Quadratic Envelopes: A method that can quadratize with a negative number of auxiliary variables

Nike Dattani[1] and Andreas Soteriou[2]

[1]*Harvard-Smithsonian Center for Astrophysics, USA*
[2]*Surrey University, Department of Mathematics, UK*

We present a quadratization method that, for all of the many cases considered, provides quadratizations that require fewer auxiliary variables, less connectivity between the variables, and *much* smaller coefficients than any previously known quadratization method. The quadratizations presented in this work, are also obtainable much more quickly (in terms of computation runtime) than quadratizatons for functions of similar complexity have traditionally been in the past. The idea is that many *very* simple quadratic functions might *almost* reproduce a degree-k function perfectly, but each of these *almost* perfect quadratic functions can compensate for each others imperfections, hence leading to a perfect quadratization when all such quadratic functions are considered collectively. This collection is called a *quadratic envelope.* We are able to quadratize positive monomials with quadratic functions that have exponentially smaller coefficients than in [Boros *et al.* (2018)], while also having far less connectivity between the variables of the quadratics, in addition to requiring fewer auxiliary variables. We will also show examples in which an envelope of quadratic functions, each with *fewer* total variables than the original degree-k function, collectively can be made to *exactly* reproduce the degree-k function.

I. INTRODUCTION

Any real-valued function of binary variables can be turned into a quadratic one that maintains all the desired properties of the original degree-k function. We call this a 'quadratization' of the degree-k function. The first quadratization technique of which we are aware, is Rosenberg's substitution method from 1975 [1], which for quadratizing a single positive monomial of degree-k, would need $k-2$ auxiliary variables (meaning that the quadratic function obtained after the quadratization, would involve $k-2$ more auxiliary variables than the original degree-k monomial). This was cut by roughly one half in 2011 by Ishikawa, who introduced a quadratization for a positive degree-k monomial, which needed only $\frac{k-1}{2}$ auxiliary variables (rounded down if k were even). In 2018 several new quadratizations were introduced for positive degree-k monomials: one required only $k/4$ auxiliary variables, one required only $\log k$, and while it might be surprising that an improvement can be made over $\log k$, a quadratization was finally shown which required only $\log(k/2)$ (all three of these were presented in [2, 3], and the numbers are rounded *up* to the nearest integer). While it was astonishing that any positive monomial can be quadratized with only $\log(k/2)$ auxiliary variables, the resulting quadratic function would have very large coefficients and all possible quadratic terms over all original and auxiliary variables; and since large coefficients and a large number of quadratic terms, are two of the factors which most severely increase the cost when optimizing a quadratic discrete function, one may hesitate to use such quadratizations in practice.

Quadratization is also possible without the addition of any 'auxiliary variables' [4–8], and while these techniques should always be attempted, they in many cases might only reproduce the ground state of the degree-k function rather than the whole spectrum [8]. One of these zero-auxiliary-variable methods that does reproduce the full spectrum, the Split-Reduc method [9], can be very powerful when quadratizing multiple terms that have common variables, but for the degree-k positive monomial alone, its application can be far more costly than the methods described in the previous paragraph (this will be discussed more later in the paper when we compare and contrast Split-Reduc, methods involving auxiliaries, and our new concept of quadratic envelopes).

In this work we introduce the concept of quadratic envelopes, which seem to be capable of 'perfectly' quadratizing functions more efficiently than any of the above methods (by 'perfectly' we mean, reproducing the whole spectrum and not just the ground state). Even for just preserving the ground state, quadratic envelopes are often the most efficient way to quadratize a function, and in other cases should likely always be considered in combination with other methods in order to achieve the most efficient quadratization possible.

II. A QUICK EXAMPLE

Let us review the idea behind most known quadratizations. Consider the equality:

$$-b_1b_2b_3 = \min_{b_a}\left(2b_a - b_1b_a - b_2b_a - b_3b_a\right), \qquad (1)$$

where all b_i are either 0 or 1 and the subscript a in b_a indicates that this is an 'auxiliary' variable because it does not appear in the original cubic function on the left side. This quadratization was first published by Kolmogorov and Zabih in 2004 [10] and generalized by Freedman and Drineas in 2005 beyond cubics and to negative monomials of any degree k. For clarity we explicitly show why Eq. 1 is true by constructing the truth tables for the left and right sides:

b_1	b_2	b_3	$-b_1b_2b_3$
0	0	0	**0**
0	0	1	**0**
0	1	0	**0**
0	1	1	**0**
1	0	0	**0**
1	0	1	**0**
1	1	0	**0**
1	1	1	**-1**

b_1	b_2	b_3	b_a	$2b_a - b_1b_a - b_2b_a - b_3b_a$	$\min_{b_a}$
0	0	0	**0**	0	**0**
0	0	0	**1**	0	
0	0	1	**0**		**0**
0	0	1	**1**		
0	1	0	**0**		**0**
0	1	0	**1**		
0	1	1	**0**		**0**
0	1	1	**1**		
1	0	0	**0**		**0**
1	0	0	**1**		
1	0	1	**0**		**0**
1	0	1	**1**		
1	1	0	**0**		**0**
1	1	0	**1**		
1	1	1	**0**		**-1**
1	1	1	**1**	-1	

It is impossible to construct a single quadratic function without any auxiliary variables, that reproduces the spectrum as seen in the tables above. However, minimizing over the quadratic function b_1b_2 and the linear function b_3, perfectly yields the full spectrum of $b_1b_2b_3$ without introducing any auxiliary variables:

b_1	b_2	b_3	b_1b_2	b_3	$\min(b_1b_2, b_3)$
0	0	0	0	0	0
0	0	1		1	0
0	1	0	0	0	0
0	1	1		1	0
1	0	0	0	0	0
1	0	1		1	0
1	1	0	1	0	0
1	1	1		1	1

We call the set $\{b_1b_2, b_3\}$ a *quadratic envelope* for $b_1b_2b_3$. At each point (b_1, b_2, b_3), the minimum over all functions in the quadratic envelope is equal to the degree-k function $b_1b_2b_3$.

