheless, the stronger upper bound in Theorem 9 can be easily derived from the proofs of these theorems when $k = n$.

Theorem 9 *Let $l = \lceil \log(n) \rceil$. Then,*

$$g(x, y) = \frac{1}{2} \left(|x| + 2^l - n - \sum_{i=1}^{l-1} 2^i y_i \right) \left(|x| + 2^l - n - \sum_{i=1}^{l-1} 2^i y_i - 1 \right) \quad (24)$$

is a quadratization of the positive monomial $P_n(x) = \prod_{i=1}^n x_i$ using $\lceil \log n \rceil - 1$ auxiliary variables.

Proof This is a direct consequence of the proofs of Theorem 7 and Theorem 8: indeed, when setting $k = n$ it is easy to verify that we can always fix $z = 1$ in the quadratizations (22) and (23). \square

As mentioned in Section 1, Theorem 9 provides a significant improvement over the best previously known quadratizations for the POSITIVE MONOMIAL, and the upper bound on the number of auxiliary variables precisely matches the lower bound presented in Section 3.

Remark 5 Although the quadratization (24), and the related expressions (22) or (23), may seem somewhat mysterious, it is instructive to realize that they derive from rather simple modifications of a more natural result: indeed, the readers may easily convince themselves that, when $n = 2^l$, then

$$g'(x, y) = (|x| - \sum_{i=0}^{l-1} 2^i y_i)^2$$

is a quadratization of P_n using $\log(n)$ auxiliary variables. This result clearly highlights the underlying intuition, which is that $|x|$ can always be expressed as $|x| = \sum_{i=0}^{l-1} 2^i y_i$, except when $|x| = n$.

When $n < 2^l$, the quadratization g' can be adjusted by fixing $2^l - n$ variables x_i to 1 in P_{2^l} and in g' . Moreover, the number of auxiliary variables can be marginally reduced by distinguishing between even and odd values of $|x|$. Altogether, this leads to Theorem 9.

Let us finally present the following family of quadratizations of the positive monomial, the best of which uses $\lceil \frac{n}{4} \rceil$ auxiliary variables (see [4] for a proof).

Theorem 10 *For all integers $n \geq 2$, if $\frac{n}{4} \leq m \leq \frac{n}{2}$, and $N = n - 2m$, then*

$$g(x, y) = \frac{1}{2} (|x| - 2|y| - (N - 2)y_1) (|x| - 2|y| - (N - 2)y_1 - 1) \quad (25)$$

is a quadratization of the positive monomial $P_n = \prod_{i=1}^n x_i$ using m auxiliary variables.

These quadratizations require a linear number of auxiliary variables but still improve the $\lfloor \frac{n-1}{2} \rfloor$ bound of (5). Notice that Ishikawa's quadratization (5) uses coefficients of absolute values varying approximately between 1 and n , while the absolute values of the coefficients in (24) and (25) vary roughly between 1 and n^2 , which might result in functions containing coefficients of very different orders of magnitude, potentially inducing numerical problems when n is large. Moreover, note that $\lceil \log n \rceil - 1$ is equal to $\lceil \frac{n}{4} \rceil$ when $3 \leq n \leq 12$, so that the difference in the number of auxiliary variables only becomes relevant for very high degrees. Finally, the number of positive quadratic terms is also different in quadratizations (5), (24), and (25), especially for large degrees, which might also impact computational performance. All in all, the behavior of these different quadratizations in an optimization setting is unclear and should be computationally tested. Some preliminary results can be found in [18].

4.4 The PARITY function.

Theorem 11 *Let $l = \lceil \log(n) \rceil$. When n is even, the function*

$$g_e(x, y) = \left(|x| - n + 2^l - \sum_{i=1}^{l-1} 2^i y_i - 1 \right)^2 \quad (26)$$

is a quadratization of the PARITY function $\pi_n(x)$.

When n is odd, the function

$$g_o(x, y) = \left(|x| - n + 2^l - \sum_{i=1}^{l-1} 2^i y_i \right)^2 \quad (27)$$

is a quadratization of the PARITY function $\pi_n(x)$.

