

Quadratization in Discrete Optimization and Quantum Mechanics

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An open source Book on quadratizations for classical computing, quantum annealing, and universal adiabatic quantum computing.

When optimizing discrete functions, it is often easier when the function is quadratic than if it is of higher degree. But notice that the cubic and quadratic functions:

$$b_1 b_2 + b_2 b_3 + b_3 b_4 - 4b_1 b_2 b_3 \quad (\text{cubic}), \quad (1)$$

$$b_1 b_2 + b_2 b_3 + b_3 b_4 + 4b_1 - 4b_1 b_2 - 4b_1 b_3 \quad (\text{quadratic}), \quad (2)$$

where each b_i can either be 0 or 1, both never go below the value of -2, and all minima occur at $(b_1, b_2, b_3, b_4) = (1, 1, 1, 0)$. Therefore if we are interested in the ground state of a discrete function of degree k , we may optimize either function and get exactly the same result. **Part I** gives more than 40 different ways to do this, almost all of them published in the last 5 years.

The binary variables b_i can be either of the eigenvalues of the matrix b below, which is related to the Pauli z matrix by $z = 2b - \mathbb{1}$. The Pauli matrices $x, y, z, \mathbb{1}$ are listed below:

$$b \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \mathbb{1} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3)$$

Any Hermitian 2×2 matrix can be written as a linear combination of the Pauli matrices, so we can therefore describe the Hamiltonian of any number of spin- $1/2$ particles by a function of Pauli matrices acting on each particle, for instance:

$$x_1 y_2 z_3 y_4 + y_1 x_2 z_3 y_4 + x_1 x_2 y_3 \quad (\text{cubic}), \quad (4)$$

$$x_1 y_4 + x_2 y_4 + x_3 \quad (\text{quadratic}), \quad (5)$$

where the coefficients tell us about the strengths of couplings between these particles. The Schrödinger equation tells us that the eigenvalues of the Hamiltonian are the allowed energy levels and their eigenvectors (wavefunctions) are the corresponding physical states. More generally these do not have to be spins but can be any type of qubits, and we can encode the solution to *any* problem in the ground state of a Hamiltonian, then solve the problem by finding the lowest energy state of the physical system (this is called adiabatic quantum computing). Eqs. (5) and (4) have exactly the same energy spectra, so Eq. (5) is one example of a type of quadratization, and many quadratizations in this book will also preserve wavefunctions.

Two-body physical interactions occur more naturally than many-body interactions so **Parts II-III** give more than 30 different ways to quadratize general Hamiltonians (some of these methods may use $d \times d$ matrices instead of only the 2×2 matrices in Eq. (3), meaning that we can have types of qudits that are not qubits). All of these methods were published during the last 15 years.

The optimization problems of Eqs. (1)-(2) are specific cases of the type in Eqs. (4)-(5), but with only b matrices.

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Part I

Diagonal Hamiltonians (pseudo-Boolean functions)

I. METHODS THAT INTRODUCE ZERO AUXILIARY VARIABLES

A. Deduction Reduction (Deduc-reduc; Tanburn, Okada, Dattani, 2015)

Summary

We look for *deductions* (e.g. $b_1 b_2 = 0$) that must hold true at the global minimum. These can be found by *a priori* knowledge of the given problem, or by enumerating solutions of a small subset of the variables. We can then substitute high-order terms using the low-order terms of the deduction, and add on a penalty term to preserve the ground states [?].

Cost

- 0 auxiliary variables needed.
- For a particular value of m , we have $\binom{n}{m}$ different m -variable subsets of the n variable problem, and $\binom{n}{m} 2^m$ evaluations of the objective function to find all possible m -variable deductions, whereas 2^n evaluations is enough to solve the entire problem. We therefore choose $m \lll n$.

Pros

- No auxiliary variables needed.

Cons

- When deductions cannot be determined naturally (as in the Ramsey number determination problem, see Example XIII), deductions need to be found by ‘brute force’, which scales exponentially with respect to m . For highly connected systems (systems with a large number of non-zero coefficients), the value of m required to find even one deduction can be prohibitively large.

Example

Consider the objective function:

$$H_{4\text{-local}} = b_1 b_2 (4 + b_3 + b_3 b_4) + b_1 (b_3 - 3) + b_2 (1 - 2b_3 - b_4) + F(b_3, b_4, b_5, \dots, b_N) \quad (6)$$

where F is any quadratic polynomial in b_i for $i \geq 3$. Since

$$H_{4\text{-local}}(1, 1, b_3, b_4, \dots) > H_{4\text{-local}}(0, 0, b_3, b_4, \dots), H_{4\text{-local}}(0, 1, b_3, b_4, \dots), H_{4\text{-local}}(1, 0, b_3, b_4, \dots),$$

it must be the case that $b_1 b_2 = 0$. Specifically, for the 4 assignments of (b_3, b_4) , we see that $b_1 b_2 = 0$ at every minimum of $H_{4\text{-local}} - F$.

Using deduc-reduc we have:

$$H_{2\text{-local}} = 6b_1 b_2 + b_1 (b_3 - 3) + b_2 (1 - 2b_3 - b_4) + F(b_3, b_4, b_5, \dots, b_N), \quad (7)$$

which has the same global minima as $H_{4\text{-local}}$ but one fewer quartic and one fewer cubic term. The coefficient of $b_1 b_2$ was chosen as 6 because $6 \geq \max(4 + b_3 + b_3 b_4)$.

Bibliography

- Original paper, with more implementation details, and application to integer factorization: [?].

B. ELC Reduction (Ishikawa, 2014)

Summary

An Excludable Local Configuration (ELC) is a partial assignment of variables that make it impossible to achieve the minimum. We can therefore add a term that corresponds to the energy of this ELC without changing the solution to the minimization problem. In practice we can eliminate all monomials with a variable in which a variable is set to 0, and reduce any variable set to 1. Given a general objective function we can try to find ELCs by enumerating solutions of a small subset of variables in the problem [?].

Cost

- 0 auxiliary variables needed.
- For a particular value of m , we have $\binom{n}{m}$ different m -variable subsets of the n variable problem, and $\binom{n}{m}2^m$ evaluations of the objective function to find all possible m -variable deductions, whereas 2^n evaluations is enough to solve the entire problem. We therefore choose $m \ll n$.
- Approximate methods exist which have been shown to be much faster and give good approximations to the global minimum [?].

Pros

- No auxiliary variables needed.

Cons

- No known way to find ELCs except by ‘brute force’, which scales exponentially with respect to m .
- ELCs do not always exist.

Example

Consider the objective function:

$$H_{3\text{-local}} = b_1 b_2 + b_2 b_3 + b_3 b_4 - 4b_1 b_2 b_3. \quad (8)$$

If $b_1 b_2 b_3 = 0$, no assignment of our variables will we be able to reach a lower energy than if $b_1 b_2 b_3 = 1$. Hence this gives us *twelve* ELCs, and one example is $(b_1, b_2, b_3) = (1, 0, 0)$ which we can use to form the polynomial:

$$H_{2\text{-local}} = H_{3\text{-local}} + 4b_1(1 - b_2)(1 - b_3) \quad (9)$$

$$= b_1 b_2 + b_2 b_3 + b_3 b_4 + 4b_1 - 4b_1 b_2 - 4b_1 b_3. \quad (10)$$

In both cases Eqs. (8) and (10), the only global minima occur when $b_1 b_2 b_3 = 1$.

Bibliography

- Original paper and application to computerized image denoising: [?].

