

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

Nike Dattani¹ and Hou Tin Chau²

¹Harvard-Smithsonian Center for Astrophysics, USA*

²Cambridge University, Churchill College, 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: we provide quadratizations for all possible 4-variable functions. There exists 4 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 5 examples of functions that can be quadratized using the result of this work. For each of the 5 examples we compare the best possible quadratization we could construct using previously known methods, to a quadratization that we construct using our new result. In the most extreme example, the quadratization using our new result needs only N auxiliary variables for a $4N$ -variable degree-4 function, whereas the previous state-of-the-art quadratization requires $2N$ (double as many) auxiliary variables and therefore we can reduce by the cost of optimizing such a function by a factor of 2^{1000} if it were to have 4000 variables before quadratization. In all 5 of our examples, the range of coefficient sizes in our quadratic function is smaller than in the previous state-of-the-art one, and our coefficient range is a factor of 7 times smaller in our 15-term, 5-variable example of a degree-4 function.

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 $k = d^2$ with $d \geq 2$ 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 d -color Ramsey number (where $k = \frac{dN(N-1)}{2}$) [11–13].

Solving such discrete optimization problems with $k > 2$ can be very difficult, and more methods have been developed for the $k = 2$ case (such as the algorithm known as “QPBO” and extensions of it [14], and quantum annealing using thousands of superconducting qubits [15] connected by graphs as complicated as Pegasus [16, 17]) 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’ [18].

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, 19, 20], but not every function can be turned into a single quadratic function with the same global optimum 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). Discovering 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 [21], and some subsequent quadratization methods were published in 2004 [22], 2005 [23], and 2011 [1, 2, 24, 25], but the rest of the methods were published in the last 5 years (from 2014–2019) [8, 13, 18–20, 26–37].

In 2018 a remarkable discovery was made [35, 36], that degree- k monomials can be quadratized with only $\log_2 \binom{k}{2}$ 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 $\log_2 \binom{k}{2}$ 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 [35, 36] that sometimes a function of n variables can entirely be quadratized with only $\log_2 \binom{k}{2}$ 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 [35, 36] 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 2 auxiliaries, which used to be the best

possible quadratization known for such a 5-term function, and is a substantial improvement over the 5 auxiliaries that would be required if quadratizing each term individually with $\log_2 (k/2)$ 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, without affecting any properties of the much larger n -variable function after minimizing over the 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 :

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

Define Q to be the set of all $\alpha = (\alpha_{1234}, \alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}) \in \mathbb{R}^5$ such that Formula 1 can be quadratized with 1 auxiliary. We want to show that $Q = \mathbb{R}^5$, which is a restatement of Theorem 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: $\alpha_{123} \leq \alpha_{124} \leq \alpha_{134} \leq \alpha_{234}$ unless otherwise stated.

We will now provide a quadratization formula for Formula 1 in Lemma 1, which is only valid when some conditions on the α coefficients hold; but we will then prove Lemmas 2 and Corollary 3 and combine them in Table I to prove Theorem 1. The explicit quadratizations for Lemma 2 1 is given below, but its proof take up a lot of space so it is given in the Appendix.

Lemma 1: If $\alpha_{ijk} \geq -\alpha_{1234}$ for all ijk , and $\alpha_{ijk} + \alpha_{lmn} \geq -\alpha_{1234}$ whenever $ijk \neq lmn$, then Formula 1 is perfectly quadratized by:

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

Define the region $S = \{(\alpha_{1234}, \alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}) \in \mathbb{R}^5 : \alpha_{ijk} \geq -\alpha_{1234} \forall ijk, \alpha_{ijk} + \alpha_{lmn} \geq -\alpha_{1234} \text{ whenever } ijk \neq lmn\}$. The Lemma then says $S \subseteq Q$.

