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 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 7 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) > 0[? ?], 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 case 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 some entire functions (no matter how many terms and how many variables they contain) can be quadratized with only $\log_2(k) - 1$ auxiliary variables. For many functions this can still be very costly though, because for example, quadratizing each monomial term with $\log_2(k) - 1$ auxiliary variables can mean the new optimization problem has far more variables than the original one.

This motivated us to look for quadratizations that are compact, but also applicable to many real-world problems. The result of this study is the theorem described in the title of this paper, and explained in more detail in the section below.

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 outcomes 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.

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 7 Lemmas which cover all such cases.

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

$\alpha_{ijk} \leq -\alpha_{1234}$	$-\alpha_{1234} \leq \alpha_{ijk} \leq -\frac{\alpha_{1234}}{2}$	$-\frac{\alpha_{1234}}{2} \leq \alpha_{ijk} \leq 0$	$0 \leq \alpha_{ijk}$	
			$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$	Lemma 1
		α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$	Lemma 1
	α_{123}		$\alpha_{124}, \alpha_{134}, \alpha_{234}$	Lemma 8
α_{123}			$\alpha_{124}, \alpha_{134}, \alpha_{234}$	Lemma 2
		$\alpha_{123}, \alpha_{124}$	$\alpha_{134}, \alpha_{234}$	Lemma 1
	α_{123}	α_{124}	$\alpha_{134}, \alpha_{234}$	Lemma 4, 5
α_{123}		α_{124}	$\alpha_{134}, \alpha_{234}$	Lemma 8
		$\alpha_{123}, \alpha_{124}, \alpha_{134}$	α_{234}	Lemma 1
	α_{123}	$\alpha_{124}, \alpha_{134}$	α_{234}	Lemma 4, 5
α_{123}		$\alpha_{124}, \alpha_{134}$	α_{234}	Lemma 3
		$\alpha_{123}, \alpha_{124}, \alpha_{134}, \alpha_{234}$		Lemma 1
	α_{123}	$\alpha_{124}, \alpha_{134}, \alpha_{234}$		Lemma 6
α_{123}		$\alpha_{124}, \alpha_{134}, \alpha_{234}$		Lemma 7

Lemma X: 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:

$$\alpha_{1234}\bar{b}_1\bar{b}_2 b_3 b_4 + \alpha_{123}\bar{b}_1\bar{b}_2 b_3 + \alpha_{124}\bar{b}_1\bar{b}_2 b_4 + \alpha_{134}\bar{b}_1 b_3 b_4 + \alpha_{234}\bar{b}_2 b_3 b_4 \tag{2}$$

$$= \alpha_{1234}\left(b_3 b_4 - \bar{b}_2 b_3 b_4 - \bar{b}_1 b_3 b_4 + \bar{b}_1\bar{b}_2 b_3 b_4\right) + \alpha_{123}\left(b_3 - \bar{b}_1 b_3 - \bar{b}_2 b_3 + \bar{b}_1\bar{b}_2 b_3\right) + \alpha_{124}\left(b_4 - \bar{b}_1 b_4 - \bar{b}_2 b_4 + \bar{b}_1\bar{b}_2 b_4\right) \tag{3}$$

$$+ \alpha_{134}\left(b_3 b_4 - \bar{b}_1 b_3 b_4\right) + \alpha_{234}\left(b_3 b_4 - \bar{b}_2 b_3 b_4\right) \tag{4}$$

$$= \alpha_{1234}\bar{b}_1\bar{b}_2 b_3 b_4 + \alpha_{123}\bar{b}_1\bar{b}_2 b_3 + \alpha_{124}\bar{b}_1\bar{b}_2 b_4 + \left(\alpha_{134} - \alpha_{1234}\right)\bar{b}_1 b_3 b_4 + \left(\alpha_{234} - \alpha_{1234}\right)\bar{b}_2 b_3 b_4 \tag{5}$$

$$+ \alpha_{1234} b_3 b_4 + \alpha_{123}\left(b_3 - \bar{b}_1 b_3 - \bar{b}_2 b_3\right) + \alpha_{124}\left(b_4 - \bar{b}_1 b_4 - \bar{b}_2 b_4\right) + \left(\alpha_{134} + \alpha_{234}\right) b_3 b_4 \tag{6}$$