C. Groebner Bases

Summary

Given a set of polynomials, a Groebner basis is another set of polynomials that have exactly the same zeros. The advantage of a Groebner basis is it has nicer algebraic properties than the original equations, in particular they tend to have smaller degree polynomials. The algorithms for calculating Groebner bases are generalizations of Euclid's algorithm for the polynomial greatest common divisor.

Work has been done in the field of 'Boolean Groebner bases', but while the variables are Boolean the coefficients of the functions are in \mathbb{F}_2 rather than \mathbb{Q} .

Cost

- 0 auxiliary variables needed.
- $\mathcal{O}(2^{2^n})$ in general, $\mathcal{O}(d^{n^2})$ if the zeros of the equations form a set of discrete points, where d is the degree of the polynomial and n is the number of variables [?].

Pros

- No auxiliary variables needed.
- General method, which can be used for other rings, fields or types of variables.

Cons

- Best algorithms for finding Groebner bases scale double exponentially in n .
- Only works for objective functions whose minimization corresponds to solving systems of discrete equations, as the method only preserves roots, not minima.

Example

Consider the following pair of equations:

$$b_1 b_2 b_3 b_4 + b_1 b_3 + b_2 b_4 - b_3 = b_1 + b_1 b_2 + b_3 - 2 = 0. \quad (11)$$

Feeding these to Mathematica's `GroebnerBasis` function, along with the binarizing $b_1(b_1 - 1) = \dots = b_4(b_4 - 1) = 0$ constraints, gives a Groebner basis:

$$\{b_4 b_3 - b_4, b_2 + b_3 - 1, b_1 - 1\}. \quad (12)$$

From this we can immediately read off the solutions $b_1 = 1$, $b_2 = 1 - b_3$ and reduce the problem to $b_3 b_4 - b_4 = 0$. Solving this gives a final solution set of: $(b_1, b_2, b_3, b_4) = (1, 0, 1, 0), (1, 0, 1, 1), (1, 1, 0, 0)$, which should be the same as the original 4-local problem.

Bibliography

- Reduction and embedding of factorizations of all bi-primes less than 200,000: [?].

D. Application of ELM (Dattani, 2018)

Summary

We use the formula from [?] for representing any function of three binary variables:

$$f(b_1, b_2, b_3) = (f(1, 1, 1) + f(1, 0, 0) - f(1, 1, 0) - f(1, 0, 1) - f(0, 1, 1) - f(0, 0, 0) + \quad (13)$$

$$f(0, 0, 1) + f(0, 1, 0)) b_1 b_2 b_3 + (f(0, 1, 1) + f(0, 0, 0) - f(0, 0, 1) - f(0, 1, 0)) b_2 b_3 + \quad (14)$$

$$(f(1, 0, 1) + f(0, 0, 0) - f(0, 0, 1) - f(1, 0, 0)) b_1 b_3 + \quad (15)$$

$$(f(1, 1, 0) + f(0, 0, 0) - f(1, 0, 0) - f(0, 1, 0)) b_1 b_2 + (f(0, 1, 0) - f(0, 0, 0)) b_2 \quad (16)$$

$$+ (f(1, 0, 0) - f(0, 0, 0)) b_1 + (f(0, 0, 1) - f(0, 0, 0)) b_3 + f(0, 0, 0). \quad (17)$$

If the cubic term is zero, then the function becomes quadratic. We can use ELM (Energy Landscape Manipulation) to change the energy landscape *without* changing the ground state [?]. In this case, we apply ELM in order to make the cubic term zero.

Cost

- No auxiliary variables.
- May require many evaluations of the cubic function, varying coefficients in order to find the right ELM coefficients.
- For a particular value of m , we have $\binom{n}{m}$ different m -variable subsets of the n variable problem, and $\binom{n}{m} 2^m$ evaluations of the objective function to find all possible m -variable deductions, whereas 2^n evaluations is enough to solve the entire problem. We therefore choose $m \ll n$.

Pros

- Can be generalized to arbitrary k -local functions, but the ELM constraints may become harder to achieve.
- Can quadratize an entire cubic function (or a cubic part of a more general function) with no auxiliary qubits.
- Can reproduce the full spectrum.

Cons

- May not always be possible.
- May require a local search to find appropriate deductions.

Example

In order to reduce the number of constraints required for the cubic term to be zero, we will assume that Deduc-Reduc told us that $(1-b_1)(1-b_2)+(1-b_2)(1-b_3)+(1-b_1)(1-b_3) = 0$ when the overall function is minimized, which means the ground state only occurs when at least two variables are 1. This does not allow us to assign the linear terms, but assigns all quadratic terms to have $b_i b_j = 1$. This also suggests that $b_1 b_2 b_3$ can also be reduced to a linear term, but we do not know whether it is b_1 , b_2 , or b_3 . So we have the following constraint on the cubic term, after setting all $f(b_1, b_2, b_3)$ to zero if there is not at least two 1's:

$$f(1, 1, 1) - f(1, 1, 0) - f(1, 0, 1) - f(0, 1, 1) = 0. \quad (18)$$

Bibliography

- The method was first presented in the first arXiv version of this book [?].

E. Split Reduction (Okada, Tanburn, Dattani, 2015)

Summary

It is possible to reduce a lot of the problem by conditioning on the most connected variables. We call each of these operations a *split*.

Cost

Usually slightly sub-exponential in the number of splits, as the number of problems to solve at most doubles with every split, but often does not double (since entire cases can get eliminated by some splits, as in the example below).

Pros

- This method can be applied to any problem and can be very effective on problems with a few very connected variables.

Cons

- Multiple runs of the optimization procedure need to be made, and the number of runs can often grow almost exponentially with respect to the number of splits.

Example

Consider the simple objective function

$$H = 1 + b_1 b_2 b_5 + b_1 b_6 b_7 b_8 + b_3 b_4 b_8 - b_1 b_3 b_4. \quad (19)$$

In order to quadratize H , we first have to choose a variable over which to split. In this case b_1 is the obvious choice since it is present in the most terms and contributes to the quartic term.

We then obtain two different problems:

$$H_0 = 1 + b_3 b_4 b_8 \quad (20)$$

$$H_1 = 1 + b_2 b_5 + b_6 b_7 b_8 + b_3 b_4 b_8 - b_3 b_4. \quad (21)$$

At this point, we could split H_0 again and solve it entirely, or use a variable we saved in the previous split to quadratize our only problem.

To solve H_1 , we can split again on b_8 , resulting in two quadratic problems:

$$H_{1,0} = 1 + b_2 b_5 - b_3 b_4 \quad (22)$$

$$H_{1,1} = 1 + b_2 b_5 + b_6 b_7. \quad (23)$$

Now both of these problems are quadratic. Hence we have reduced our original, hard problem into 3 easy problems, requiring only 2 extra (much easier) runs of our minimization algorithm, and without needing any auxiliary variables.

Note that the number of quadratic problems to solve is 3, which is smaller than 2^2 which would be the "exponential" cost if the number of problems were (hypothetically) to double with each split. This is a good example of the typical *sub*-exponential scaling of split-reduc.

Bibliography

- Original paper and application to Ramsey number determination: [?].

II. METHODS THAT INTRODUCE AUXILIARY VARIABLES TO QUADRATIZE A SINGLE NEGATIVE TERM (NEGATIVE TERM REDUCTIONS, NTR)

A. NTR-KZFD (Kolmogorov & Zabih, 2004; Freedman& Drineas, 2005)

Summary

For a negative term $-b_1 b_2 \dots b_k$, introduce a single auxiliary variable b_a and make the substitution:

$$-b_1 b_2 \dots b_k \rightarrow (k-1)b_a - \sum_i b_i b_a. \quad (24)$$

Cost

- 1 auxiliary variable for each k -local term.