In the Appendix, Lemma 1 is proven. However with ‘bit-flipping’ (a strategy described in [1] and on Pg. 27 of the current version of [18]) we can extend their applicability to more general conditions for which a laborious proof was not performed explicitly. Lemma 2 will describe the effect of flipping one bit in Eq. 1. By 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 2: 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 $\bar{\alpha}_{1234} \equiv -\alpha_{1234}$, $\bar{\alpha}_{123} \equiv -\alpha_{123}$, $\bar{\alpha}_{124} \equiv -\alpha_{124}$, $\bar{\alpha}_{134} \equiv -\alpha_{134}$, $\bar{\alpha}_{234} \equiv \alpha_{234} + \alpha_{1234}$, 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:

$$\alpha_{1234}\bar{b}_1b_2b_3b_4 + \alpha_{123}\bar{b}_1b_2b_3 + \alpha_{124}\bar{b}_1b_2b_4 + \alpha_{134}\bar{b}_1b_3b_4 + \alpha_{234}b_2b_3b_4. \quad (3)$$

Expanding \bar{b}_1 as $1 - b_1$, and completely expanding the expressions for each term of Eq. 3, we get:

$$\alpha_{1234}(b_2b_3b_4 - b_1b_2b_3b_4) + \alpha_{123}(b_2b_3 - b_1b_2b_3) + \alpha_{124}(b_2b_4 - b_1b_2b_4) + \alpha_{134}(b_3b_4 - b_1b_3b_4) + \alpha_{234}b_2b_3b_4 \quad (4)$$

We can now regroup everything in Eq. 4 such that it is back in the form of Eq. 1, except with new coefficients:

$$- \alpha_{1234}b_1b_2b_3b_4 - \alpha_{123}b_1b_2b_3 - \alpha_{124}b_1b_2b_4 - \alpha_{134}b_1b_3b_4 + (\alpha_{1234} + \alpha_{234})b_2b_3b_4 + \alpha_{123}b_2b_3 + \alpha_{124}b_2b_4 + \alpha_{134}b_3b_4 \quad (5)$$

$$= \bar{\alpha}_{1234}b_1b_2b_3b_4 + \bar{\alpha}_{123}b_1b_2b_3 + \bar{\alpha}_{124}b_1b_2b_4 + \bar{\alpha}_{134}b_1b_3b_4 + \bar{\alpha}_{234}b_2b_3b_4 + f_{\text{quadratic},1}(b_1, b_2, b_3, b_4). \quad (6)$$

Corollary 3: Define the ‘bit-flip’ map $\varphi_1 : \mathbb{R}^5 \rightarrow \mathbb{R}^5$ given by $\varphi_1(\alpha) = (-\alpha_{1234}, -\alpha_{123}, -\alpha_{124}, -\alpha_{134}, \alpha_{234} + \alpha_{1234})$ which is the transformation acting on the tuple of coefficients when we flip b_1 in Lemma 4, and similarly φ_2, φ_3 , and φ_4 for the corresponding map when we flip b_2, b_3 , and b_4 respectively. Then for each i , we have $\alpha \in Q \iff \varphi_i(\alpha) \in Q$.

Proof: If $\alpha \in Q$, then for some quadratic g we have

$$\alpha_{1234}\bar{b}_1b_2b_3b_4 + \alpha_{123}\bar{b}_1b_2b_3 + \alpha_{124}\bar{b}_1b_2b_4 + \alpha_{134}\bar{b}_1b_3b_4 + \alpha_{234}b_2b_3b_4 = \min_{b_a} g(\bar{b}_1, b_2, b_3, b_4, b_a),$$

so

$$\bar{\alpha}_{1234}b_1b_2b_3b_4 + \bar{\alpha}_{123}b_1b_2b_3 + \bar{\alpha}_{124}b_1b_2b_4 + \bar{\alpha}_{134}b_1b_3b_4 + \bar{\alpha}_{234}b_2b_3b_4 = \min_{b_a} g(1 - b_1, b_2, b_3, b_4, b_a) - f_{\text{quadratic},1}(\bar{b}_1, b_2, b_3, b_4),$$

so $\varphi_1(\alpha) \in Q$. The other direction comes from the fact that $\varphi_1(\varphi_1(\alpha)) = \alpha$.

The same holds for other indices $i = 2, 3, 4$.