III. GENERALIZATIONS OF THE QUICK EXAMPLE

The simple example from the previous section, of a quadratic envelope reproducing $b_1b_2b_3$, can be generalized:

$$b_1b_2b_3\dots b_k = \min\left(b_1b_2\dots b_{k_1}, b_{k_1+1}b_{k_1+2}\dots b_{k_2}, b_{k_2+1}b_{k_2+2}\dots b_{k_3}, \dots, b_{k_n+1}b_{k_n+2}\dots b_k\right), \quad (2)$$

where $k_1, k_2, \dots, k_n$ can be chosen arbitrarily between 1 and k (if $k_1 > 2$ or if any $k_i > k_{i-1}+2$ then it is no longer a quadratic envelope but an envelope of a higher degree). One interesting quadratic envelope which is an example of Eq. 2 is:

$$b_1b_2b_3\dots b_k = \min\left(b_1, b_2, b_3, \dots, b_k\right), \quad (3)$$

which is also an example of a *linear envelope.*

IV. USAGE

If we wished to minimize the function of binary variables:

$$b_1b_2b_3 - b_1b_2\dots, \quad (4)$$

using the wealth of techniques we have available for minimizing *quadratic* functions of binary variables (such as the classical algorithm 'QPBO' and extensions of it [11], or quantum annealing using thousands of qubits [12] connected by graphs as complicated as Pegasus [13, 14]), we can quadratize the cubic term with the quadratic envelope...., and we get two optimization problems:

$$b_1b_2b_3 - b_1b_2\dots, \quad (5)$$

Running the optimization procedure on both functions would result in the following two minima:

$$b_1b_2b_3 - b_1b_2\dots, \quad (6)$$

The lower minimum is (), so this is the minimum of the original cubic function (this can be verified by simply optimizing the original cubic function, but for more complicated super-quadratic functions, the algorithms to optimize a super-quadratic function can be very costly and it would be *preferred* to optimize the quadratic problem instead).

A. Quadratizing multiple parts of a function using quadratic envelopes

To show that the method of using quadratic envelopes can be applied many times for the same degree-k objective function, consider the example:

$$b_1b_2b_3 - b_1b_2..., \tag{7}$$

Here we quadratize bbb with the envelope $\{bb, bb\}$ and bbb with the envelope $\{bb, bb\}$. This gives us four possible objective functions to consider:

$$b_1b_2b_3 - b_1b_2..., \tag{8}$$
$$b_1b_2b_3 - b_1b_2..., \tag{9}$$
$$b_1b_2b_3 - b_1b_2..., \tag{10}$$
$$b_1b_2b_3 - b_1b_2...,. \tag{11}$$

Running the optimization procedure on all four functions would result in the following four minima:

$$b_1b_2b_3 - b_1b_2..., \tag{12}$$

The lowest minimum is $()$, so this is the minimum of the original degree-k function (again, this can be verified by simply optimizing the original cubic function, but for more complicated super-quadratic functions, the algorithms to optimize a super-quadratic function can be very costly and it would be *preferred* to optimize the quadratic problem instead).

V. COST ANALYSIS AND CLAIMS OF SUPERIORITY OVER ALL PREVIOUSLY KNOWN METHODS

The cost is ....

Compare BCR to ours (20 vs 32 and connectivity etc.).

VI. MORE EXAMPLES AND POTENTIAL APPLICATIONS

A. Positive degree-8 monimial

One of our favorite examples is:

$$b_1b_2b_3b_4b_5b_6b_7b_8: \tag{13}$$
$$\longrightarrow\ 3b_a + b_1b_2 + b_1b_3 + b_1b_4 + b_2b_3 + b_2b_4 \tag{14}$$
$$+ b_3b_4 - 2b_a(b_1 + b_2 + b_3 + b_4) \tag{15}$$
$$\longrightarrow\ 3b_a + b_5b_6 + b_5b_7 + b_5b_8 + b_6b_7 + b_6b_8 \tag{16}$$
$$+ b_7b_8 - 2b_a(b_5 + b_6 + b_7 + b_8) \tag{17}$$

B. Computer vision problem and LHZ lattice

3-runs/0-aux case to be applied in Computer Vision and LHZ lattice:

$$b_1b_2b_3b_4 + b_3b_4b_5b_6 = \min(b_2b_3 + b_3b_6, b_1b_4 + b_4b_5, \tag{18}$$
$$b_1b_2 + b_5b_6 - b_3 - b_4 + 2) \tag{19}$$

3-runs/0-aux case:

$$b_1b_2b_3b_4 + b_2b_3b_4b_5 + b_3b_4b_5b_6: \tag{20}$$
$$\longrightarrow 3b_3b_4 + b_3b_5 + b_4b_5 - b_3 - b_4 - b_5 + 1 \tag{21}$$
$$\longrightarrow b_1b_4 + b_3b_5 + b_4b_5 \tag{22}$$
$$\longrightarrow b_1b_2 + b_2b_6 + b_3b_5 + b_5b_6 + b_2 - b_3 - b_4 - b_5 + 2 \tag{23}$$

One more example which is the best one we can come up with for cost savings.

VII. DISCUSSION

Negative variables. Reinforcement learning.

VIII. ACKNOWLEDGMENTS

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