Pros

- All resulting quadratic terms are submodular (have negative coefficients).
- Can reduce arbitrary order terms with only 1 auxiliary.
- Reproduces the full spectrum.

Cons

- Only works for negative terms.

Example

$$H_{6\text{-local}} = -2b_1 b_2 b_3 b_4 b_5 b_6 + b_5 b_6, \quad (25)$$

has a unique minimum energy of -1 when all $b_i = 1$.

$$H_{2\text{-local}} = 2(5b_a - b_1 b_a - b_2 b_a - b_3 b_a - b_4 b_a - b_5 b_a - b_6 b_a) + b_5 b_6 \quad (26)$$

has the same unique minimum energy, and it occurs at the same place (all $b_i = 1$), with $b_a = 1$.

Alternate Forms

$$-b_1 b_2 \dots b_k = \min_{b_a} \left((k-1 - \sum_i b_i) b_a \right) \quad (27)$$

$$\rightarrow \left((k-1 - \sum_i b_i) b_a \right). \quad (28)$$

Alternate Names

- "Standard quadratization" of negative monomials [?].
- $s_k(b, b_a)$ [?]

Bibliography

- 2004: Kolmogorov and Zabih presented this for cubic terms [?].
- 2005: Generalized to arbitrary order by Freedman and Drineas [?].
- Discussion: [?], [?].

B. NTR-ABCG (Anthony, Boros, Crama, Gruber, 2014)

Summary

For a negative term $-b_1 b_2 \dots b_k$, introduce a single auxiliary variable b_a and make the substitution:

$$-b_1 b_2 \dots b_k \rightarrow \sum_i^{k-1} b_i - \sum_i^{k-1} b_i b_k - \sum_i^k b_i b_a + (k-1) b_k b_a. \quad (29)$$

Cost

- 1 auxiliary variable for each k -local term.
- 1 non-submodular term for each k -local term (and it is quadratic).

Pros

- Can reduce arbitrary order terms with only 1 auxiliary.
- Reproduces the full spectrum.

Cons

- Only works for negative terms.
- Turns a symmetric term into a non-symmetric term (but only b_k is asymmetric).

Example

$$H_{6\text{-local}} = -2b_1 b_2 b_3 b_4 b_5 b_6 + b_5 b_6, \quad (30)$$

has a unique minimum energy of -1 when all $b_i = 1$.

$H_{2\text{-local}}$ has the same unique minimum energy, and it occurs at the same place (all $b_i = 1$), with $b_a = 1$.

Alternate Forms

$$-b_1 b_2 \dots b_k \rightarrow (k-1) b_k b_a - \sum_i b_i (b_a + b_k - 1) \quad (31)$$

$$= (k-2) b_k b_a - \sum_i^{k-1} b_i (b_a + b_k - 1) \quad (32)$$

Alternate Names

- "Extended standard quadratization" of negative monomials (see Eqs. 25-26 of [?]).
- $s_k(b, b_a)^+ [?]$.

Bibliography

- 2014, First presentation: [? ?].
- Further discussion: [?].

C. NTR-ABCG-2 (Anthony, Boros, Crama, Gruber, 2016)

Summary

For a negative term $-b_1 b_2 \dots b_k$, introduce a single auxiliary variable b_a and make the substitution:

$$-b_1 b_2 \dots b_k \rightarrow (2k - 1) b_a - 2 \sum_i b_i b_a \quad (33)$$

Cost

- 1 auxiliary variable for each k -local term.
- 1 non-submodular term for each k -local term (and it is linear).

Pros

- Can reduce arbitrary order terms with only 1 auxiliary.
- Reproduces the full spectrum.
- The non-submodular term is linear as opposed to NTR-ABCG-1 whose non-submodular term is quadratic.
- Symmetric with respect to all non-auxiliary variables.

Cons

- Only works for negative terms.
- Turns a symmetric term into a non-symmetric term (but only b_k is asymmetric).
- Coefficients of quadratic terms are twice the size of their size in NTR-KZFD or NTR-ABCG-1, and roughly twice the size for the linear term.

Example

$$\begin{aligned} H_{6\text{-local}} &= -2b_1 b_2 b_3 b_4 b_5 b_6 + b_5 b_6 \\ &= 2((2(6) - 1)b_a - 2(\sum_{i=1}^6 b_i b_a)) + b_5 b_6 \end{aligned} \quad (34)$$

has a unique minimum energy of -1 when all $b_i = 1$.

$H_{2\text{-local}}$ has the same unique minimum energy, and it occurs at the same place (all $b_i = 1$), with $b_a = 1$.

Alternate Forms

$$-b_1 b_2 \dots b_k = 2b_a \left(k - \frac{1}{2} - \sum_{i=1}^k b_i \right) \quad (35)$$

(33) can be generalized as follows:

$$-b_1 b_2 \dots b_k \rightarrow (Ck - 1) b_a - C \sum_i b_i b_a \quad (36)$$

where $C \geq 1$ is a constant. NTR-KZFD is a particular case of (36) where $C = 1$.

Bibliography

- Discussion: [?].

D. NTR-GBP (“Asymmetric cubic reduction”, Gallagher, Batra, Parikh, 2011)

Summary

$$-b_1 b_2 b_3 \rightarrow b_a (-b_1 + b_2 + b_3) - b_1 b_2 - b_1 b_3 + b_1 \quad (37)$$

$$\rightarrow b_a (-b_2 + b_1 + b_3) - b_1 b_2 - b_2 b_3 + b_2 \quad (38)$$

$$\rightarrow b_a (-b_3 + b_1 + b_2) - b_2 b_3 - b_1 b_3 + b_3 \quad (39)$$

Cost

- 1 auxiliary variable per negative cubic term.

Pros

- Asymmetric which allows more flexibility in cancelling with other quadratics.

Cons

- Only works for negative cubic monomials.

Example

$$-b_1 b_2 b_3 + b_1 b_3 - b_2 = \min_{b_a} (b_a - b_1 b_a - b_3 b_a + b_2 b_a + 2b_1 b_3) - b_2 \quad (40)$$

Alternate Forms

$$-b_1 b_2 b_3 = \min_{b_a} (b_a - b_1 + b_2 + b_3 - b_1 b_2 - b_1 b_3 + b_1) \quad (41)$$

- By starting with (39), and flipping b_a (i.e. setting $b_a \rightarrow 1 - \bar{b}_a$ and relabelling $b_a \rightarrow \bar{b}_a$ since b_a does not appear anywhere else in the function being quadratized), we see that NTR-GBP can actually be derived from NTR-ABCG with $k = 3$).

Bibliography

- First introduced in: [?].

E. NTR-YXKK (Yip, Xu, Koenig and Kumar, 2019)

Summary

For $\alpha > 1$ we can quadratize a degree- k negative term with one auxiliary variable b_a :

$$-b_1 b_2 \cdots b_k \rightarrow b_a + \alpha \sum_{i=1}^k (1 - b_i) (1 - b_a) - 1. \quad (42)$$

Cost

- 1 auxiliary variable to quadratize any degree- k negative term.

Pros

- The coefficient α is adjustable, so there is flexibility in its size.
- Many of the introduced quadratic terms are submodular.
- It is a ‘perfect’ quadratization, meaning that after minimizing over the auxiliary variable, the original function is exactly reproduced.