We can also flip more than one bit. The corresponding transformations are given by:

$$\varphi_2(\varphi_1(\alpha)) = (\alpha_{1234}, \alpha_{123}, \alpha_{124}, -\alpha_{1234} - \alpha_{134}, -\alpha_{1234} - \alpha_{234}),$$

$$\varphi_3(\varphi_2(\varphi_1(\alpha))) = (-\alpha_{1234}, -\alpha_{123}, \alpha_{1234} + \alpha_{124}, \alpha_{1234} + \alpha_{134}, \alpha_{1234} + \alpha_{234}),$$

$$\varphi_4(\varphi_3(\varphi_2(\varphi_1(\alpha)))) = (\alpha_{1234}, -\alpha_{1234} - \alpha_{123}, -\alpha_{1234} - \alpha_{124}, -\alpha_{1234} - \alpha_{134}, -\alpha_{1234} - \alpha_{234}).$$

We can also verify that $\varphi_1 \circ \varphi_2 = \varphi_2 \circ \varphi_1$ so any φ_i and φ_j commute and we do not have to consider the order of such transformations.

Corollary 3 allows us to assume from now on that $\alpha_{1234} \geq 0$, because if $\alpha_{1234} < 0$ then $\alpha' = \varphi_1(\alpha)$ has $\alpha'_{1234} \geq 0$, and by Corollary 3, $\alpha \in Q \iff \alpha' \in Q$. 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 . We then have 35 different cases (see Table I) 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. Some of these cases needs to be further broken down into two subcases depending on some sum $\alpha_{ijk} + \alpha_{lmn}$. Only for some of these cases, Lemma 1 can be applied immediately (i.e. $\alpha \in S$), but thanks to Lemma 2 and Corollary 3, Lemma 1 can be applied to more cases after bit-flipping appropriately (i.e. there is some sequence i_1, \dots, i_k such that $\varphi_{i_k} \circ \dots \circ \varphi_{i_1}(\alpha) \in S \subseteq Q$, which implies $\alpha \in Q$). Table I summarizes which bits have to be flipped to reduce the problem to one that is that is solved by Lemma 1. Since so many neighboring cases are often covered by a same transformation, we were also able to make Table II, which is a more compact version of Table I.

Table I. All 35 possible cases of 4-variable functions with $\alpha_{1234} \geq 0$, and the corresponding lemma (or lemmas) of this paper that provide a quadratization for each case.

$\alpha_{ijk} \leq -\alpha_{1234}$	$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$	$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$	$0 \leq \alpha_{ijk}$	Other conditions	Bit flips required
			$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$		-
α_{123}	α_{123}	α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{124}, \alpha_{134}, \alpha_{234}$		- - b_1, b_2, b_4
α_{123}	α_{123}	$\alpha_{123}, \alpha_{124}$ α_{124} α_{124}	$\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$	$\alpha_{123} + \alpha_{124} \geq -\alpha_{1234}$ $\alpha_{123} + \alpha_{124} \leq -\alpha_{1234}$	- - b_3, b_4 b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$	$\alpha_{123}, \alpha_{124}$ α_{124}		$\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$		b_3, b_4 b_3, b_4 b_3, b_4
α_{123}	α_{123}	$\alpha_{123}, \alpha_{124}, \alpha_{134}$ $\alpha_{124}, \alpha_{134}$ $\alpha_{124}, \alpha_{134}$	α_{234} α_{234} α_{234}	$\alpha_{123} + \alpha_{124} \geq -\alpha_{1234}$ $\alpha_{123} + \alpha_{124} \leq -\alpha_{1234}$	- - b_3, b_4 b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$	$\alpha_{123}, \alpha_{124}$ α_{124}	α_{134} α_{134} α_{134}	α_{234} α_{234} α_{234}		b_3, b_4 b_3, b_4 b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$ $\alpha_{123}, \alpha_{124}, \alpha_{134}$	$\alpha_{123}, \alpha_{124}, \alpha_{134}$ $\alpha_{124}, \alpha_{134}$ α_{134}		α_{234} α_{234} α_{234}		b_3, b_4 b_3, b_4 b_3, b_4 b_1
α_{123}	α_{123}	$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{124}, \alpha_{134}, \alpha_{234}$		$\alpha_{123} + \alpha_{124} \geq -\alpha_{1234}$ $\alpha_{123} + \alpha_{124} \leq -\alpha_{1234}$	- - b_3, b_4 b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$	$\alpha_{123}, \alpha_{124}$ α_{124}	$\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$			b_3, b_4 b_3, b_4 b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$ $\alpha_{123}, \alpha_{124}, \alpha_{134}$	$\alpha_{123}, \alpha_{124}, \alpha_{134}$ $\alpha_{124}, \alpha_{134}$ α_{134}	α_{234} α_{234} α_{234}		$\alpha_{134} + \alpha_{234} \geq -\alpha_{1234}$ $\alpha_{134} + \alpha_{234} \leq -\alpha_{1234}$ $\alpha_{134} + \alpha_{234} \geq -\alpha_{1234}$ $\alpha_{134} + \alpha_{234} \leq -\alpha_{1234}$ $\alpha_{134} + \alpha_{234} \geq -\alpha_{1234}$ $\alpha_{134} + \alpha_{234} \leq -\alpha_{1234}$	b_3, b_4 b_1, b_2, b_3, b_4 b_3, b_4 b_1, b_2, b_3, b_4 b_3, b_4 b_1, b_2, b_3, b_4 b_1, b_2, b_3, b_4
α_{123} $\alpha_{123}, \alpha_{124}$ $\alpha_{123}, \alpha_{124}, \alpha_{134}$ $\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$	$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{124}, \alpha_{134}, \alpha_{234}$ $\alpha_{134}, \alpha_{234}$ α_{234}				b_1, b_2, b_3, b_4 b_1, b_2, b_3, b_4 b_1, b_2, b_3, b_4 b_1, b_2, b_3, b_4 b_1, b_2, b_3, b_4

