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

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

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:

$$\left(3\alpha_{1234} + \sum_{ijk}\alpha_{ijk}\right)b_a + \alpha_{1234}\sum_{ij}b_ib_j + \sum_{lmn}\alpha_{lmn}\sum_{ij\subset lmn}b_ib_j - \sum_i\left(2\alpha_{1234} + \sum_{jkl\ni i}\alpha_{jkl}\right)b_ib_a. \tag{2}$$

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

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

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:

$$\alpha_{123}\left(-b_1 + b_1b_2 + b_1b_3\right) + \alpha_{234}\left(-b_4 + b_2b_4 + b_3b_4\right) + \left(\alpha_{134} + \alpha_{124} + \alpha_{1234}\right)b_1b_4 \tag{4}$$
$$+b_a\left(\alpha_{123}\left(b_1 - b_2 - b_3\right) + \alpha_{234}\left(-b_2 - b_3 + b_4\right) + \alpha_{134}\left(1 - b_1 + b_3 - b_4\right) + \alpha_{124}\left(1 - b_1 + b_2 - b_4\right) + \alpha_{1234}\left(1 - b_1 - b_4\right)\right). \tag{5}$$

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

$$\sum_{ijk}\alpha_{ijk}\left(1 - \sum_{l\in ijk}b_l + \sum_{lm\subset ijk}b_lb_m\right) + \alpha_{1234}\left(3 - 2\sum_i b_i + \sum_{ij}b_ib_j\right) + b_a\left(\sum_{ijk}\alpha_{ijk}\left(\sum_{l\in ijk}b_l - 1\right) + \alpha_{1234}\left(2\sum_i b_i - 3\right)\right). \tag{6}$$

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:

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

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

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:

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

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:

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

$$+ b_a \left(\sum_{\substack{ijk=123,\\423}} \alpha_{ijk}\left(b_j + b_k - b_i\right) + \sum_{\substack{ijk=134,\\124}} \left(b_i - b_j + b_k - 1\right) + \alpha_{1234}\left(b_1 + b_4 - 1\right) \right) \tag{11}$$

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