All 4-variable functions can be perfectly quadratized with only 1 auxiliary variable

Nike Dattani[1] and Hou Tin Chau[2]

[1] *Harvard-Smithsonian Center for Astrophysics, USA*
[2] *Cambridge University, Department of Mathematics, UK*

We prove that any function with real-valued coefficients, whose input is 4 binary variables and whose output is a real number, is perfectly equivalent to a *quadratic* function whose input is 5 binary variables and is minimized over the new variable. Our proof is constructive, so we provide quadratic functions that quadratize any 4-variable function, but there exists 5 different classes of 4-variable functions that each have their own 5-variable quadratization formula. Since we provide 'perfect' quadratizations, we can apply these formulas to any 4-variable subset of an n-variable function even if $n \gg 4$. We provide a simple example function where a termwise quadratization method would require 15 auxiliary variables to perfectly quadratize, whereas with the results of this paper, we only need 5 auxiliary variables (so each application of our theorem saves 10 auxiliary variables).

I. INTRODUCTION

Many problems can be solved by minimizing a real-valued degree-k function of binary variables with $k > 2$. Some examples include image de-blurring (where typically $k = 4$ but in general we can have $k = m^2$ with $m \geq 2$ being the length in pixels of the square-shaped mask) [1, 2], integer factoring (where typically $k = 4$) [3–10], and determining whether or not a number N is an m-color Ramsey number (where $k = \frac{mN(N-1)}{2}$) [11–13].

Solving such discrete optimization problems with $k > 2$ can be very difficult, and more algorithms have been developed for the $k = 2$ case (such as the algorithm known as "QPBO" and extensions of it [14]) than for the $k > 2$ case. Fortunately it is possible to turn any k-degree binary optimization problem into a 2-degree binary optimization problem, by a transformation called "quadratization" [15].

Quadratization methods exist which can turn an n-variable degree-k problem into an n-variable quadratic problem (i.e. the number of variables does not change) [8, 13, 16, 17], but not every function can be quadratized without adding some auxiliary variables (so the number of variables in the quadratic problem is usually much more than in the original degree-k problem). Coming up with better quadratizations (for example with fewer auxiliary variables) has been a very active area of research recently: The first quadratization method was published in 1975 [18], and some subsequent quadratization methods were published in 2004 [19], 2005 [20], and 2011 [1, 2, 21], but the rest of the methods were published in the last 5 years (from 2014-2018) [8, 13, 15–17, 22–32].

In the most recent of these papers [31, 32], a remarkable discovery was made, that degree-k monomials can be quadratized with only $\log_2 k - 1$ auxiliary variables. For many functions this can still be prohibitively costly though: If a 44-variable function has 1 million degree-5 terms and each term requires $\log_2 k - 1$ auxiliary variables for quadratization, the quadratic function will have more than 2 million variables (the search space increases from $2^{44} \approx 10^{13}$ to $2^{2,000,044} \approx 10^{602,073}$).

It was also shown in [31, 32] that sometimes a function of n variables can entirely be quadratized with only $\log_2 k - 1$ auxiliary variables no matter how many terms and how many variables it contains (so a 44-variable, degree-5 function with 1 million degree-5 terms would only need 2 auxiliary variables rather than 2 million!). However, it is only known how to do this very 'compact' quadratization for a very specific class of functions called "at-least-k-of-n" (AkON) functions, which includes functions consisting of only a single positive monomial term.

Learning from [31, 32] that it is possible to quadratize multi-term functions so compactly inspired us, and the fact that such 'compact' quadratizations are only known for a very specific category of functions (the AkON functions), motivated us to look for quadratizations that are 'compact', but also applicable to a much wider class of functions. The result of this study is the theorem described in the title of this paper, and explained in more detail in the section below. It allows up to 5 terms of a function (1 of them can be of degree-4 and the other 4 can be of degree-3) to be quadratized with only 1 auxiliary variable rather than 5 auxiliaries (which is what would be required if quadratizing each term individually with $\log_2 k$-1 auxiliary variables for each term).

II. RESULTS

Theorem 1: All 4-variable functions of binary variables with real-valued coefficients can be quadratized perfectly with only 1-auxiliary variable.

By 'perfect' quadratization we mean all 2^4 output values of the 4-variable function are exactly preserved when minimizing over the auxiliary variable in the 5-variable quadratic function. Therefore any 4-variable subset of an n-variable problem can be quadratized with only 1-auxiliary variable.

We prove the theorem by providing an explicit quadratization for various different cases, of the following function of binary variables $b_i \in \{0,1\}$ with real-valued coefficients α:

$$\alpha_{1234}b_1b_2b_3b_4 + \alpha_{123}b_1b_2b_3 + \alpha_{124}b_1b_2b_4 + \alpha_{134}b_1b_3b_4 + \alpha_{234}b_2b_3b_4. \tag{1}$$

Since $\alpha_{123}, \alpha_{124}, \alpha_{134}$ and α_{234} are completely symmetric (they can be switched with each other and have their subscripts relabeled without any effect on the function), we can order them however we desire, so for convenience we choose for the rest of this paper: $\alpha_{123} \le \alpha_{124} \le \alpha_{134} \le \alpha_{234}$.