III. EXAMPLES

A. 11-term, 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-the-art methods:

$$b_1 b_2 b_3 b_4 + b_1 b_2 b_3 + b_1 b_2 b_4 + 2b_1 b_3 b_4 + 3b_2 b_3 b_4 - b_5 b_6 b_7 b_8 - 2b_5 b_6 b_7 - 3b_5 b_6 b_8 - 4b_5 b_7 b_8 - 5b_6 b_7 b_8 + b_1 b_8. \quad (7)$$

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:

$$b_1 b_2 b_3 b_4 + b_1 b_2 b_3 + b_1 b_2 b_4 + 2b_1 b_3 b_4 + 3b_2 b_3 b_4 - b_5 b_6 b_7 b_8 - 2b_5 b_6 b_7 - 3b_5 b_6 b_8 - 4b_5 b_7 b_8 - 5b_6 b_7 b_8 + b_1 b_8. \quad (8)$$

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

Table II. Simplified version of Table I.

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

$$b_1 b_2 b_3 b_4 + b_1 b_2 b_3 + b_1 b_2 b_4 + 2b_1 b_3 b_4 + 3b_2 b_3 b_4 \rightarrow 3b_1 b_2 + 4b_1 b_3 + 4b_1 b_4 + 5b_2 b_3 + 5b_2 b_4 + 6b_3 b_4 + b_{a_1} (10 - 6b_1 - 7b_2 - 8b_3 - 8b_4) \quad (9)$$

$$-b_5 b_6 b_7 b_8 - 2b_5 b_6 b_7 - 3b_5 b_6 b_8 - 4b_5 b_7 b_8 - 5b_6 b_7 b_8 \rightarrow b_{a_2} (31 - 10b_5 - 11b_6 - 12b_7 - 13b_8). \quad (10)$$

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 [18], 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 [21] with the following auxiliary variables defined:

$$b_{a_1} \equiv b_1 b_2, \quad b_{a_2} \equiv b_3 b_4, \quad b_{a_3} \equiv b_5 b_6, \quad b_{a_4} \equiv b_7 b_8, \quad (11)$$

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

$$b_{a_1} b_{a_2} + b_{a_1} b_3 + b_{a_1} b_4 + 2b_1 b_{a_2} + 3b_2 b_{a_2} + 3(b_{a_1} - 2b_{a_1} b_1 - 2b_{a_1} b_2 + 3b_{a_1}) + 6(b_{a_2} - 2b_{a_2} b_3 - 2b_{a_2} b_4 + 3b_{a_2}) \quad (12)$$

$$-b_{a_3} b_{a_4} - 2b_{a_3} b_7 - 3b_{a_3} b_8 - 4b_5 b_{a_4} - 5b_6 b_{a_4} + b_1 b_8 + 6(b_{a_3} - 2b_{a_3} b_5 - 2b_{a_3} b_6 + 3b_{a_3}) + 10(b_{a_4} - 2b_{a_4} b_7 - 2b_{a_4} b_8 + 3b_{a_4}). \quad (13)$$

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:

$$f = -2b_1 b_2 b_3 b_4 + b_1 b_2 b_3 + 5b_4 b_5 - 2b_5 b_6 b_7 b_8 + b_5 b_6 b_7 + 5b_8 b_9 - 2b_9 b_{10} b_{11} b_{12} + b_9 b_{10} b_{11} + \dots + 5b_{4N-4} b_{4N-3} - 2b_{4N-3} b_{4N-2} b_{4N-1} b_{4N} + b_{4N-3} b_{4N-2} b_{4N-1} \quad (14)$$

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 at least $2N$ 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.