Both $g_e(x, y)$ and $g_o(x, y)$ use $\lceil \log(n) \rceil - 1$ auxiliary variables.

Proof Assume that n is even. Then, $2^l - n$ is even and the parity of $|x|$ and $|x| - n + 2^l$ is the same.

If $|x|$ is odd, we only have to show that for each x , there exists a y such that $g_e(x, y) = 0$, because $g_e(x, y) \geq 0$ holds for all (x, y) . Since $|x| - n + 2^l$ is odd, we have that $0 \leq |x| - n + 2^l \leq 2^l - 1$. Now, Remark 3 implies that for the right choice of y , $g_e(x, y) = 0$ is satisfied.

If $|x|$ is even, $g_e(x, y) \geq 1$ holds for all (x, y) , because $|x| - n + 2^l - \sum_{i=1}^{l-1} 2^i y_i - 1$ is odd. Moreover, since $0 \leq |x| - n + 2^l \leq 2^l$ we obtain $\min_{y \in \{0,1\}^{l-1}} g_e(x, y) = 1$ with an appropriate choice of y .

When n is odd, the proof is analogous by considering I_{even}^l instead of I_{odd}^l and by noticing that $|x|$ and $|x| - n + 2^l$ have different parities. \square

5 Further lower bounds.

This last section presents lower bounds on the number of variables required to define a quadratization for a class of pseudo-Boolean functions generalizing AT LEAST k -OUT-OF- n , EXACT k -OUT-OF- n , PARITY functions and a particular type of SYMMETRIC functions. These functions are called d -SUBLINEAR, and are characterized by the fact that they take value zero everywhere, except on d hyperplanes. The main result of this section is Theorem 12, which gives a logarithmic lower bound on the number of auxiliary variables required to define a quadratization for d -SUBLINEAR functions. We choose to present these results in a separate section because the bounds derived from Theorem 12 are in general weaker than those presented in Section 3. Nevertheless, Theorem 12 may prove useful in other situations, and establishes an interesting link with results obtained by Linial and Radhakrishnan [17] in a different context (see also Alon and Füredi [1]).

Definition 8 A pseudo-Boolean function $f : \{0, 1\}^n \rightarrow \mathbb{R}$ is d -SUBLINEAR, if there exist linear functions q_1, \dots, q_d such that $\prod_{j=1}^d q_j(x) = 0$ whenever $f(x) \neq 0$. We say that the linear functions q_1, \dots, q_d *dominate* f .

We say that a pseudo-Boolean function is SUBLINEAR if it is 1-SUBLINEAR.

In other words, f is d -SUBLINEAR if every point x^* such that $f(x^*) \neq 0$ belongs to at least one of the hyperplanes $q_1(x) = 0, \dots, q_d(x) = 0$.

For a linear function $q = a_0 + \sum_{i=1}^n a_i x_i$, let $\beta(q)$ denote the number of variables with a non-zero coefficient in q , that is,

$$\beta(q) = |\{i \in \{1, \dots, n\} \text{ such that } a_i \neq 0\}|.$$

We are going to use the following lemma.

Lemma 1 (Lemma 2 in [17]) *Assume that $r : \{0, 1\}^n \rightarrow \mathbb{R}$ is a SUBLINEAR function dominated by a linear function q , and assume that there exists a point x^* such that $r(x^*) \neq 0$. Then,*

$$\deg(r) \geq \frac{\beta(q)}{2}.$$

Theorem 12 *Assume that f is a d -SUBLINEAR function dominated by linear functions q_1, \dots, q_d , and that there exists $x^* \in \{0, 1\}^n$ such that $f(x^*) > 0$, $q_1(x^*) = 0$ and $\prod_{j=2}^d q_j(x^*) \neq 0$. Then, the number m of auxiliary variables in any quadratization of f is such that*

$$2^{m+1} \geq \frac{\beta(q_1)}{2} - d + 1.$$

Proof Let us define

$$r(x) = \prod_{j=2}^d q_j(x) \prod_{y \in \{0, 1\}^m} g(x, y),$$

and note that

$$\deg(r) \leq d - 1 + 2^{m+1},$$

because r is a product of $d - 1$ linear functions and 2^m quadratic functions.