We will now provide 4 different quadratization formulas for Eq. 1 (Lemmas 1-4), which each are only valid for their own specific conditions on the α coefficients; but we will then prove with Lemmas 6-8 that these 4 cases for the coefficients, cover every possible case. The explicit quadratizations for Lemmas 1-4 are given below, but their proofs take up a lot of space so they are given in the Appendix.

Lemma 1: Suppose $\alpha_{1234} \ge 0$. If $\alpha_{ijk} \ge -\frac{\alpha_{1234}}{2}$ for all ijk, or $-\alpha_{1234} \le \alpha_{123} \le -\frac{\alpha_{1234}}{2} \le 0 \le \alpha_{234} \le \alpha_{134} \le \alpha_{124}$, or both $-\alpha_{1234} \le \alpha_{123} \le -\frac{\alpha_{1234}}{2} \le \alpha_{124} \le \alpha_{134} \le \alpha_{234} \le 0$, and $\alpha_{123} + \alpha_{124} \ge -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\left(3\alpha_{1234} + \sum\nolimits_{ijk} \alpha_{ijk}\right) b_a + \alpha_{1234} \sum_{ij} b_i b_j + \sum_{ij} \sum_{k \notin ij} \alpha_{ijk} b_i b_j - \sum_i \left(2\alpha_{1234} + \sum\nolimits_{jk, i \neq jk} \alpha_{ijk}\right) b_i b_a. \tag{2}$$

Lemma 2: If $\alpha_{1234} \le 0$ and $\alpha_{ijk} \le 0$, then Eq. 1 is perfectly quadratized by:

$$\left(\alpha_{1234}\left(\sum\nolimits_i b_i - 3\right) + \sum_{ijk} \alpha_{ijk} \left(\sum\nolimits_{l \in ijk} b_l - 2\right)\right) b_a. \tag{3}$$

Lemma 3: If $\alpha_{1234} \ge 0$, $\alpha_{123} \le -\alpha_{1234}$, and $-\frac{\alpha_{1234}}{2} \le \alpha_{124} \le \alpha_{134} \le 0 \le \alpha_{234}$, then Eq. 1 is perfectly quadratized by:

$$\alpha_{1234} - \sum_i \left(\alpha_{12i} + \alpha_{1234}\right) b_i + \sum_i \alpha_{i34} b_a + \sum_{\substack{ijk \\ i,j \neq 1,2}} \alpha_{ijk} b_i b_j + \alpha_{1234} b_3 b_4 - \sum_{\substack{i=p,q \\ p,q=1,2 \text{ or } 3,4}} \left(\sum\nolimits_{\substack{j=r,s \\ r,s=3,4 \text{ or } 1,2}} \alpha_{pqj} - \alpha_{irs}\right) b_i b_a. \tag{4}$$

Lemma 4: If $\alpha_{1234} \ge 0$, $\alpha_{123} \le -\frac{\alpha_{1234}}{2} \le \alpha_{124} \le \alpha_{134} \le \alpha_{234} \le 0$, and $\alpha_{123} + \alpha_{124} \le -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\alpha_{1234} - \sum_i (\alpha_{12i} + \alpha_{1234}) b_i + \sum_i \alpha_{i34} b_a + \sum_{ijk} \alpha_{ijk} b_i b_j + \alpha_{1234} b_3 b_4 - \sum_{\substack{i=p,q \\ p,q=1,2 \text{ or } 3,4}} \left(\sum\nolimits_{\substack{j=r,s \\ r,s=3,4 \text{ or } 1,2}} \alpha_{pqj} - \alpha_{irs}\right) b_i b_a \tag{5}$$

$$- \sum_i \alpha_{12i} \left(b_1 + b_2\right) - \sum_i \alpha_{i34} \left(b_3 + b_4 - 1 - b_i\right) - \alpha_{1234} \left(b_3 + b_4 - 1\right) b_a. \tag{6}$$

In the Appendix, Lemmas 1-4 are each proven for their own specific conditions on the coefficients α. However with 'bit-flipping' (a strategy described in [1] and on Pg. 27 of the current version of [15]) we can extend their applicability to more general conditions for which a laborious proof was not peformed explicitly. Lemma 6 will describe the effect of flipping one bit in Eq. 1, and Lemma 7 will describe the effect of flipping two. Since the function is completely symmetric with respect to the four variables b_1, b_2, b_3 and b_4, these Lemmas depend only on the number of bits flipped and not at all on which bits are flipped.

Lemma 6: If one bit is flipped ($b_1 \rightarrow \bar{b}_1 \equiv 1 - b_1$) everywhere in Eq. 1, then the function remains exactly the same except with $\bar{\alpha}_{1234} \equiv -\alpha_{1234}$, $\bar{\alpha}_{123} = -\alpha_{123}$, $\bar{\alpha}_{124} = -\alpha_{124}$, $\bar{\alpha}_{134} = -\alpha_{134}$, $\bar{\alpha}_{234} = \alpha_{234} + \alpha_{1234}$, **and some extra quadratic terms:** $f_{\text{quadratic},1}(b_1, b_2, b_3, b_4) \equiv \alpha_{123}b_2b_3 + \alpha_{124}b_2b_4 + \alpha_{134}b_3b_4$.

