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

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We prove that any function 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 $n \gg 4$.

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) [**? ?**], integer factoring (where typically $k = 4$) [**? ? ? ? ? ? ? ? ?**], and determining whether or not a number N is an m-color Ramsey number (where $k = \frac{mN(N-1)}{2}$) [**? ? ?**].

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 [**?**]) 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" [**?**].

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) [**? ? ? ?**], 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 [**?**], and some subsequent quadratization methods were published in 2004 [**?**], 2005 [**?**], and 2011 [**? ? ?**], but the rest of the methods were published in the last 5 years (from 2014-2018) [**? ? ? ? ? ? ? ? ? ? ?**].

In the most recent of these papers [**? ?**], 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 [**? ?**] that sometimes the entire function of n variables can 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 the case of a single positive monomial term.

Learning from [**? ?**] that it is possible to quadratize very large 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 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 $b_i \in \{0, 1\}$:

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

First we reduce to the case where $\alpha_{1234} \geq 0$, and $\alpha_{123} \leq \alpha_{124} \leq \alpha_{134} \leq \alpha_{234}$ and $-\frac{\alpha_{1234}}{2} \leq \alpha_{124} \leq \alpha_{134} \leq \alpha_{234}$. Then we will prove 5 Lemmas which cover all such cases.

Table I. All possible cases of 4-variable functions.

$\alpha_{ijk} \leq -\alpha_{1234}$	$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$	$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$	$0 \leq \alpha_{ijk}$	Bits flipped	
			$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$		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
		$\alpha_{123}, \alpha_{124}, \alpha_{134}$	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
$\alpha_{123}\alpha_{124}$		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 5
α_{123}		$\alpha_{124}, \alpha_{134}, \alpha_{234}$			Lemma 4
$\alpha_{123}, \alpha_{124}$		$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
$\alpha_{123}\alpha_{124}$		$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
$\alpha_{123}, \alpha_{124}$		$\alpha_{134}, \alpha_{234}$		b_3, b_4	Lemma 1
	$\alpha_{123}, \alpha_{124}, \alpha_{134}$	α_{234}		b_3, b_4	Lemma 5
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

$\alpha_{ijk} \leq -\alpha_{1234}$	$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$	$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$	$0 \leq \alpha_{ijk}$	Bits flipped	
			$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$		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 5
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 5
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

Lemma 0: If a function of the form in Eq. 1 can be perfectly quadratized, then the function obtained by flipping two bits in the original function, can also be perfectly quadratized. Here is how:

$$\alpha_{1234}\bar{b}_1\bar{b}_2b_3b_4 + \alpha_{123}\bar{b}_1\bar{b}_2b_3 + \alpha_{124}\bar{b}_1\bar{b}_2b_4 + \alpha_{134}\bar{b}_1b_3b_4 + \alpha_{234}\bar{b}_2b_3b_4 \tag{2}$$

$$\begin{aligned}
&= \alpha_{1234}\left(b_3b_4 - b_2b_3b_4 - b_1b_3b_4 + b_1b_2b_3b_4\right) + \alpha_{123}\left(b_3 - b_1b_3 - b_2b_3 + b_1b_2b_3\right) + \alpha_{124}\left(b_4 - b_1b_4 - b_2b_4 + b_1b_2b_4\right) && (3)\\
&\quad + \alpha_{134}\left(b_3b_4 - b_1b_3b_4\right) + \alpha_{234}\left(b_3b_4 - b_2b_3b_4\right) && (4)\\
&= \alpha_{1234}b_1b_2b_3b_4 + \alpha_{123}b_1b_2b_3 + \alpha_{124}b_1b_2b_4 + \left(-\alpha_{134} - \alpha_{1234}\right)b_1b_3b_4 + \left(-\alpha_{234} - \alpha_{1234}\right)b_2b_3b_4 && (5)\\
&\quad + \alpha_{1234}b_3b_4 + \alpha_{123}\left(b_3 - b_1b_3 - b_2b_3\right) + \alpha_{124}\left(b_4 - b_1b_4 - b_2b_4\right) + \left(\alpha_{134} + \alpha_{234}\right)b_3b_4 && (6)\\
&= \alpha_{1234}b_1b_2b_3b_4 + \alpha_{123}b_1b_2b_3 + \alpha_{124}b_1b_2b_4 + \bar{\alpha}_{134}b_1b_3b_4 + \bar{\alpha}_{234}b_2b_3b_4 + f_{\text{quadratic}}\left(b_1, b_2, b_3, b_4\right) && (7)
\end{aligned}$$