Using Theorem 1, we can quadratise $-2b_1b_2b_3b_4 + b_1b_2b_3$ as $2b_1 + 2b_2 + 2b_3 + b_1b_2 + b_1b_3 + b_2b_3 - 2b_1b_4 - 2b_2b_4 - 2b_3b_4 + b_a(5 - 3b_1 - 3b_2 - 3b_3 + 4b_4)$, so f can be quadratised as

$$\begin{aligned} & 2b_1 + 2b_2 + 2b_3 + b_1b_2 + b_1b_3 + b_2b_3 - 2b_1b_4 - 2b_2b_4 - 2b_3b_4 + b_a(5 - 3b_1 - 3b_2 - 3b_3 + 4b_4) + 5b_4b_5 \\ & + 2b_5 + 2b_6 + 2b_7 + b_5b_6 + b_5b_7 + b_6b_7 - 2b_5b_8 - 2b_6b_8 - 2b_7b_8 + b_a(5 - 3b_5 - 3b_6 - 3b_7 + 4b_8) + 5b_8b_9 + \dots \\ & + 2b_{4N-3} + 2b_{4N-2} + 2b_{4N-1} + b_{4N-3}b_{4N-2} + b_{4N-3}b_{4N-1} + b_{4N-2}b_{4N-1} - 2b_{4N-3}b_{4N} - 2b_{4N-2}b_{4N} - 2b_{4N-3}b_{4N} + b_a(5 - 3b_{4N-3} \end{aligned}$$

Previous state-of-the-art

There are exactly two non-isomorphic to quadratise $-2b_1b_2b_3b_4 + b_1b_2b_3$ using pairwise cover with two auxiliaries: $\{12, 123\}$ and $\{12, 34\}$ are both covers. The first gives the quadratisation

$$-2b_{a_2}b_4 + b_{a_1}b_3 + 3(b_{a_1}(3 - 2b_1 - 2b_2) + b_1b_2) + 2(b_{a_2}(5 - 2b_1 - 2b_2 - 2b_3) + b_{a_1}b_3),$$

and the second gives

$$-2b_{a_1}b_{a_2} + b_{a_1}b_3 + 3(b_{a_1}(3 - 2b_1 - 2b_2) + b_1b_2) + 2(b_{a_2}(3 - 2b_3 - 2b_4) + b_3b_4).$$

The second is better it has fewer quadratic terms.

The original function can thus be quadratised as

$$\begin{aligned} & -2b_{a_1}b_{a_2} + b_{a_1}b_3 + 3(b_{a_1}(3 - 2b_1 - 2b_2) + b_1b_2) + 2(b_{a_2}(3 - 2b_3 - 2b_4) + b_3b_4) + 5b_4b_5 \\ & -2b_{a_3}b_{a_4} + b_{a_3}b_7 + 3(b_{a_3}(3 - 2b_5 - 2b_6) + b_5b_6) + 2(b_{a_2}(3 - 2b_7 - 2b_8) + b_7b_8) + 5b_8b_9 + \dots \\ & -2b_{a_{2N-1}}b_{a_{2N}} + b_{a_{2N-1}}b_{4N-1} + 3(b_{a_{2N-1}}(3 - 2b_{4N-3} - 2b_{4N-2}) + b_{4N-3}b_{4N-2}) + 2(b_{a_{2N}}(3 - 2b_{4N-1} - 2b_{4N}) + b_{4N-1}b_{4N}). \end{aligned}$$

Comparison

Number of auxiliary variables: Previous state-of-the-art ($2N$), Present (N).

Number of quadratic terms in quadratization result: Previous state-of-the-art ($9N - 1$), Present ($11N - 1$).