Proof: We start with Eq. 1 but with every occurrence of b_1 replaced by its flipped version:

$$\alpha_{1234}\bar{b}_1b_2b_3b_4 + \alpha_{123}\bar{b}_1b_2b_3 + \alpha_{124}\bar{b}_1b_2b_4 + \alpha_{134}\bar{b}_1b_3b_4 + \alpha_{234}b_2b_3b_4. \tag{7}$$

Expanding $\bar{b}_1$ as $1 - b_1$, and completely expanding the expressions for each term of Eq. 7, we get:

$$\alpha_{1234}(b_2b_3b_4 - b_1b_2b_3b_4) + \alpha_{123}(b_2b_3 - b_1b_2b_3) + \alpha_{124}(b_2b_4 - b_1b_2b_4) + \alpha_{134}(b_3b_4 - b_1b_3b_4) + \alpha_{234}b_2b_3b_4 \tag{8}$$

We can now regroup everything in Eq. 8 such that it is back in the form of Eq. 1, except with new coefficients:

$$-\alpha_{1234}b_1b_2b_3b_4 - \alpha_{123}b_1b_2b_3 - \alpha_{124}b_1b_2b_4 - \alpha_{134}b_1b_3b_4 + (\alpha_{1234} + \alpha_{234})b_2b_3b_4 + \alpha_{123}b_2b_3 + \alpha_{124}b_2b_4 + \alpha_{134}b_3b_4 \tag{9}$$

$$= \bar{\alpha}_{1234}b_1b_2b_3b_4 + \bar{\alpha}_{123}b_1b_2b_3 + \bar{\alpha}_{124}b_1b_2b_4 + \bar{\alpha}_{134}b_1b_3b_4 + \bar{\alpha}_{234}b_2b_3b_4 + f_{\text{quadratic},1}(b_1, b_2, b_3, b_4). \tag{10}$$

Lemma 7: If two bits are flipped ($b_1 \rightarrow \bar{b}_1 \equiv 1 - b_1, b_2 \rightarrow \bar{b}_2 \equiv 1 - b_2$) everywhere in Eq. 1, the function remains exactly the same except with $\bar{\alpha}_{134} \equiv -(\alpha_{134} + \alpha_{1234})$, $\bar{\alpha}_{234} \equiv -(\alpha_{234} + \alpha_{1234})$, **and some extra quadratic terms:** $f_{\text{quadratic},2}(b_1, b_2, b_3, b_4) \equiv \alpha_{1234}b_3b_4 + \alpha_{123}(b_3 - b_1b_3 - b_2b_3) + \alpha_{124}(b_4 - b_1b_4 - b_2b_4) + (\alpha_{134} + \alpha_{234})b_3b_4$.

Proof: We start with Eq. 1 but with every occurrence of b_1 and b_2 replaced by their flipped versions:

$$\alpha_{1234}\bar{b}_1\bar{b}_2b_3b_4 + \alpha_{123}\bar{b}_1\bar{b}_2b_3 + \alpha_{124}\bar{b}_1\bar{b}_2b_4 + \alpha_{134}\bar{b}_1b_3b_4 + \alpha_{234}\bar{b}_2b_3b_4. \tag{11}$$

Expanding $\bar{b}_1$ and $\bar{b}_2$ as $1 - b_1$ and $1 - b_2$ respectively, and completely expanding the expressions for each term of Eq. 11, we get:

$$\alpha_{1234}(b_3b_4 - b_2b_3b_4 - b_1b_3b_4 + b_1b_2b_3b_4) + \alpha_{123}(b_3 - b_1b_3 - b_2b_3 + b_1b_2b_3) + \alpha_{124}(b_4 - b_1b_4 - b_2b_4 + b_1b_2b_4) \tag{12}$$
$$+ \alpha_{134}(b_3b_4 - b_1b_3b_4) + \alpha_{234}(b_3b_4 - b_2b_3b_4).$$

We can now regroup everything in Eq. 12 such that it is back in the form of Eq. 1, except with new coefficients for two of the terms, and some extra quadratic terms:

$$\alpha_{1234}b_1b_2b_3b_4 + \alpha_{123}b_1b_2b_3 + \alpha_{124}b_1b_2b_4 - (\alpha_{134} + \alpha_{1234})b_1b_3b_4 - (\alpha_{234} + \alpha_{1234})b_2b_3b_4 \tag{13}$$
$$+ \alpha_{1234}b_3b_4 + \alpha_{123}(b_3 - b_1b_3 - b_2b_3) + \alpha_{124}(b_4 - b_1b_4 - b_2b_4) + (\alpha_{134} + \alpha_{234})b_3b_4.$$

$$= \alpha_{1234}b_1b_2b_3b_4 + \alpha_{123}b_1b_2b_3 + \alpha_{124}b_1b_2b_4 + \bar{\alpha}_{134}b_1b_3b_4 + \bar{\alpha}_{234}b_2b_3b_4 + f_{\text{quadratic},2}(b_1, b_2, b_3, b_4). \tag{14}$$