Example

$$-b_1 b_2 b_3 b_4 b_5 \rightarrow b_a + 2 \sum_{i=1}^5 (1 - b_i) (1 - b_a) - 1. \quad (43)$$

Bibliography

- Original paper (Theorem 1): [?].
- Inspired by Theorem 3 of [?].
- More technical details (Constraint Composite Graph): [?].

F. NTR-RBL (Rocchetto, Benjamin, Li, 2016)

Summary

Using a ternary variable $t_q \in -1, 0, 1$ we have:

$$-z_1 z_2 z_3 \rightarrow (1 + 4t_a + z_1 + z_2 + z_3)^2 - 1. \quad (44)$$

Cost

- 1 auxiliary ternary variable

Pros

- One of the only methods designed specifically for z variables.
- Symmetric with respect to all variables.

Cons

- The auxiliary variable required is ternary (a qutrit).
- Requires all possible quadratic terms and they are all non-submodular.
- Only reproduces the ground state manifold.

Example

$$-b_1 b_2 b_3 = \min_{b_a} b_a - b_1 + b_2 + b_3 - b_1 b_2 - b_1 b_3 + b_1 \quad (45)$$

Alternate Forms

$$-z_1 z_2 z_3 z_4 \rightarrow 16 t_a^2 + 4 t_a \sum_{i=1}^4 z_i + 2 \sum_{i=1}^4 \sum_{j>i}^4 z_i z_j + 4 \quad (46)$$

Bibliography

- Original paper where they introduce this gadget for the *end points* in the LHZ lattice: [?].

G. NTR-LHZ (Lechner, Hauke, Zoller, 2015)

Summary

Extra binary or ternary variable is added to ensure that the energy of the even parity sector is zero and the energy of the odd sector is higher:

Cost

- 1 auxiliary ternary variable (see appendix for transformation to a binary variable)

Pros

- One of the only methods designed specifically for z variables.

Cons

- Only reproduces the ground state manifold, not higher excited states.
- Requires all possible quadratic terms and they are all non-submodular.
- Only reproduces the ground state manifold.

Example

$$\begin{aligned}
 -z_1 z_2 z_3 z_4 &= -16 b_1 b_2 b_3 b_4 + 8 (b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) - \\
 &4 (b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) + 2 (b_1 + b_2 + b_3 + b_4) - 1 \\
 &\rightarrow 16 t_a^2 + 8 t_a \sum_{i=1}^4 b_i + 8 \sum_{i=1}^4 \sum_{j>i}^4 b_i b_j + 16
 \end{aligned} \tag{47}$$

Alternate Forms

$$-z_1 z_2 z_3 z_4 \rightarrow 16 t_a^2 + 4 t_a \sum_{i=1}^4 z_i + 2 \sum_{i=1}^4 \sum_{j>i}^4 z_i z_j + 4 \tag{48}$$

Bibliography

- Original paper: [?] (Eq. 4).
- Also given in Eq. 10 of [?] for $i + 2 < j$.

III. METHODS THAT INTRODUCE AUXILIARY VARIABLES TO QUADRATIZE A SINGLE POSITIVE TERM (POSITIVE TERM REDUCTIONS, PTR)

A. PTR-BG (Boros and Gruber, 2014)

Summary

By considering the negated literals $\bar{b}_i = 1 - b_i$, we recursively apply NTR-KZFD to $b_1 b_2 \dots b_k = -\bar{b}_1 b_2 \dots b_k + b_2 b_3 \dots b_k$. The final identity is:

$$b_1 b_2 \dots b_k \rightarrow \left(\sum_{i=1}^{k-2} b_{a_i} (k - i - 1 + b_i - \sum_{j=i+1}^k b_j) \right) + b_{k-1} b_k \quad (49)$$

Cost

- $k - 2$ auxiliary variables for each k -local term.

Pros

- Works for positive monomials.

Cons

- $k - 1$ non-submodular quadratic terms.

Example

$$b_1 b_2 b_3 b_4 \rightarrow b_{a_1} (2 + b_1 - b_2 - b_3 - b_4) + b_{a_2} (1 + b_2 - b_3 - b_4) + b_3 b_4 \quad (50)$$

Notes

- Based on the way Eq. (49) is written, the gadget graph will have an extra edge between the last two logical qubits, and a missing edge between the first logical qubit and second auxiliary qubit (for the $k = 4$ case), but a slightly different graph is also possible.

Bibliography

- Summary: [?].

B. PTR-Ishikawa (Ishikawa, 2011)

Summary

This method re-writes a positive monomial using symmetric polynomials, so all possible quadratic terms are produced and they are all non-submodular:

$$b_1 \dots b_k \rightarrow \left(\sum_{i=1}^{n_k} b_{a_i} \left(c_{i,d} \left(- \sum_{j=1}^k b_j + 2i \right) - 1 \right) + \sum_{i < j} b_i b_j \right) \quad (51)$$

where $n_k = \lfloor \frac{k-1}{2} \rfloor$ and $c_{i,k} = \begin{cases} 1, & i = n_d \text{ and } k \text{ is odd,} \\ 2, & \text{else.} \end{cases}$

Cost

- $\lfloor \frac{k-1}{2} \rfloor$ auxiliary variables for each k -order term
- $\mathcal{O}(kt)$ for a k -local objective function with t terms.

Pros

- Works for positive monomials.
- About half as many auxiliary variables for each k -order term as the previous method.
- Reproduces the full spectrum.

Cons

- $\mathcal{O}(k^2)$ quadratic terms are created, which may make chimerization more costly.
- $\frac{k(k-1)}{2}$ non-submodular terms.
- Worse than the previous method for quartics, with respect to submodularity.

Example

$$b_1 b_2 b_3 b_4 \rightarrow (3 - 2b_1 - 2b_2 - 2b_3 - 2b_4) b_a + b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4 \quad (52)$$

Alternate Forms

For even k , and equivalent expression is given in [?]:

$$b_1 b_2 \dots b_k \rightarrow \sum_i b_i + \sum_{ij} b_i b_j + \sum_{2i} b_{a_{2i}} \left(4i - 2 - \sum_j b_j \right) \quad (53)$$

$$\rightarrow \sum_i b_i + 2 \sum_{2i} b_{a_{2i}} (2i - 1) + \sum_{ij} b_i b_j - \sum_{2i,j} b_j b_{a_{2i}} \quad (54)$$

Alternate Names

- "Ishikawa's Symmetric Reduction" [?].
- "Ishikawa Reduction"
- "Ishikawa"

Bibliography

- Original paper and application to image denoising: [?].
- Equivalent way of writing it for even k , shown in [?].

C. PTR-ABCG (Anthony, Boros, Crama, Gruber, 2014)

Summary

This is very similar to the alternative form of Ishikawa Reduction, but works for odd values of k , and is different from Ishikawa Reduction:

$$b_1 b_2 \dots b_k \rightarrow \sum_i b_i + \sum_{2i-1} (4i-3) b_{a_{2i-1}} + \sum_{ij} b_i b_j - \sum_{2i-1, j} b_j b_{a_{2i-1}} \quad (55)$$

Cost

- Same number of auxiliaries as Ishikawa Reduction.

Pros

- Same as for Ishikawa Reduction.

Cons

- Same as for Ishikawa Reduction.
- Only works for odd k , but for even k we have an analogous method which is equivalent to Ishikawa Reduction.