where we have defined:

$$\begin{aligned}
\bar{\alpha}_{134} &\equiv -\alpha_{134} - \alpha_{1234}, && (8)\\
\bar{\alpha}_{234} &\equiv -\alpha_{234} - \alpha_{1234}, && (9)\\
f_{\text{quadratic}}\left(b_1, b_2, b_3, b_4\right) &\equiv \alpha_{1234}b_3b_4 + \alpha_{123}\left(b_3 - b_1b_3 - b_2b_3\right) + \alpha_{124}\left(b_4 - b_1b_4 - b_2b_4\right) + \left(\alpha_{134} + \alpha_{234}\right)b_3b_4. && (10)
\end{aligned}$$

Lemma 1: If $\alpha_{1234} \geq 0$, and either $\alpha_{ijk} \geq -\frac{\alpha_{1234}}{2}$ for all ijk, or $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq 0 \leq \alpha_{234} \leq \alpha_{134} \leq \alpha_{124}$, then Eq. 1 is perfectly quadratized by:

$$\left(3\alpha_{1234} + \sum_{ijk} \alpha_{ijk}\right) b_a + \alpha_{1234} \sum_{ij} b_i b_j + \sum_{ij} \sum_{k \notin ij} \alpha_{ijk} b_i b_j - \sum_{i} \left(2\alpha_{1234} + \sum_{jk, i \neq jk} \alpha_{ijk}\right) b_i b_a. \tag{11}$$

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

$$\left(\alpha_{1234}\left(\sum_i b_i - 3\right) + \sum_{ijk} \alpha_{ijk}\left(\sum_{l \in ijk} b_l - 2\right)\right) b_a. \tag{12}$$

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

$$-\sum_i \alpha_{12i} b_i + \sum_{\substack{i=3,4 \\ j=1,2}} \alpha_{12i} b_i b_j + (\alpha_{134} + \alpha_{234} + \alpha_{1234})\, b_3 b_4 + \sum_i \alpha_{12i}\left(b_i - b_1 - b_2\right) b_a + \sum_i \alpha_{i34}\left(1 - b_3 + b_i - b_4\right) b_a + \alpha_{1234}(1 - b_3 - b_4). \tag{13}$$

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

$$\sum_{i=3,4} \alpha_{12i}\left(-b_1 - b_2 + b_1 b_i + b_2 b_i\right) + \sum_{i=1,2} \alpha_{i34}\left(1 + b_i - b_3 - b_4 + b_3 b_4\right) + \alpha_{1234}\left(1 - b_3 - b_4 + b_3 b_4\right) \tag{14}$$

$$+\, b_a \left(\sum_{i=3,4} \alpha_{12i}\left(b_1 + b_2 - b_i\right) + \sum_{i=1,2} \alpha_{i34}\left(-b_i + b_3 + b_4 - 1\right) + \alpha_{1234}\left(b_3 + b_4 - 1\right)\right) \tag{15}$$

Lemma 5: If $\alpha_{1234} \geq 0$, $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq \alpha_{124} \leq \alpha_{134} \leq \alpha_{234} \leq 0$, and $\alpha_{123} + \alpha_{124} \geq -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\sum_{ijk} \alpha_{ijk} \sum_{lm \subset ijk} b_l b_m + \alpha_{1234} \sum_{ij} b_i b_j + b_a \left(\sum_{ijk} \alpha_{ijk}\left(1 - \sum_{l \in ijk} b_l\right) + \alpha_{1234}\left(3 - 2\sum_i b_i\right)\right). \tag{16}$$