Lemma 6 allows us to assume from now on that $\alpha_{1234} \geq 0$, because every case with $\alpha_{1234} < 0$ can be turned into a case with $\alpha_{1234} > 0$ by fipping only one bit. With $\alpha_{1234} \geq 0$, we can categorize all cubic coefficients α_{ijk} according to whether they are $\leq -\alpha_{1234}$, or $\leq -\frac{\alpha_{1234}}{2}$, or whether they are simply just ≤ 0 or ≥ 0. There's then 35 different cases for how the four cubic coefficients α_{ijk} can fit into the four different non-overlapping intervals that can be made on the number line with $-\alpha_{1234}$, $-\frac{\alpha_{1234}}{2}$ and 0 as partition points. For some of these cases, Lemma 1, 3, 4 or 5 can be applied immediately. Due to the conditions used to prove Lemma 2, it cannot be applied directly to any of the 35 cases, but thanks to Lemmas 6 and 7, Lemma 2 can be applied to two of the 35 cases after bit-flipping appropriately. Lemma 1, 3, 4 or 5 can be applied for the rest of the 35 cases if 2, 3, or 4 bits are flipped (meaning either one application of Lemma 7, one application of Lemma 6 combined with one application of Lemma 7, or two applications of Lemma 7, is done). This means that one of Lemmas 1-5 can be applied for all of the 35 possible cases, as long as Lemmas 6 and/or 7 are applied appropriately. Table I summarizes which bits have to be flipped using Lemma 6 and/or Lemma 7, and which of Lemmas 1-5 can be applied, for each of the 35 possible cases.

Table I. All possible cases of 4-variable functions with $\alpha_{1234} \geq 0$.

$\alpha_{ijk} \leq -\alpha_{1234}$	$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$	$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$	$0 \leq \alpha_{ijk}$	Bits flipped	Quadratization
			$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$	-	Lemma 1
		α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$	-	Lemma 1
	α_{123}		$\alpha_{124}, \alpha_{134}, \alpha_{234}$	-	Lemma 1
α_{123}			$\alpha_{124}, \alpha_{134}, \alpha_{234}$	b_4	Lemma 2
		$\alpha_{123}, \alpha_{124}$	$\alpha_{134}, \alpha_{234}$	-	Lemma 1
	α_{123}	α_{124}	$\alpha_{134}, \alpha_{234}$	b_2, b_4	Lemma 3
α_{123}		α_{124}	$\alpha_{134}, \alpha_{234}$	b_3, b_4	Lemma 1
	$\alpha_{123}, \alpha_{124}$		$\alpha_{134}, \alpha_{234}$	b_3, b_4	Lemma 1
α_{123}	α_{124}		$\alpha_{134}, \alpha_{234}$	b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}$			$\alpha_{134}, \alpha_{234}$	b_3, b_4	Lemma 1
		$\alpha_{123}, \alpha_{124}, \alpha_{134}$	α_{234}	-	Lemma 1
	α_{123}	$\alpha_{124}, \alpha_{134}$	α_{234}	b_1, b_4	Lemma 4
α_{123}		$\alpha_{124}, \alpha_{134}$	α_{234}	-	Lemma 3
	$\alpha_{123}, \alpha_{124}$	α_{134}	α_{234}	b_3, b_4	Lemma 1
α_{123}	α_{124}	α_{134}	α_{234}	b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}$		α_{134}	α_{234}	b_3, b_4	Lemma 1
	$\alpha_{123}, \alpha_{124}, \alpha_{134}$		α_{234}	b_1, b_2, b_3, b_4	Lemma 4
α_{123}	$\alpha_{124}, \alpha_{134}$		α_{234}	b_2, b_3	Lemma 3
$\alpha_{123}, \alpha_{124}$	α_{134}		α_{234}	b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}, \alpha_{134}$			α_{234}	b_2, b_3, b_4	Lemma 2
		$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$		-	Lemma 1
	α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$		-	Lemma 1, 4
α_{123}		$\alpha_{124}, \alpha_{134}, \alpha_{234}$		-	Lemma 4
	$\alpha_{123}, \alpha_{124}$	$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
α_{123}	α_{124}	$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}$		$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
	$\alpha_{123}, \alpha_{124}, \alpha_{134}$	α_{234}		b_3, b_4	Lemma 1, 4
α_{123}	$\alpha_{124}, \alpha_{134}$	α_{234}		b_2, b_3	Lemma 4
$\alpha_{123}, \alpha_{124}$	α_{134}	α_{234}		b_2, b_3	Lemma 3
$\alpha_{123}, \alpha_{124}, \alpha_{134}$		α_{234}		b_1, b_2, b_3, b_4	Lemma 1
	$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$			b_1, b_2, b_3, b_4	Lemma 1
α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$			b_1, b_2, b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}$	$\alpha_{134}, \alpha_{234}$			b_1, b_2, b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}, \alpha_{134}$	α_{234}			b_1, b_2, b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$				b_1, b_2, b_3, b_4	Lemma 1

Table II. Simplified version of Table I.