Alternate Forms

$$b_1 b_2 \dots b_k \rightarrow \sum_i b_i + \sum_{ij} b_i b_j + \sum_{2i-1} b_{a_{2i-1}} \left(4i-3 - \sum_j b_j \right) \quad (56)$$

Bibliography

- Original paper (Theorem 4.3): [?].

D. PTR-BCR-1 (Boros, Crama, and Rodríguez-Heck, 2018)

Summary

Let $\lceil \frac{k}{4} \rceil \leq m \leq \lceil \frac{k}{2} \rceil$,

$$\begin{aligned}
 b_1 b_2 \cdots b_k \rightarrow & \alpha^b \sum_i b_i + \alpha^{b_{a,1}} \sum_i b_{a_i} + \alpha^{b_{a,2}} b_{a_m} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha^{bb_{a,1}} \sum_i \sum_j^{m-1} b_i b_{a_j} + \\
 & \alpha^{bb_{a,2}} \sum_i b_i b_{a_m} + \alpha^{b_{a,1} b_{a,1}} \sum_{ij}^{m-1} b_{a_i} b_{a_j} + \alpha^{b_{a,1} b_{a,2}} \sum_i^{m-1} b_{a_i} b_{a_m},
 \end{aligned} \tag{57}$$

where:

$$\begin{pmatrix} \alpha^b & \alpha^{bb_{a,1}} \\ \alpha^{b_{a,1}} & \alpha^{bb_{a,2}} \\ \alpha^{b_{a,2}} & \alpha^{b_{a,1} b_{a,1}} \\ \alpha^{bb} & \alpha^{b_{a,1} b_{a,2}} \end{pmatrix} = \begin{pmatrix} -1/2 & -1 \\ 1 & -2 \\ \frac{1}{2}(n-m+n^2-2mn+m^2) & -(n-m) \\ 1/2 & 4(n-m) \end{pmatrix}. \tag{58}$$

Cost

- $\lceil \frac{k}{4} \rceil$ to $\lceil \frac{k}{2} \rceil$ auxiliary qubits per positive monomial.

Pros

- Smallest number of auxiliary coefficients that scales linearly with k .
- Smaller coefficients than the logarithmic reduction.

Cons

- Introduces many non-submodular terms.

Example

We quadratize a quartic term with only 1 auxiliary (half as many as in PTR-Ishikawa):

$$b_1 b_2 b_3 b_4 \rightarrow \frac{1}{2} (b_1 + b_2 + b_3 + b_4 - 2b_{a_1}) (b_1 + b_2 + b_3 + b_4 - 2b_{a_1} - 1) \tag{59}$$

Bibliography

- Original appears in: Theorem 7 of [?], and Theorem 10 of [?].

E. PTR-BCR-2 (Boros, Crama, and Rodríguez-Heck, 2018)

Summary

Pick m such that $k < 2^{m+1}$,

$$b_1 b_2 \dots b_k \rightarrow \alpha + \alpha^b \sum_i b_i + \alpha^{b_{a_i}} \sum_i 2^{i-1} b_{a_i} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha^{bb_a} \sum_{ij} b_i b_{a_j} + \alpha^{b_{a_i} b_{a_j}} b_{a_i} b_{a_j}, \quad (60)$$

where,

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha^{bb_a} \\ \alpha^{b_a} & \alpha^{b_a b_a} \end{pmatrix} = \begin{pmatrix} (2^m - k)^2 & 1 \\ 2(2^m - k) & 2^{j-1} \\ -2(2^m - k) & 2^{i+j-2} \end{pmatrix}. \quad (61)$$

Cost

$\lceil \log k \rceil$ auxiliary qubits per positive monomial.

Pros

- Logarithmic number of auxiliary variables.

Cons

- Introduces all terms non-submodular except for the term linear in auxiliaries.

Example

$$b_1 b_2 b_3 b_4 \rightarrow \frac{1}{2} (4 + b_1 + b_2 + b_3 + b_4 - b_{a_1} - 2b_{a_2}) (3 + b_1 + b_2 + b_3 + b_4 - b_{a_1} - 2b_{a_2}) \quad (62)$$

Alternate Forms

$$b_1 b_2 \dots b_k \rightarrow \left(2^m - k + \sum_i b_i - \sum_i 2^{i-1} b_{a_i} \right)^2 \quad (63)$$

Bibliography

- Original paper (Theorem 4, special case of Theorem 1): [?].

F. PTR-BCR-3 (Boros, Crama, and Rodríguez-Heck, 2018)

Summary

Pick m such that $k \leq 2^{m+1}$,

$$b_1 \dots b_k \rightarrow \frac{1}{2} \left(2^{m+1} - k + \sum_i b_i - \sum_i^m 2^i b_{a_i} \right) \left(2^{m+1} - k + \sum_i b_i - \sum_i^m 2^i b_{a_i} - 1 \right). \quad (64)$$

Cost

- $\lceil \log k/2 \rceil$ auxiliary qubits per positive monomial.
- coefficients range from $-\frac{k}{4}$ to $\frac{k^2}{8}$ when k is a power of 2 (best case scenario) and from $-\frac{(k-1)(k-2)}{2}$ to $\frac{(k-1)^2}{2}$ when k is not a power of 2 (worst case scenario).

Pros

- Logarithmic number of auxiliary variables.
- From the original paper: "As mentioned in Section 1, Theorem 9 provides a significant improvement over the best previously known quadratizations for the Positive monomial, and the upper bound on the number of auxiliary variables precisely matches the lower bound presented in Section 3."

Cons

- Introduces many non-submodular terms.

Example

$$b_1 b_2 b_3 b_4 \rightarrow \frac{1}{2} (b_1 + b_2 + b_3 + b_4 - 2b_a) (b_1 + b_2 + b_3 + b_4 - 2b_a - 1) \quad (65)$$

Alternate Forms

Let $X = \sum b_i$ and $N = 2^{m+1} - k$,

$$b_1 \dots b_k = \min_{b'_1, \dots, b'_n} \frac{1}{2} \left(N + X - \sum_{i=1}^n 2^i b'_i \right) \left(N + X - \sum_{i=1}^n 2^i b'_i - 1 \right). \quad (66)$$

Bibliography

- Original paper (Theorem 5): [?], Also in (Theorem 9): [?].

G. PTR-BCR-4 (Boros, Crama, and Rodríguez-Heck, 2018)

Summary

This is a more general form of the previous reduction, PTR-BCR-4, in which $k = 2^{m+1}$:

$$b_1 \dots b_k \rightarrow \sum_{ij} b_i b_j + \sum_{ij} 2^{i+j} b_{a_i} b_{a_j} - \sum_i \sum_j 2^{j+1} b_i b_{a_i}. \quad (67)$$

Cost

$\log(n)$ auxiliary qubits per positive monomial.

Pros

- Logarithmic number of auxiliary variables.

Cons

- Introduces many non-submodular terms.

Example

$$b_1 b_2 b_3 b_4 \rightarrow (b_1 + b_2 + b_3 + b_4 - 2b_a)^2 \quad (68)$$

Alternate Forms

Let $|x| = \sum_{i=1}^n b_i$

$$b_1 \dots b_k = \left(|x| - \sum_{i=0}^m 2^i b_{a_i} \right)^2. \quad (69)$$

Bibliography

- Original paper (Remark 5): [?].

H. PTR-KZ (Kolmogorov & Zabih, 2004)

Summary

This method can be used to re-write positive or negative cubic terms in terms of 6 quadratic terms. The identity is given by:

$$b_1 b_2 b_3 \rightarrow 1 - (b_a + b_1 + b_2 + b_3) + b_a (b_1 + b_2 + b_3) + b_1 b_2 + b_1 b_3 + b_2 b_3 \quad (70)$$

Cost

- 1 auxiliary variable per positive or negative cubic term.

