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

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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 $\log k$ (both of these were presented in[2]), and while it might be surprising that an improvement can be made over $\log k$, a subsequent 2018 paper finally showed a quadratization which required only $\log(k/2)$ [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:

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

where $k_1, k_2, \dots, k_p$ 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. WORST-CASE COST ANALYSIS AND CLAIMS OF SUPERIORITY OVER ALL PREVIOUSLY KNOWN METHODS

Envelope quadratizations can *always* be better than (or at least as efficient as) the previous state-of-the-art quadratization method for quadratizing a single positive degree-k monomial. The state-of-the-art method for this was the 2018 method requiring only $\log_2(k/2)$ auxiliary variables (rounded up) [2, 3], and in the handbook of quadratizations [8] it was called PTR-BCR-4.

Unless there is some property of the function making it easier, optimizing a function of n binary variables by brute force requires 2^n queries, so if m binary variables are added in the quadratization process, the cost becomes 2^n2^m (meaning the cost is increased by a factor of 2^m). While it is true that better optimization algorithms exist than doing brute force queries (hence the reason for quadratizing the original function at the expense of a possible 2^m increase in cost!), all general-purpose methods for optimizing such functions still cost $\mathcal{O}(2^x)$ for x binary variables (this includes quantum annealing, where the scaling up to ~1000 variables can be seen in the figures of [15] and [16]), so we claim that a factor of 2^m increase in cost is not unfair (especially in the absence of any better measure of the added cost to the optimization due to adding auxiliary variables) for analyzing costs of quadratizations.

Having established our notion of how much adding m auxiliary variables increases the cost of optimizing a quadratic function of binary variables, for the positive degree-k monomial we compare the added cost of envelope quadratizations to the added cost of PTR-BCR-4 (which was previously the state-of-the-art). PTR-BCR-4 adds $m = \lceil \log_2(k/2) \rceil$ auxiliary variables, which means that the added cost of optimization can be increased by up to a factor of k (see footnote: [1]).

Using Eq. 2 we can split the positive monomial into k/p pieces: $b_1b_2 \dots b_{k/p}$, and each piece can be quadratized with PTR-BCR-4 with $\log_2\lceil k/2p \rceil$ auxiliary variables, incurring a cost of $\lceil k/2p \rceil$ for each of the k/p pieces. Since to optimize the original function containing $b_1b_2 \dots b_k$, we would need to do our optimization procedure once for each piece that is being substituted, in the worst case the cost of the optimization procedure will be increased by a factor equal to the number of pieces, which is k/p.

For example if we wish to optimize a function in which we quadratize a positive degree-40 monomial using PTR-BCR-4, we would be adding $\lceil \log_2 {}^{40}/_2 \rceil = \lceil \log_2 20 \rceil = 5$ auxiliary variables, and therefore increase the cost of optimizing the original function by a factor of $2^5 = 32$. However the positive degree-40 monomial can be split into 20 quadratic pieces: $\{b_1b_2, b_3b_4, \cdots, b_{39}b_{40}\}$, and doing 20 different optimizations (replacing $b_1b_2 \dots b_{40}$ in the original function by one of each of the 20 total pieces) would cost at most only 20 times more than doing one such optimization. Likewise the positive degree-40 monomial can be split into 10 pieces, each of degree-4: $\{b_1b_2b_3b_4, b_5b_6b_7b_8, \cdots, b_{37}b_{38}b_{39}b_{40}\}$, and then each dergree-4 term can be quadratized using PTR-BCR-4 with only 1 auxiliary variables (increasing the cost by a factor of 2, leading to having 10 optimization problems each being 2 times more expensive than they would have been without auxiliary variables, meaning that again the cost is only increased by a factor of 20). Finally the same would be true if we used 5 pieces, each of degree-8: $\{b_1b_2 \cdots b_8, b_9b_{10} \cdots b_{16}, \cdots, b_{33}b_{34} \cdots b_{40}\}$,and then quadratized each degree-8 term using PTR-BCR-4 with

[1] $x \le \lceil x \rceil \le 1 + \lfloor x \rfloor$, because if x is an integer then $\lceil x \rceil = x = \min\lceil x \rceil$ and if x is not an integer then we have $\lceil x \rceil = 1 + \lfloor x \rfloor = \max\lceil x \rceil$. So if we have $m = \lceil \log_2 k/2 \rceil = \lceil \log_2 k \rceil - 1$ and we are interested in 2^m, we have $\min(2^m) = 2^{\min\lceil \log_2 k \rceil - 1} = 2^{\log_2 k - 1} = k/2$ in the case of k being a power of 2, and $\max(2^m) = 2^{\max\lceil \log_2 k \rceil - 1} = 2^{1 + \lfloor \log_2 k \rfloor - 1} = 2^{\lfloor \log_2 k \rfloor} =$.

only 2 auxiliary variables each (increasing the cost by a factor of 4, leading to having 5 optimization problems each being 4 times more expensive than they would have been without auxiliary variables, meaning that again the cost is only increased by a factor of 20).

In general we can get up to a factor of 2 improvement over BCR, equivalent to effectively using only log(k/4) auxiliaries, and even better if the other variables don't appear in positive/negative coefficients of other terms? And what about cases that are not monomials? Furthermore compare the coefficients and connectivity in BCR to COMIGs

VI. MORE EXAMPLES AND POTENTIAL APPLICATIONS

A. Positive degree-8 monimial

It has been known for some time that no positive monomial with degree greater than 4 can be quadratized by a single function with fewer than 2 auxiliary variables. We therefore found it quite fascinating that we could find an envelope quadratization for the positive degree-8 monomial which involves at most 1 auxiliary variable in the two pieces:

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

Here the added cost of a factor of 4 is still the same as it would be with PTR-BCR-4 (which would need only 2 auxiliary variables and therefore an added cost of a factor of $2^2 = 4$). However the quadratic function arising from PTR-BCR-4 contains all possible quadratic terms for the 8 original variables and the 2 auxiliary variables, which would result in a *gadget graph* [14] of K_{10}, whereas the above envelope quadratization would for both quadratic functions involve the much simpler gadget graph of K_5. Furthermore, the quadratic terms resulting from the PTR-BCR-4 quadratization the above envelope quadratization would have coefficients ranging from X to X, and in the above envelope quadratization, they range from -2 to 1, which means the coefficient range is X times smaller in the envelope quadratization case. Submodularity?

B. Application to a computer vision algorithm

The image deblurring algorithm of [] involves degree-k terms with $k = d^2$ with $d \geq 2$ being the length in pixels of the square-shaped mask) [17, 18]. In all known applications so far, $d = 2$ and $k = 4$ (though larger masks can be used, it would just be more difficult since the optimization problem would involve much higher-degree terms). With $d = 2$, this optimizaton problem involves degree-4 terms for every set of pixels that can be covered by the 2×2 pixel mask, so we can have neighboring degree-4 terms such as.....

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

3-runs/0-aux case:

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

C. 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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