Range of coefficients: Previous state-of-the-art (-6 to $+9$), Present (-3 to $+5$).

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

We can quadratize the following function:

$$5b_1b_2b_3b_4 + 4b_1b_2b_3b_5 + 3b_1b_2b_4b_5 - 3b_1b_2b_3 - b_1b_2b_4 - 5b_1b_2b_5 - b_1b_3b_4 - b_1b_3b_5 - b_1b_4b_5 - 2b_2b_3b_4 - b_2b_3b_5 - 4b_2b_4b_5, \quad (15)$$

with only 3 auxiliary variables. To do this we will apply Theorem 1 for three sub-functions (displayed below in three different colors) that contain only 4 variables:

$$5b_1b_2b_3b_4 + 4b_1b_2b_3b_5 + 3b_1b_2b_4b_5 - 3b_1b_2b_3 - b_1b_2b_4 - 5b_1b_2b_5 - b_1b_3b_4 - b_1b_3b_5 - b_1b_4b_5 - 2b_2b_3b_4 - b_2b_3b_5 - 4b_2b_4b_5. \quad (16)$$

We now quadratize these 3 sub-functions with only 1 auxiliary variable for each sub-function by Theorem 1:

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

$$4b_1b_2b_3b_5 - 5b_1b_2b_5 - b_1b_3b_5 - b_2b_3b_5 \rightarrow -3b_1 + 6b_2 - 3b_3 + 5b_5 - 5b_1b_2 + 3b_1b_3 - 5b_1b_5 - b_2b_3 - b_3b_5 \quad (18)$$

$$-b_{a_2}(-8b_1 + 6b_2 - 4b_3 + 5b_5 + 3) + 3 \quad (19)$$

$$3b_1b_2b_4b_5 - b_1b_4b_5 - 4b_2b_4b_5 \rightarrow b_1 + 4b_2 + 3b_1b_2 - b_1b_4 - b_1b_5 - 4b_2b_4 - 4b_2b_5 + b_{a_3}(-4b_1 - 7b_2 + 5b_4 + 5b_5 + 3) \quad (20)$$

The final quadratic function contains only 8 variables (the 5 original ones and the 3 new auxiliary variables).

Previous state-of-the-art

Pairwise covers would require at least 4 auxiliary variables. It is not possible with only 3 auxiliary variables because we cannot cover all 9 cubic terms with only 3 auxiliary variables. 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:

$$b_{a_1} \equiv b_1b_2, \quad b_{a_2} \equiv b_3b_4, \quad b_{a_3} \equiv b_3b_5, \quad b_{a_4} \equiv b_4b_5. \quad (21)$$

Then we have the following quadratic function (and coefficients chosen based on the recommendation in Eq. (3.44) in Gruber's thesis):

$$5b_{a_1}b_{a_2} + 4b_{a_1}b_{a_3} + 3b_{a_1}b_{a_4} - 3b_{a_1}b_3 - b_{a_1}b_4 - 5b_{a_1}b_5 - b_1b_{a_2} - b_1b_{a_3} - b_1b_{a_4} - 2b_2b_{a_2} - b_2b_{a_3} - 4b_2b_{a_4} + 21(b_1b_2 - 2b_{a_1}b_1 - 2b_{a_1}b_2 + 3b_{a_1}) \quad (22)$$

$$+ 8(b_3b_4 - 2b_{a_2}b_3 - 2b_{a_2}b_4 + 3b_{a_2}) + 6(b_3b_5 - 2b_{a_3}b_3 - 2b_{a_3}b_5 + 3b_{a_3}) + 8(b_4b_5 - 2b_{a_4}b_4 - 2b_{a_4}b_5 + 3b_{a_4}). \quad (23)$$

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:

$$5b_1b_2b_3b_4 - 3b_1b_2b_3 - b_1b_2b_4 - 5b_1b_2b_5 - b_1b_3b_4 - b_1b_3b_5 - b_1b_4b_5 - 2b_2b_3b_4 - b_2b_3b_5 - 4b_2b_4b_5 - 3b_3b_4b_5 + 4b_1b_2b_3b_5 + 3b_1b_2b_4b_5 + 2b_1b_3b_4b_5 + b_2b_3b_4b_5. \quad (24)$$