Pros

- Works on positive or negative monomials.
- Reproduces the full spectrum.

Cons

- Introduces all 6 possible non-submodular quadratic terms.

Alternate Names

- "Reduction by Minimum Selection" [? ?].

Bibliography

- Original paper: [?].

I. PTR-KZ (in terms of z)

Summary

The formula is almost the same as in the version of PTR-KZ on the previous page (which is written in terms of b), but with a factor of 2, a change of sign for the linear terms, and a slight change in the constant term. This formula can be obtained directly from the PTR-KZ quadratization formula in terms of b , by starting with $8b_1b_2b_3$ on the left-side, making the substitution $b_i \rightarrow (1 + z_i)/2$, and removing all terms that appear on both sides of the equation. The result is:

$$\pm z_1 z_2 z_3 \rightarrow 3 \pm (z_1 + z_2 + z_3 + z_a) + 2z_a (z_1 + z_2 + z_3) + z_1 z_2 + z_1 z_3 + z_2 z_3. \quad (71)$$

Cost

- 1 auxiliary variable per positive or negative cubic term.

Pros

- Works on positive or negative monomials.
- Reproduces the full spectrum.

Cons

- Introduces all 6 possible non-submodular quadratic terms.

Bibliography

- 2004: published by Kolmogorov and Zabih in terms of b variables: [?].
- 31 March 2016: published by Chancellor, Zohren, and Warburton in terms of z , and without the constant term: [?].
- 8 April 2016: published independently by Leib, Zoller, and Lechner in terms of z , and without the constant term [? ?].

J. PTR-GBP ("Asymmetric reduction", Gallagher, Batra, Parikh, 2011)

Summary

Similar to other methods of reducing one term, this method can reduce a positive cubic monomial into quadratic terms using only one auxiliary variable, while introducing fewer non-submodular terms than the symmetric version.

The identity is given by:

$$b_1 b_2 b_3 \rightarrow b_a - b_2 b_a - b_3 b_a + b_1 b_a + b_2 b_3 \quad (72)$$

$$\rightarrow b_a - b_1 b_a - b_3 b_a + b_2 b_a + b_1 b_3 \quad (73)$$

$$\rightarrow b_a - b_1 b_a - b_2 b_a + b_3 b_a + b_1 b_2. \quad (74)$$

$$(75)$$

Cost

1 auxiliary variable per positive cubic term.

Pros

- Works on positive monomials.
- Fewer non-submodular terms than Ishikawa Reduction.

Cons

- Only been shown to work for cubics.

Example

$$b_1 b_2 b_3 + b_1 b_3 - b_2 \rightarrow (b_a - b_1 b_a - b_3 b_a + b_2 b_a + 2b_1 b_3) - b_2 \quad (76)$$

Bibliography

- Original paper and application to computer vision: [?].

K. PTR-RBL-(3→2) (Rocchetto, Benjamin, Li, 2016)

Summary

Using a ternary variable $t_q \in -1, 0, 1$ we have:

$$z_1 z_2 z_3 \rightarrow (1 + 4t_a + z_1 + z_2 + z_3)^2 - 1. \quad (77)$$

Cost

- 1 auxiliary ternary variable

Pros

- One of the only methods designed specifically for z variables.
- Symmetric with respect to all variables.

Cons

- The auxiliary variable required is ternary (a qutrit).
- Requires all possible quadratic terms and they are all non-submodular.
- Only reproduces the ground state manifold.

Example

$$-b_1 b_2 b_3 = \min_{b_a} b_a - b_1 + b_2 + b_3 - b_1 b_2 - b_1 b_3 + b_1 \quad (78)$$

Alternate Forms

$$-z_1 z_2 z_3 z_4 \rightarrow 16 t_a^2 + 4 t_a \sum_{i=1}^4 z_i + 2 \sum_{i=1}^4 \sum_{j>i}^4 z_i z_j + 4 \quad (79)$$

Bibliography

- Original paper where they introduce this gadget for the *end points* in the LHZ lattice: [?].

L. PTR-RBL-(4→2) (Rocchetto, Benjamin, Li, 2016)

Summary

Extra binary or ternary variable is added to ensure that the energy of the even parity sector is zero and the energy of the odd sector is higher:

$$z_1 z_2 z_3 z_4 \rightarrow 16 t_a^2 + 4 t_a \sum_{i=1}^4 z_i + 2 \sum_{i=1}^4 \sum_{j>i}^4 z_i z_j + 4. \quad (80)$$

Cost

- 1 auxiliary ternary variable

Pros

- One of the only methods designed specifically for z variables.

Cons

- Only reproduces the ground state manifold, not higher excited states.
- Requires all possible quadratic terms and they are all non-submodular.
- Only reproduces the ground state manifold.

Example

$$\begin{aligned} -z_1 z_2 z_3 z_4 &= -16 b_1 b_2 b_3 b_4 + 8 (b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) - \\ &4 (b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) + 2 (b_1 + b_2 + b_3 + b_4) - 1 \\ &\rightarrow 16 t_a^2 + 8 t_a \sum_{i=1}^4 b_i + 8 \sum_{i=1}^4 \sum_{j>i}^4 b_i b_j + 16 \end{aligned} \quad (81)$$

Bibliography

- Original paper: [?].

M. PTR-YXKK (Yip, Xu, Koenig and Kumar, 2019)

Summary

For $\alpha_1 \geq \alpha_2 > 1$ we can reduce a degree- k positive term to a degree- $(k-1)$ positive term, plus some extra terms which are at most quadratic:

$$b_1 b_2 \cdots b_k \rightarrow b_1 b_2 \cdots b_{k-1} + b_{a_1} + \alpha_1 b_{a_2} + \alpha_2 \sum_{i=1}^{k-1} (1 - b_i) (1 - b_{a_1}) + \quad (82)$$

$$\alpha_2 (1 - b_k) (1 - b_{a_2}) + \alpha_2 (1 - b_{a_2}) (1 - b_{a_1}) - \alpha_1 (1 - b_k) - 1. \quad (83)$$

Cost

- 2 auxiliary variables for each reduction from degree- k to degree- $(k-1)$.
- $2(k-2)$ auxiliary variables to quadratize a degree- k term.

Pros

- The coefficients α_1 and α_2 are adjustable, so there is flexibility in the size of the coefficients.
- Many terms are submodular.
- It is a ‘perfect’ quadratization, meaning that after minimizing over the auxiliary variables, the original function is exactly reproduced.
- Can in some very special cases, also eliminate up to $(k-3)$ negative terms (at most one of each from 3-local to $(k-1)$ -local) of the user’s choice, without any extra auxiliary qubits, if all of the variables in these negative terms are included in the higher-degree terms being reduced in the appropriate intermediate application of Eq. (82)-(83).

Cons

- Uses a lot of auxiliary variables.

Example

$$b_1 b_2 b_3 + b_1 b_3 - b_2 \rightarrow b_1 b_2 + b_{a_1} + 2b_{a_2} + 2(1 - b_1)(1 - b_{a_1}) + 2(1 - b_2)(1 - b_{a_1}) \quad (84)$$

$$+ 2(1 - b_3)(1 - b_{a_2}) + 2(1 - b_{a_2})(1 - b_{a_1}) - 2(1 - b_3) - 1 + b_1 b_3 - b_2. \quad (85)$$

Bibliography

- Original paper (Theorem 1): [?].
- Inspired by Theorem 3 of [?].
- More technical details (Constraint Composite Graph): [?].