<table>
<tr><th>$\alpha_{ijk} \leq -\alpha_{1234}$</th><th>$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$</th><th>$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$</th><th>$0 \leq \alpha_{ijk}$</th><th>$\alpha_{123} + \alpha_{124}$</th><th>Bits flipped</th><th>Quadratization</th></tr>
<tr><td rowspan="2"></td><td></td><td colspan="2">$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$</td><td rowspan="6">-</td><td rowspan="2">-</td><td rowspan="2">Lemma 1</td></tr>
<tr><td colspan="2">α_{123}</td><td>$\alpha_{124}, \alpha_{134}, \alpha_{234}$</td></tr>
<tr><td>α_{123}</td><td colspan="2"></td><td>$\alpha_{124}, \alpha_{134}, \alpha_{234}$</td><td>$b_4$</td><td>Lemma 2</td></tr>
<tr><td></td><td>α_{123}</td><td>α_{124}</td><td>$\alpha_{134}, \alpha_{234}$</td><td>$b_2, b_3$</td><td>Lemma 3</td></tr>
<tr><td>α_{123}</td><td></td><td>α_{124}</td><td>$\alpha_{134}, \alpha_{234}$</td><td>$b_3, b_4 b_3, b_4$</td><td>Lemma 1</td></tr>
<tr><td colspan="2">$\alpha_{123}, \alpha_{124}$</td><td colspan="2">$\alpha_{134}, \alpha_{234}$</td><td>$b_3, b_4 b_3, b_4$</td><td>Lemma 1</td></tr>
<tr><td></td><td>α_{123}</td><td>$\alpha_{124}, \alpha_{134}$</td><td>$\alpha_{234}$</td><td>$\leq -\alpha_{1234}$</td><td>$b_1, b_4$</td><td>Lemma 4</td></tr>
<tr><td>α_{123}</td><td></td><td>$\alpha_{124}, \alpha_{134}$</td><td>$\alpha_{234}$</td><td>-</td><td>-</td><td>Lemma 3</td></tr>
<tr><td></td><td>$\alpha_{123}, \alpha_{124}, \alpha_{134}$</td><td></td><td>$\alpha_{234}$</td><td>$\leq -\alpha_{1234}$</td><td>$b_1, b_2, b_3, b_4$</td><td>Lemma 4</td></tr>
<tr><td>α_{123}</td><td>$\alpha_{124}, \alpha_{134}$</td><td></td><td>$\alpha_{234}$</td><td>-</td><td>$b_2, b_3$</td><td>Lemma 3</td></tr>
<tr><td>$\alpha_{123}, \alpha_{124}$</td><td>$\alpha_{134}$</td><td></td><td>$\alpha_{234}$</td><td>-</td><td>$b_3, b_4$</td><td>Lemma 1</td></tr>
<tr><td>$\alpha_{123}, \alpha_{124}, \alpha_{134}$</td><td></td><td></td><td>α_{234}</td><td>-</td><td>b_2, b_3, b_4</td><td>Lemma 2</td></tr>
<tr><td></td><td>α_{123}</td><td rowspan="2">$\alpha_{124}, \alpha_{134}, \alpha_{234}$</td><td rowspan="2"></td><td>$\geq -\alpha_{1234}$</td><td rowspan="2">-</td><td>Lemma 1</td></tr>
<tr><td colspan="2">α_{123}</td><td>$\leq -\alpha_{1234}$</td><td>Lemma 4</td></tr>
<tr><td rowspan="2"></td><td rowspan="2">$\alpha_{123}, \alpha_{124}, \alpha_{134}$</td><td rowspan="2">$\alpha_{234}$</td><td rowspan="2"></td><td>$\geq -\alpha_{1234}$</td><td rowspan="2">b_3, b_4</td><td>Lemma 1</td></tr>
<tr><td>$\leq -\alpha_{1234}$</td><td>Lemma 4</td></tr>
<tr><td>α_{123}</td><td>$\alpha_{124}, \alpha_{134}$</td><td>$\alpha_{234}$</td><td rowspan="3"></td><td>-</td><td rowspan="2">b_2, b_3</td><td>Lemma 4</td></tr>
<tr><td>$\alpha_{123}, \alpha_{124}$</td><td>$\alpha_{134}$</td><td>$\alpha_{234}$</td><td>-</td><td>Lemma 3</td></tr>
<tr><td>$\alpha_{123}, \alpha_{124}, \alpha_{134}$</td><td></td><td>$\alpha_{234}$</td><td>-</td><td>$b_1, b_2, b_3, b_4$</td><td>Lemma 1</td></tr>
<tr><td colspan="2">$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$</td><td colspan="2"></td><td>-</td><td>b_1, b_2, b_3, b_4</td><td>Lemma 1</td></tr>
</table>

A. 8-variable, degree-4, function

The following function can be quadratized using only *two* auxiliary variables when using Theorem 1 of the present paper, but would require a minimum of *four* auxiliary variables when using the previous state-of-of-the-art methods:

$$b_1b_2b_3b_4 + b_1b_2b_3 + b_1b_2b_4 + 2b_1b_3b_4 + 3b_2b_3b_4 - b_5b_6b_7b_8 - 2b_5b_6b_7 - 3b_5b_6b_8 - 4b_5b_7b_8 - 5b_6b_7b_8 + b_1b_8. \tag{15}$$

To apply Theorem 1 of the present paper, we will first split the super-quadratic terms into two categories, each involving a different set of 4 variables:

$$b_1b_2b_3b_4+b_1b_2b_3+b_1b_2b_4+2b_1b_3b_4+3b_2b_3b_4-b_5b_6b_7b_8-2b_5b_6b_7-3b_5b_6b_8-4b_5b_7b_8-5b_6b_7b_8 + b_1b_8. \tag{16}$$