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

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

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

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

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

$$2b_1b_3b_4b_5 - 3b_3b_4b_5 \rightarrow b_{a_4}(2b_1 - 3b_3 - 3b_4 - 3b_5 + 6) \quad (29)$$

$$b_2b_3b_4b_5 \rightarrow b_2b_3 + b_2b_4 + b_2b_5 + b_3b_4 + b_3b_5 + b_4b_5 + b_{a_5}(3 - 2b_2 - 2b_3 - 2b_4 - 2b_5). \quad (30)$$

Previous state-of-the-art

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

$$b_{a_1} \equiv b_1 b_2, b_{a_2} \equiv b_1 b_3, b_{a_3} \equiv b_4 b_5, b_{a_4} \equiv b_2 b_3, b_{a_5} \equiv b_1 b_2 b_3, \quad (31)$$

we arrive at the following quadratic function:

$$-3b_{a_1}b_3 - b_{a_1}b_4 - 5b_{a_1}b_5 - b_{a_2}b_4 - b_{a_2}b_5 - b_1b_{a_3} - 2b_{a_4}b_4 - b_{a_4}b_5 - 4b_2b_{a_3} - 3b_3b_{a_3} + 5b_{a_5}b_4 + 4b_{a_5}b_5 + 3b_{a_1}b_{a_3} + 2b_{a_2}b_{a_3} + b_{a_4}b_{a_3} \quad (32)$$

$$+ 9(b_{a_5}(5 - 2b_1 - 2b_2 - 2b_3) + b_{a_1}b_3) + 21(b_{a_1}(3 - 2b_1 - 2b_2) + b_1b_2) + 4(b_{a_2}(3 - 2b_1 - 2b_3) + b_1b_3) \quad (33)$$

$$+ 4(b_{a_4}(3 - 2b_2 - 2b_3) + b_2b_3) + 14(b_{a_3}(3 - 2b_4 - 2b_5) + b_4b_5). \quad (34)$$

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 +10).

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:

$$\arctan(b_1 + b_2)e^{\min(b_2, b_3)}\sqrt{5b_4}. \quad (35)$$

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 [38], and we get the polynomial:

$$\sqrt{5}b_4 \left(\frac{\pi}{4}b_1 + \frac{\pi}{4}b_2 + b_1b_2 \left(\arctan(2) - \frac{\pi}{2} \right) + \frac{\pi}{4}(e-1)b_2b_3 + b_1b_2b_3(e-1) \left(\arctan(2) - \frac{\pi}{4} \right) \right) \quad (36)$$

$$= \frac{\sqrt{5}\pi}{4}b_1b_4 + \frac{\sqrt{5}\pi}{4}b_2b_4 + \sqrt{5} \left(\arctan(2) - \frac{\pi}{2} \right) b_1b_2b_4 + \frac{\sqrt{5}\pi}{4}(e-1)b_2b_3b_4 + \sqrt{5}(e-1) \left(\arctan(2) - \frac{\pi}{4} \right) b_1b_2b_3b_4. \quad (37)$$

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):

$$0.20b_1b_2 + 1.24b_1b_3 + 0.20b_1b_4 + 4.25b_2b_3 + 3.22b_2b_4 + 4.25b_3b_4 + 5.70b_a - 1.44b_1b_a - 4.45b_2b_a - 5.49b_3b_a - 4.45b_4b_a. \quad (38)$$

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

$$b_{a_1} \equiv b_1b_3, \quad b_{a_2} \equiv b_2b_4, \quad (39)$$

and get the following quadratic function:

$$1.76b_{a_2} + 1.76b_1b_4 - 1.04b_1b_{a_2} + 3.02b_3b_{a_2} + 1.24b_{a_1}b_{a_2} + 5.30(b_2b_4 - 2b_2b_{a_2} - 2b_4b_{a_2} + 3b_{a_2}) + 1.24(b_1b_3 - 2b_1b_{a_1} - 2b_3b_{a_1} + 3b_{a_1}). \quad (40)$$

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 they have the same number of auxiliary qubits. Therefore, while Lemmas 1 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 yet found them.

V. ACKNOWLEDGMENTS

We wish to thank Elisabeth Rodríguez-Heck for helpful comments on an early version of this paper.

* nik.dattani@gmail.com

† houtinchau@gmail.com

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* nik.dattani@gmail.com

† houtinchau@gmail.com

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