N. PTR-CZW (Chancellor, Zohren, Warburton, 2017)

Summary

Auxilliary qubits can be made to “count” the number of logical qubits in the 1 configuration. By applying single qubit terms to the auxilliary qubits, the spectrum of *any* permutation symmetric objective function can be reproduced.

Cost

- For a k local coupler requires k auxilliary qubits.

Pros

- Natural flux qubit implementation [?].
- Single gadget can reproduce any permutation symmetric spectrum.
- High degree of symmetry means this method is natural for some kinds of quantum simulations [?].

Cons

- Requires coupling between all logical bits and from all logical bits to all auxilliary bits.
- Requires single body terms of increasing strength as k is increased.

Example

A 4 qubit gadget guarantees that the number of auxillary bits in the -1 state is equal to the number of logical bits in the 1 state

$$H_{4\text{-count}} = 4 \sum_{i=2}^4 \sum_{j=1}^{i-1} b_i b_j + 4 \sum_{i=1}^4 \sum_{j=1}^4 b_i b_{a_j} - 15 \sum_{i=1}^4 b_i - 8 \sum_{i=1}^4 b_{a_i} + (5 b_{a_1} + b_{a_2} - 3 b_{a_3} - 7 b_{a_4}) + 26 \quad (86)$$

This gadget can be expressed more naturally in terms of z :

$$H_{4\text{-count}} = \sum_{i=2}^4 \sum_{j=1}^{i-1} z_i z_j - \frac{1}{2} \sum_{i=1}^4 z_i + \sum_{i=1}^4 \sum_{j=1}^4 z_i z_{a_j} + \frac{1}{2} (5 z_{a_1} + z_{a_2} - 3 z_{a_3} - 7 z_{a_4}). \quad (87)$$

To replicate the spectrum of $b_1 b_2 b_3 b_4$, we add

$$H_{2\text{-local}} = -b_{a_4} + \lambda H_{4\text{-count}}. \quad (88)$$

where λ is a large number.

For the spectrum of

$$z_1 z_2 z_3 z_4 = 16 b_1 b_2 b_3 b_4 - 8 (b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) + 4 (b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) - 2 (b_1 + b_2 + b_3 + b_4) + 1, \quad (89)$$

we implement,

$$H_{2\text{-local}} = 2 b_{a_1} - 2 b_{a_2} + 2 b_{a_3} - 2 b_{a_4} + \lambda H_{4\text{-count}}, \quad (90)$$

Bibliography

- Paper on flux qubit implementation: [?]
- Paper on MAX- k -SAT mapping: [?] (published in a journal earlier than [?] but put on arXiv 1 month later).
- Talk including use in quantum simulation: [?]

O. Bit flipping (Ishikawa, 2011)

Summary

For any variable b , we can consider the negation $\bar{b} = 1 - b$. The process of exchanging b for \bar{b} is called *flipping*. Using bit-flipping, an arbitrary function in n variables can be represented using at most $2^{(n-2)}(n-3) + 1$ variables, though this is a gross overestimate.

Can be used in many different ways:

1. Flipping positive terms and using **II A**, recursively;
2. For $\alpha < 0$, we can reduce $\alpha \bar{b}_1 \bar{b}_2 \dots \bar{b}_k$ very efficiently to submodular form using **II A**. A generalized version exists for arbitrary combinations of flips in the monomial which makes reduction entirely submodular [?];
3. When we have quadratized we can minimize the number of non-submodular terms by flipping.
4. We can make use of both b_i and \bar{b}_i in the same objective function by adding on a sufficiently large penalty term: $\lambda(b_i + \bar{b}_i - 1)^2 = \lambda(1 + 2b_i \bar{b}_i - b_i - \bar{b}_i)$. This is similar to the ideas in reduction by substitution or deduc-reduc. In this way, given a quadratic in n variables we can make sure it only has at most n nonsubmodular terms if we are willing to use the extra n negation variables as well (so we have $2n$ variables in total).

Cost

- None, as replacing b_i with it's negation \bar{b}_i costs nothing except a trivial symbolic expansion.

Pros

- Cheap and effective way of improving submodularity.
- Can be used to combine terms in clever ways, making other methods more efficient.

Cons

- Unless the form of the objective function is known, spotting these 'factorizations' using negations is difficult.
- We need an auxiliary variable for each b_i for which we also want to use \bar{b}_i in the same objective function.

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (91)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (92)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- Original paper: [?].

IV. METHODS THAT QUADRATIZE MULTIPLE TERMS WITH THE SAME AUXILIARIES (CASE 1: SYMMETRIC FUNCTION REDUCTIONS, SFR)

A symmetric function is one where if we switch any of the variable names (for example $b_1 \rightarrow b_5 \rightarrow b_8 \rightarrow b_1$), the function's output is unaffected.

A. SFR-ABCG-1 (Anthony, Boros, Crama, Gruber, 2014)

Summary

Any n -variable symmetric function $f(b_1, b_2, \dots, b_n) \equiv f(b)$ can be quadratized with $n - 2$ auxiliaries:

$$f(b) \rightarrow -\alpha_0 - \alpha_0 \sum_i b_i + a_2 \sum_{ij} b_i b_j + 2 \sum_i (\alpha_i - c) b_{a_i} \left(2i - \frac{1}{2} - \sum_j b_j \right) \quad (93)$$

$$c = \begin{cases} \min(\alpha_{2j}) & , i \in \text{even} \\ \min(\alpha_{2j-1}) & , i \in \text{odd} \end{cases} \quad (94)$$

$$a_2 = \text{Determined from Page 12 of [?]} \quad (95)$$

Cost

- $n - 2$ auxiliaries for any n -variable symmetric function.
- n^2 non-submodular quadratic terms (of the non-auxiliary variables).
- $n - 2$ non-submodular linear terms (of the auxiliary variables).

Pros

- Quadratization is symmetric in all non-auxiliary variables (this is not always true, for example some of the methods in the NTR section).
- Reproduces the full spectrum.
- When there's a large number of terms, there's fewer auxiliary variables than quadratizing each positive monomial separately.

Cons

- Only works on a specific class of functions, although the quadratizations of arbitrary functions can be related to the quadratizations of symmetric functions on a larger number of variables.
- All quadratic terms of the non-auxiliary variables are non-sub-modular.
- All linear terms of the auxiliaries are non-submodular.
- Not meant so much to be practical, but rather an easy proof of an upper bound on the number of needed auxiliaries.

Bibliography

- 2014, original paper (Theorem 4.1, with α_i from Corollary 2.3): [?].