The two sub-functions can be quadratized using Lemma 1 (with the addition of the auxiliary variable b_{a_1}) and 2 (with the addition of the auxiliary variable b_{a_2}) respectively:

$$b_1b_2b_3b_4+b_1b_2b_3+b_1b_2b_4+2b_1b_3b_4+3b_2b_3b_4 \rightarrow 3b_1b_2+4b_1b_3+4b_1b_4+5b_2b_3+5b_2b_4+6b_3b_4+b_{a_1}(10-6b_1-7b_2-8b_3-8b_4) \tag{17}$$

$$-b_5b_6b_7b_8-2b_5b_6b_7-3b_5b_6b_8-4b_5b_7b_8-5b_6b_7b_8 \rightarrow -b_{a_2}(31-10b_5-11b_6-12b_7-13b_8). \tag{18}$$

Previous state-of-the-art

Prior to the present paper, a minimum of *four* auxiliary variables would be needed because out of all the methods described in the book of quadratizations [15], no method can quadratize the terms involving (b_1, b_2, b_3, b_4) and the terms involving (b_5, b_6, b_7, b_8) with fewer than two auxiliary variables each, which is what can be done with Rosenberg's substitution method [18] with the following auxiliary variables defined:

$$b_{a_1} \equiv b_1b_2, \quad b_{a_2} \equiv b_3b_4, \quad b_{a_3} \equiv b_5b_6, \quad b_{a_4} \equiv b_7b_8, \tag{19}$$

which leads to the following quadratic terms (and coefficients chosen based on the recommendation in Gruber's thesis):

$$b_{a_1}b_{a_2}+b_{a_1}b_3+b_{a_1}b_4+2b_1b_{a_2}+3b_2b_{a_2}+3(b_{a_1}-2b_{a_1}b_1-2b_{a_1}b_2+3b_{a_1})+6(b_{a_2}-2b_{a_2}b_3-2b_{a_2}b_4+3b_{a_2}) \tag{20}$$

$$-b_{a_3}b_{a_4}-2b_{a_3}b_7-3b_{a_3}b_8-4b_5b_{a_4}-5b_6b_{a_4}+b_1b_8+6(b_{a_3}-2b_{a_3}b_5-2b_{a_3}b_6+3b_{a_3})+10(b_{a_4}-2b_{a_4}b_7-2b_{a_4}b_8+3b_{a_4}). \tag{21}$$

Comparison

Number of auxiliary variables: Previous state-of-the-art (4), Present (2).
Number of quadratic terms in quadratization result: Previous state-of-the-art (19), Present (14).
Range of coefficients: Previous state-of-the-art (-20 to +30), Present (-13 to +31).

B. $4N$-variable, degree-4 function:

Consider the function:

$$2b_1b_2b_3b_4-b_1b_2b_4-b_4b_5+2b_5b_6b_7b_8-b_5b_6b_8-b_8b_9+2b_9b_{10}b_{11}b_{12}-b_9b_{10}b_{12}-\cdots-b_{4N-4}b_{4N-3}+2b_{4N-3}b_{4N-2}b_{4N-1}b_{4N}-b_{4N-2}b_{4N-1}b_{4N}. \tag{22}$$

With Theorem 1, we can quadratize this function with only N auxiliary variables (one for each set of 4 variables). A term-wise quadratization would need $2N$ variables (one for each of the N degree-4 terms, and one for each of the N degree-3 terms). Pairwise covers would also need $2N$ variables because the degree-4 terms alone would require 2 auxiliary variables each.

C. 12-term, 5-variable, degree-4, function with all terms at least cubic:

To quadratize the following function:

$$5b_1b_2b_3b_4 + 4b_1b_2b_3b_5 + 3b_1b_2b_4b_5 - 3b_1b_2b_3 - b_1b_2b_4 - 5b_1b_2b_5 - b_1b_3b_4 - b_1b_3b_5 - b_1b_4b_5 - 2b_2b_3b_4 - b_2b_3b_5 - 4b_2b_4b_5 \quad (23)$$

normally we would need at least 12 auxiliary variables (at least one for each term). Instead we quadratize the whole function with only 3 auxiliary variables. To do this we will apply Theorem 1 for 3 sub-functions (displayed below in five different colors) that contain only 4 variables:

$$5b_1b_2b_3b_4 + 4b_1b_2b_3b_5 + 3b_1b_2b_4b_5 - 3b_1b_2b_3 - b_1b_2b_4 - 5b_1b_2b_5 - b_1b_3b_4 - b_1b_3b_5 - b_1b_4b_5 - 2b_2b_3b_4 - b_2b_3b_5 - 4b_2b_4b_5. \quad (24)$$