Since g is a quadratization of f and $f(x^*) > 0$, we have $g(x^*, y) > 0$ for all $y \in \{0, 1\}^m$. By assumption, $\prod_{j=2}^d q_j(x^*) \neq 0$, and hence $r(x^*) \neq 0$.

Moreover, r is SUBLINEAR dominated by the function q_1 . Indeed, for points x with $r(x) \neq 0$, the definition of r implies that $q_j(x) \neq 0$ for all $j = 2, \dots, d$ and $g(x, y) \neq 0$ for all $y \in \{0, 1\}^m$, thus $f(x) \neq 0$. But f is d -SUBLINEAR, thus $q_1(x) = 0$, which implies that $r(x)$ is SUBLINEAR.

The conditions of Lemma 1 are satisfied, therefore

$$\deg(r) \geq \frac{\beta(q_1)}{2},$$

which together with $\deg(r) \leq d - 1 + 2^{m+1}$ proves the claim. \square

The bound of Theorem 12 is of interest when d is small. In particular, for the special case of EXACT k -OUT-OF- n functions (including the POSITIVE MONOMIAL), we can take $d = 1$ and $q_1(x) = \sum_{i=1}^n x_i - k$. This yields a lower bound $\log(n) - 2$ that is only slightly weaker than the bound established in Theorem 4. More generally, for arbitrary symmetric functions, we have the following corollary.

Corollary 5 *If f is a SYMMETRIC function, the value of which is strictly above its minimum value for at most d different Hamming weights $|x|$, where $d \leq \mu n + 1$ and $0 \leq \mu < \frac{1}{2}$, then the number m of auxiliary variables in any quadratization of f is such that*

$$m \geq \log\left(\frac{1}{2} - \mu\right) + \log(n) - 1.$$

Proof As in the proof of Corollary 4, let α be the minimum value of f . Then, $h = f - \alpha$ is strictly positive for d values of $|x|$, and Theorem 12 applies directly to h with d dominating linear functions of the form $q_i(x) = \sum_{i=1}^n x_i - k_i$, for $i = 1, \dots, d$. \square

Again, this bound is relatively weak when compared, for instance, to the upper bound in Corollary 4, but it could prove useful in some cases.

6 Conclusions

In this paper we have established new upper and lower bounds on the number of auxiliary variables required to define a quadratization for several classes of specially structured pseudo-Boolean functions defined on n binary variables. These bounds greatly improve the best bounds previously proposed in the literature. Most remarkably, the best upper bound published so far for the POSITIVE MONOMIAL was linear in n , whereas our new upper bound is logarithmic. Moreover, for the POSITIVE MONOMIAL and for the PARITY function, we have also established lower bounds that exactly match the upper bounds.

Furthermore, we have provided logarithmic upper and lower bounds for EXACT k -OUT-OF- n and AT LEAST k -OUT-OF- n functions. For SYMMETRIC functions we have proved an upper bound of the order of $O(\sqrt{n})$, matching the order of magnitude of the best lower bound proposed in the literature.

For the more general class of ZERO UNTIL k functions, we have established two different types of lower bounds, namely, a logarithmic bound in k which is valid for all functions in this class, and an exponential bound in n , which is valid for almost all ZERO UNTIL k functions and which implies that the upper bounds available for general pseudo-Boolean functions are also applicable for this class.

Many additional questions arise from these results. From a theoretical point of view, it would be interesting to explore further generalizations and classes of pseudo-Boolean functions. For EXACT k -OUT-OF- n and AT LEAST k -OUT-OF- n functions, the lower and upper bounds are of the same order of magnitude,

but it would be nice to close the remaining unit gap. From an experimental perspective, it would be worth to examine the computational behavior of the different proposed quadratizations when applied to generic pseudo-Boolean optimization problems.

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