$$= \alpha_{1234} b_1 b_2 b_3 b_4 + \alpha_{123} b_1 b_2 b_3 + \alpha_{124} b_1 b_2 b_4 + \bar{\alpha}_{134} b_1 b_3 b_4 + \bar{\alpha}_{234} b_2 b_3 b_4 + f_{\text{quadratic}}\left(b_1, b_2, b_3, b_4\right) \tag{7}$$

where we have defined:

$$\bar{\alpha}_{134} \equiv \alpha_{134} - \alpha_{1234}, \tag{8}$$

$$\bar{\alpha}_{234} \equiv \alpha_{234} - \alpha_{1234}, \tag{9}$$

$$f_{\text{quadratic}}\left(b_1, b_2, b_3, b_4\right) \equiv \alpha_{1234} b_3 b_4 + \alpha_{123}\left(b_3 - \bar{b}_1 b_3 - \bar{b}_2 b_3\right) + \alpha_{124}\left(b_4 - \bar{b}_1 b_4 - \bar{b}_2 b_4\right) + \left(\alpha_{134} + \alpha_{234}\right) b_3 b_4. \tag{10}$$

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

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

$$\tag{13}$$

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

$$\sum_{ijk} \alpha_{ijk} \left(1 - \sum_{l \in ijk} b_l + \sum_{lm \subset ijk} b_l b_m\right) + \alpha_{1234} \left(3 - 2\sum_i b_i + \sum_{ij} b_i b_j\right) + b_a \left(\sum_{ijk} \alpha_{ijk} \left(\sum_{l \in ijk} b_l - 1\right) + \alpha_{1234} \left(2\sum_i b_i - 3\right)\right). \quad (14)$$

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

$$\sum_{i=3,4} \alpha_{12i} \left(b_1 b_i + b_2 b_i - b_i\right) + \left(\alpha_{134} + \alpha_{234} + \alpha_{1234}\right) b_3 b_4 \quad (15)$$

$$+ b_a \left(\sum_{i=3,4} \alpha_{12i} \left(b_i - b_1 - b_2\right) + \sum_{i=1,2} \alpha_{i34} \left(1 + b_i - b_3 - b_4\right) + \alpha_{1234} \left(1 - b_3 - b_4\right)\right). \quad (16)$$

Lemma 6: If $-\alpha_{1234} \le \alpha_{123} \le -\frac{\alpha_{1234}}{2} \le \alpha_{124} \le \alpha_{134} \le \alpha_{234} \le 0$ **and** $\alpha_{123} + \alpha_{124} \ge -\alpha_{1234}$**, then Eq. 1 is perfectly quadratized by:**

$$\sum_{ijk} \alpha_{ijk} \sum_{lm \subset ijk} b_l b_m + \alpha_{1234} \sum_{ij} b_i b_j + b_a \left(\sum_{ijk} \alpha_{ijk} \left(1 - \sum_{l \in ijk} b_l\right) + \alpha_{1234} \left(3 - 2\sum_i b_i\right)\right). \quad (17)$$

Lemma 7: If $\alpha_{123} \le -\frac{\alpha_{1234}}{2} \le \alpha_{124} \le \alpha_{134} \le \alpha_{234} \le 0$ **and** $\alpha_{123} + \alpha_{124} \le -\alpha_{1234}$**, then Eq. 1 is perfectly quadratized by:**

$$\sum_{i=3,4} \alpha_{12i} \left(-b_1 - b_2 + b_1 b_i + b_2 b_i\right) + \sum_{i=1,2} \alpha_{i34} \left(1 + b_i - b_3 - b_4 + b_3 b_4\right) + \alpha_{1234} \left(1 - b_3 - b_4 + b_3 b_4\right) \quad (18)$$

$$+ b_a \left(\sum_{i=3,4} \alpha_{12i} \left(b_1 + b_2 - b_i\right) + \sum_{i=1,2} \alpha_{i34} \left(-b_i + b_3 + b_4 - 1\right) + \alpha_{1234} \left(b_3 + b_4 - 1\right)\right) \quad (19)$$

Lemma 8: If $-\alpha_{1234} \le \alpha_{123} \le -\frac{\alpha_{1234}}{2}$ **and** $0 \le \alpha_{234} \le \alpha_{134} \le \alpha_{124}$**, then Eq. 1 is perfectly quadratized by 11**