We now quadrtize these 5 sub-functions with only 1 auxiliary variable for each sub-function, using Lemmas 5, 4, and 3 in that order:

$$5b_1b_2b_3b_4-3b_1b_2b_3-b_1b_2b_4-b_1b_3b_4-2b_2b_3b_4 \rightarrow b_1b_2 + b_1b_3 + 3b_1b_4 + 2b_2b_4 + 2b_3b_4 - b_{a_1}(5b_1 + 4b_2 + 4b_3 + 6b_4 - 8) \quad (25)$$

$$4b_1b_2b_3b_5-5b_1b_2b_5-b_1b_3b_5-b_2b_3b_5 \rightarrow -3b_1 + 6b_2 - 3b_3 + 5b_5 - 5b_1b_2 + 3b_1b_3 - 5b_1b_5 - b_2b_3 - b_3b_5 \quad (26)$$

$$-b_{a_2}(-8b_1 + 6b_2 - 4b_3 + 5b_5 + 3) + 3 \quad (27)$$

$$3b_1b_2b_4b_5-b_1b_4b_5-4b_2b_4b_5 \rightarrow b_1+4b_2+3b_1b_2-b_1b_4-b_1b_5-4b_2b_4-4b_2b_5+b_{a_3}(-4b_1-7b_2+5b_4+5b_5+3) \quad (28)$$

The final quadratic function contains only 8 variables (the 5 original ones and the 3 new auxiliary variables), whereas applying a termwise quadratization technique would in the best case result in a quadratic function with 17 variables (the 5 original ones and the 12 new auxiliary variables).

Previous state-of-the-art

Pairwise covers would require 4 auxiliary variables. It is not possible with only 3 auxiliary variables because we cannot cover all 9 cubic terms in (this sentence isn't complete?). One pairwise cover for the index combinations of this function is $\{12, 34, 35, 45\}$ and since none of the elements contain more than two indices, the quadratization can be done by Rosenberg's substitution. We first define the auxiliary variables:

$$b_{a_1} \equiv b_1b_2, \quad b_{a_2} \equiv b_3b_4 \quad b_{a_3} \equiv b_3b_5 \quad b_{a_4} \equiv b_4b_5. \quad (29)$$

Then we have the following quadratic function (and coefficients chosen based on the recommendation in Gruber's thesis):

$$5b_{a_1}b_{a_2}+4b_{a_1}b_{a_3}+3b_{a_1}b_{a_4}-3b_{a_1}b_3-b_{a_1}b_4-5b_{a_1}b_5-b_1b_{a_2}-b_1b_{a_3}-b_1b_{45}-2b_2b_{a_2}-b_2b_{a_3}-4b_2b_{a_4}+21(b_1b_2-2b_{a_1}b_1-2b_{a_1}b_2+3b_{a_1}) \quad (30)$$

$$+8(b_3b_4-2b_{a_2}b_3-2b_{a_2}b_4+3b_{a_2})+6(b_3b_5-2b_{a_3}b_3-2b_{a_3}b_5+3b_{a_3})+8(b_4b_5-2b_{a_4}b_4-2b_{a_4}b_5+3b_{a_4}). \quad (31)$$

Comparison

Number of auxiliary variables: Previous state-of-the-art (4), Present (3).
Number of quadratic terms in quadratization result: Previous state-of-the-art (24), Present (27).
Range of coefficients: Previous state-of-the-art (-42 to +63), Present (-7 to +10).

D. 15-term, 5-variable, degree-4, function with all terms at least cubic (i.e. all possible super-quadratic terms):

We will present the function with the colors already assigned, for applying Theorem 1:

$$5b_1b_2b_3b_4-3b_1b_2b_3-b_1b_2b_4-5b_1b_2b_5-b_1b_3b_4-b_1b_3b_5-b_1b_4b_5-2b_2b_3b_4-b_2b_3b_5-4b_2b_4b_5-3b_3b_4b_5+5b_1b_2b_3b_4+4b_1b_2b_3b_5+3b_1b_2b_4b_5+2b_1b_3b_4b_5+b_2b_3b_4b_5. \quad (32)$$

We then apply Theorem 1 five times, once for the terms of each color:

$$5b_1b_2b_3b_4 - 3b_1b_2b_3 - b_1b_2b_4 - b_1b_3b_4 - 2b_2b_3b_4 \to b_1b_2 + b_1b_3 + 3b_1b_4 + 2b_2b_4 + 2b_3b_4 - b_{a_1}(5b_1 + 4b_2 + 4b_3 + 6b_4 - 8) \tag{33}$$

$$4b_1b_2b_3b_5 - 5b_1b_2b_5 - b_1b_3b_5 - b_2b_3b_5 \to -3b_1 + 6b_2 - 3b_3 + 5b_5 - 5b_1b_2 + 3b_1b_3 - 5b_1b_5 - b_2b_3 - b_3b_5 \tag{34}$$

$$-b_{a_2}(-8b_1 + 6b_2 - 4b_3 + 5b_5 + 3) + 3 \tag{35}$$

$$3b_1b_2b_4b_5 - b_1b_4b_5 - 4b_2b_4b_5 \to b_1 + 4b_2 + 3b_1b_2 - b_1b_4 - b_1b_5 - 4b_2b_4 - 4b_2b_5 + b_{a_3}(-4b_1 - 7b_2 + 5b_4 + 5b_5 + 3) \tag{36}$$

$$2b_1b_3b_4b_5 - 3b_3b_4b_5 \to b_{a_4}(2b_1 - 3b_3 - 3b_4 - 3b_5 + 6) \tag{37}$$

$$b_2b_3b_4b_5 \to b_2b_3 + b_2b_4 + b_2b_5 + b_3b_4 + b_3b_5 + b_4b_5 + b_{a_5}(3 - 2b_2 - 2b_3 - 2b_4 - 2b_5). \tag{38}$$

