

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 8 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) [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 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 [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, 22–30].

In the most recent of these papers [29, 30], 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. Unfortunately those functions are either extremely obscure functions that would rarely come up in a real-world problem, or they are just monomials (meaning that for a real-world problem containing many terms, each of these terms would be quadratized separately, with $\log_2(k) - 1$ new auxiliary variables being added each time, and adding up to a potentially untractable number of total variables in the quadratic optimization problem).

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 $b_i \in \{0, 1\}$:

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

Case 1: An even number (2 or 4) of α_{ijk} are $\leq -\alpha_{1234}/2$ or $\geq -\alpha_{1234}/2$.

Case 2: An odd number (1 or 3) of α_{ijk} are $\leq -\alpha_{1234}/2$ or $\geq -\alpha_{1234}/2$.

Case 2.1: 0 of α_{ijk} are in $[-\alpha_{1234}, 0]$.

Case 2.2: 1 of α_{ijk} is in $[-\alpha_{1234}, 0]$.

Case 2.3: 2 of α_{ijk} are in $[-\alpha_{1234}, 0]$, one is $\leq -\alpha_{1234}$.

Case 2.4: 2 of α_{ijk} are in $[-\alpha_{1234}, 0]$, none are $\leq -\alpha_{1234}$, the lowest two α_{ijk} sum to $\geq -\alpha_{1234}$.

Case 2.5: 2 or 3 of α_{ijk} are in $[-\alpha_{1234}, 0]$, none are $\leq -\alpha_{1234}$, the lowest two α_{ijk} sum to $\leq -\alpha_{1234}$.

Case 2.6: 3 of α_{ijk} are in $[-\alpha_{1234}, 0]$, none are $\leq -\alpha_{1234}$, the lowest two α_{ijk} sum to $\geq -\alpha_{1234}$.

Case 2.7: All 4 of α_{ijk} are in $[-\alpha_{1234}, 0]$, the lowest two α_{ijk} sum to $\geq -\alpha_{1234}$.

Case 2.8: 3 or all 4 of α_{ijk} are in $[-\alpha_{1234}, 0]$, the lowest two α_{ijk} sum to $\leq -\alpha_{1234}$.

Lemma (Case 1): If $\alpha_{1234} \geq 0$, $\alpha_{ijk} \geq -\frac{\alpha_{1234}}{2}$, then Eq. 1 is perfectly quadratized by:

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

Lemma (Case 2.1): If $\alpha_{ijkl} \leq 0$ and $\alpha_{ijk} \leq 0$, then Eq. 1 is perfectly quadratized by:

$$b_a \left(\alpha_{1234} \left(\sum_i b_i - 3 \right) + \sum_{ijk} \alpha_{ijk} \left(\sum_{j \in ijk} b_j - 2 \right) \right). \quad (3)$$

Lemma (Case 2.2): If $\alpha_{1234} \geq 0$, $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2}$ and $\alpha_{234}, \alpha_{134}, \alpha_{124} \geq 0$, then Eq. 1 is perfectly quadratized by Eq. 2.

Lemma (Case 2.3): If $\alpha_{123} \leq -\alpha_{1234}$ and $-\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq \alpha_{134} \leq 0 \leq \alpha_{124}$, then Eq. 1 is perfectly quadratized by:

$$\alpha_{123}(-b_1 + b_1b_2 + b_1b_3) + \alpha_{234}(-b_4 + b_2b_4 + b_3b_4) + (\alpha_{134} + \alpha_{124} + \alpha_{1234})b_1b_4 \quad (4)$$

$$+ b_a(\alpha_{123}(b_1 - b_2 - b_3) + \alpha_{234}(-b_2 - b_3 + b_4) + \alpha_{134}(1 - b_1 + b_3 - b_4) + \alpha_{124}(1 - b_1 + b_2 - b_4) + \alpha_{1234}(1 - b_1 - b_4)). \quad (5)$$

Lemma (Case 2.4): If $\alpha_{123} \leq -\alpha_{1234}$ and $-\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq \alpha_{134} \leq 0 \leq \alpha_{124}$, then Eq. 1 is perfectly quadratized by:

$$\sum_{ijk} \alpha_{ijk} \left(1 - \sum_{i \in ijk} b_i + \sum_{ij \in ijk} b_i b_j \right) + \alpha_{1234} \left(3 - 2 \sum_i b_i + \sum_{ij} b_i b_j \right) + b_a \left(\sum_{ijk} \alpha_{ijk} \left(\sum_{l \in ijk} b_l - 1 \right) + \alpha_{1234} \left(2 \sum_i b_i - 3 \right) \right). \quad (6)$$

Lemma (Case 2.5): If $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq 0 \leq \alpha_{124}$ and $\alpha_{234} \leq \alpha_{134} \leq \alpha_{124}$, and $\alpha_{123} + \alpha_{234} \leq -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\sum_{ijk=\substack{123, \\ 423}} \alpha_{ijk} (b_i b_j + b_i b_k - b_i) + (\alpha_{134} + \alpha_{124} + \alpha_{1234}) b_1 b_4 \quad (7)$$

$$+ b_a \left(\sum_{ijk=\substack{123, \\ 423}} \alpha_{ijk} (b_i - b_j - b_k) + \sum_{ijk=\substack{134, \\ 124}} (1 - b_i + b_j - b_k) + \alpha_{ijkl} (1 - b_1 - b_4) \right). \quad (8)$$

Lemma (Case 2.6): If $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq \alpha_{134} \leq 0 \leq \alpha_{124}$ and $\alpha_{123} + \alpha_{234} \leq -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by Eq. 6.

Lemma (Case 2.7): If $-\alpha_{1234} \leq \alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq \alpha_{134} \leq \alpha_{124} \leq 0$ and $\alpha_{123} + \alpha_{234} \geq -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\sum_{ijk} \alpha_{ijk} \sum_{lm \in ijk} b_l b_m + \alpha_{1234} \sum_{ij} b_i b_j + b_a \left(\sum_{ijk} \alpha_{ijk} \left(1 - \sum_{l \in ijk} b_l \right) + \alpha_{1234} \left(3 - 2 \sum_i b_i \right) \right). \quad (9)$$

Lemma (Case 2.8): If $\alpha_{123} \leq -\frac{\alpha_{1234}}{2} \leq \alpha_{234} \leq \alpha_{134} \leq \alpha_{124} \leq 0$ and $\alpha_{123} + \alpha_{234} \leq -\alpha_{1234}$, then Eq. 1 is perfectly quadratized by:

$$\sum_{ijk=\substack{123, \\ 423}} \alpha_{ijk} (b_j + b_k + b_i b_j + b_i b_k) + \sum_{ijk=\substack{134, \\ 124}} \alpha_{ijk} (1 - b_i + b_j - b_k + b_i b_k) + \alpha_{1234} (1 - b_1 - b_4 + b_1 b_4) \quad (10)$$

$$+ b_a \left(\sum_{ijk=\substack{123, \\ 423}} \alpha_{ijk} (b_j + b_k - b_i) + \sum_{ijk=\substack{134, \\ 124}} (b_i - b_j + b_k - 1) + \alpha_{ijkl} (b_1 + b_4 - 1) \right) \quad (11)$$

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