Previous state-of-the-art

Applying the method of pairwise covers with the following definitions for auxiliary variables:

$$b_{a_1} \equiv b_1b_2, b_{a_2} \equiv b_1b_3, b_{a_3} \equiv b_4b_5, b_{a_4} \equiv b_2b_3, b_{a_5} \equiv b_1b_2b_3, \tag{39}$$

we arrive at the following quadratic function:

$$-3b_{a_1}b_3 - b_{a_1}b_4 - 5b_{a_1}b_5 - b_{a_2}b_4 - b_{a_2}b_5 - b_1b_{a_3} - 2b_{a_4}b_4 - b_{a_4}b_5 - 4b_2b_{a_3} - 3b_3b_{a_3} + 5b_{a_5}b_4 + 4b_{a_5}b_5 + 3b_{a_1}b_{a_3} + 2b_{a_2}b_{a_3} + b_{a_4}b_{a_3} \tag{40}$$

$$+ 9\left(b_{a_5}(5 - 2b_1 - 2b_2 - 2b_3) + b_{a_1}b_3\right) + 21\left(b_{a_1}(3 - 2b_1 - 2b_2) + b_1b_2\right) + 4\left(b_{a_2}(3 - 2b_1 - 2b_3) + b_1b_3\right) \tag{41}$$

$$+ 4\left(b_{a_4}(3 - 2b_2 - 2b_3) + b_2b_3\right) + 14\left(b_{a_3}(3 - 2b_4 - 2b_5) + b_4b_5\right). \tag{42}$$

Comparison

Number of auxiliary variables: Previous state-of-the-art (5), Present (5).
Number of quadratic terms in quadratization result: Previous state-of-the-art (31), Present (37).
Range of coefficients: Previous state-of-the-art (-42 to +63), Present (-7 to +8).

E. 4-variable function that is not written as a polynomial

To emphasize that literally any real-valued 4-variable function of boolean variables can be quadratized with only one auxiliary variable, we present here an example that is not written in the form of Eq. 1:

$$\arctan(b_1 + b_2)e^{\min(b_2,b_3)}\sqrt{5b_4}. \tag{43}$$

To quadratize this 4-variable function with 1 auxiliary variable, we first convert it into polynomial form using the observation first made by Hammer in 1963 and presented as Proposition 2 in [33], and we get the polynomial:

$$\sqrt{5}b_4\left(\frac{\pi}{4}b_1 + \frac{\pi}{4}b_2 + b_1b_2\left(\arctan(2) - \frac{\pi}{2}\right) + \frac{\pi}{4}(e-1)b_2b_3 + b_1b_2b_3(e-1)\left(\arctan(2) - \frac{\pi}{4}\right)\right) \tag{44}$$

$$= \frac{\sqrt{5}\pi}{4}b_1b_4 + \frac{\sqrt{5}\pi}{4}b_2b_4 + \sqrt{5}\left(\arctan(2) - \frac{\pi}{2}\right)b_1b_2b_4 + \frac{\sqrt{5}\pi}{4}(e-1)b_2b_3b_4 + (e-1)\left(\arctan(2) - \frac{\pi}{4}\right)b_1b_2b_3b_4. \tag{45}$$

The last three terms have degree larger than 2, but we can quadratize all three of them with one application of Lemma 1. We thus obtain the quadratic function (after rounding the coefficients):

$$-5.70 + 0.20b_1b_2 + 1.24b_1b_3 + 1.96b_1b_4 + 4.26b_2b_3 + 4.98b_2b_4 + 4.26b_3b_4 - 1.44b_1b_a + 4.46b_2b_a + 5.50b_3b_a + 4.46b_4b_a. \tag{46}$$

The best alternative quadratization as far as we are aware, uses Rosenberg's substitution, in which we first define the auxiliary variables:

$$b_{a_1} \equiv b_1 b_3, \quad b_{a_2} \equiv b_2 b_4, \tag{47}$$

and get the following quadratic function:

$$1.76b_{a_2} + 1.76b_1b_4 - 1.04b_1b_{a_2} + 3.02b_3b_{a_2} + 1.24b_{a_1}b_{a_2} + 5.30\left(b_2b_4 - 2b_2b_{a_2} - 2b_4b_{a_2} + 3b_{a_2}\right) + 1.24\left(b_1b_3 - 2b_1b_{a_1} - 2b_3b_{a_1} + 3b_{a_1}\right). \tag{48}$$

Comparison

Number of auxiliary variables: Previous state-of-the-art (2), Present (1).
Number of quadratic terms in quadratization result: Previous state-of-the-art (10), Present (10).
Range of coefficients: Previous state-of-the-art (-10.60 to +15.90), Present (-1.44 to +5.50).

IV. DISCUSSION

A. Non-uniqueness

We note that functions can have multiple different quadratizations, even when with the same number of auxiliary qubits. Therefore, while Lemmas 1-4 constitute the only quadratization formulas needed for proving Theorem 1, we considered the possibility that alternative quadratization formulas exist, but it turned out that all quadratization formulas that we found, could by bit-flipping be turned exactly into one of our presented formulas. Nevertheless, we do not rule out the possibility that other quadratization formulas involving only one auxiliary variable can exist: it may just be that we have not found them.

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