B. SFR-BCR-1 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

Any n -variable symmetric function $f(b_1, b_2, \dots, b_n) \equiv f(b)$ that is non-zero only when $\sum b_i = c$ where $n/2 \leq c \leq n$, can be quadratized with $m = \lceil \log_2 c \rceil + 1$ auxiliary variables:

$$f(b) \rightarrow \alpha + \alpha^b \sum_i b_i + \alpha_1^{b_a} \sum_i^{m-1} b_{a_i} + \alpha_2^{b_a} b_{a_m} + \alpha^{bb} \sum_{i,j} b_i b_j + \alpha_1^{bb_a} \sum_i^{m-1} \sum_j b_i b_{a_j} + \alpha_2^{bb_a} \sum_i b_i b_{a_m} + \alpha_1^{b_a b_a} \sum_{i,j}^{m-1} b_{a_i} b_{a_j} + \alpha_2^{b_a b_a} \sum_i^{m-1} b_{a_i} b_{a_m}, \quad (96)$$

where:

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha_1^{bb_a} \\ \alpha_1^{b_a} & \alpha_2^{bb_a} \\ \alpha_2^{b_a} & \alpha_1^{b_a b_a} \\ \cdot & \alpha_2^{b_a b_a} \end{pmatrix} = \begin{pmatrix} (c+1)^2 & 1 \\ -2(c+1) & -2^i \\ (c+1)2^i & 2(1+2^{m-1}) \\ (1+2^{m-1})(2^{m-1}-2c-1) & 2^{i+j-1} \\ \cdot & -(1+2^{m-1})2^i \end{pmatrix}. \quad (97)$$

Cost

- $m = \lceil \log_2 c \rceil + 1$ auxiliary variables.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

For $n = 4$ and $c = 2$, we have $m = 2$, and

$$(b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) - 3(b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) + 6b_1 b_2 b_3 b_4 \quad (98)$$

$$\rightarrow (-3 + b_1 + b_2 + b_3 + b_4 - b_{a_1} + 3b_{a_2})^2 \quad (99)$$

using the alternate form below.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \left(-(c+1) + \sum_i b_i - \sum_i^{m-1} 2^{i-1} b_{a_i} + (1+2^{m-1}) b_{a_m} \right)^2 \quad (100)$$

Bibliography

- 2018, original paper (Theorem 1): [?].

C. SFR-BCR-2 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

Any n -variable symmetric function $f(b_1, b_2, \dots, b_n) \equiv f(b)$ that is non-zero only when $\sum b_i = c$ where $0 \leq c \leq n/2$, can be quadratized with $m = \lceil \log_2(n - c) \rceil + 1$ auxiliary variables:

$$f(b) \rightarrow \alpha + \alpha^b \sum_i b_i + \alpha_1^{b_a} \sum_i^{m-1} b_{a_i} + \alpha_2^{b_a} b_{a_m} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha_1^{bb_a} \sum_{ij}^{m-1} b_i b_{a_j} + \alpha_2^{bb_a} \sum_i b_i b_{a_m} + \alpha_1^{b_a b_a} \sum_{ij}^{m-1} b_{a_i} b_{a_j} + \alpha_2^{b_a b_a} \sum_i^{m-1} b_{a_i} b_{a_m}, \quad (101)$$

where:

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha_1^{bb_a} \\ \alpha_1^{b_a} & \alpha_2^{bb_a} \\ \alpha_2^{b_a} & \alpha_1^{b_a b_a} \\ \cdot & \alpha_2^{b_a b_a} \end{pmatrix} = \begin{pmatrix} (c-1)^2 & 1 \\ -2(c-1) & +2^i \\ (1-c)2^i & -2(1+2^{m-1}) \\ (1+2^{m-1})(2^{m-1}+2c-1) & 2^{i+j-1} \\ \cdot & -(1+2^{m-1})2^i \end{pmatrix}. \quad (102)$$

Cost

- $m = \lceil \log_2(n - c) \rceil + 1$ auxiliary variables.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

For $n = 4$ and $c = 2$, we have $m = 2$, and

$$(b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) - 3(b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) + 6b_1 b_2 b_3 b_4 \quad (103)$$

$$\rightarrow (1 - b_1 - b_2 - b_3 - b_4 - b_{a_1} + 3b_{a_2})^2 \quad (104)$$

using the alternate form below.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \left((c-1) - \sum_i b_i - \sum_i^{m-1} 2^{i-1} b_{a_i} + (1+2^{m-1}) b_{a_m} \right)^2 \quad (105)$$

Bibliography

- 2018, original paper (Theorem 1): [?].

D. SFR-BCR-3 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

Any n -variable symmetric function $f(b_1, b_2, \dots, b_n) \equiv f(b)$ that is non-zero only when $\sum b_i = c$ where $n/2 \leq c \leq n$, can be quadratized with $m = \lceil \log_2 c \rceil$ auxiliary variables $f \rightarrow$:

$$f(b) \rightarrow \alpha + \alpha^b \sum_i b_i + \alpha_1^{b_a} \sum_i^{m-1} b_{a_i} + \alpha_2^{b_a} b_{a_m} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha_1^{bb_a} \sum_i^{m-1} \sum_j b_i b_{a_j} + \alpha_2^{bb_a} \sum_i b_i b_{a_m} + \alpha_1^{b_a b_a} \sum_{ij}^{m-1} b_{a_i} b_{a_j} + \alpha_2^{b_a b_a} \sum_i^{m-1} b_{a_i} b_{a_m}, \quad (106)$$

where:

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha_1^{bb_a} \\ \alpha_1^{b_a} & \alpha_2^{bb_a} \\ \alpha_2^{b_a} & \alpha_1^{b_a b_a} \\ \cdot & \alpha_2^{b_a b_a} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(c^2 + 3c + 2) & \frac{1}{2} \\ -c - \frac{3}{2} & -2^i \\ (3+c)2^{i-1} & (1+2^m) \\ (1+2^m)(2^{m-1} - c - 1) & 2^{i+j-1} \\ \cdot & -(1+2^m)2^i \end{pmatrix}. \quad (107)$$

Cost

- $m = \lceil \log_2 c \rceil$ auxiliary variables.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

For $n = 4$ and $c = 2$, we have $m = 1$, and

$$(b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) - 3(b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) + 6b_1 b_2 b_3 b_4 \quad (108)$$

$$\rightarrow \binom{-3 + b_1 + b_2 + b_3 + b_4 + 3b_{a_1}}{2} \quad (109)$$

using the alternate form below.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \binom{-(c+1) + \sum_i b_i - \sum_i^{m-1} 2^i b_{a_i} + (1+2^m) b_{a_m}}{2} \quad (110)$$

Bibliography

- 2018, original paper (Theorem 2): [?] and (Theorem 7): [?].

E. SFR-BCR-4 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

Any n -variable symmetric function $f(b_1, b_2, \dots, b_n) \equiv f(b)$ that is non-zero only when $\sum b_i = c$ where $0 \leq c \leq n/2$, can be quadratized with $m = \lceil \log_2(n - c) \rceil$ auxiliary variables $f \rightarrow$:

$$f(b) \rightarrow \alpha + \alpha^b \sum_i b_i + \alpha_1^{b_a} \sum_i^{m-1} b_{a_i} + \alpha_2^{b_a} b_{a_m} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha_1^{bb_a} \sum_i^{m-1} b_i b_{a_j} + \alpha_2^{bb_a} \sum_i b_i b_{a_m} + \alpha_1^{b_a b_a} \sum_{ij}^{m-1} b_{a_i} b_{a_j} + \alpha_2^{b_a b_a} \sum_i^{m-1} b_{a_i} b_{a_m}, \quad (111)$$

where:

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha_1^{bb_a} \\ \alpha_1^{b_a} & \alpha_2^{bb_a} \\ \alpha_2^{b_a} & \alpha_1^{b_a b_a} \\ \cdot & \alpha_2^{b_a b_a} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(c^2 - 3c + 2) & \frac{1}{2} \\ -c + \frac{3}{2} & +2^i \\ (3 - c)2^{i-1} & -(1 + 2^m) \\ (1 + 2^m)(2^{m-1} + c - 1) & 2^{i+j-1} \\ \cdot & -(1 + 2^m)2^i \end{pmatrix}. \quad (112)$$

Cost

- $m = \lceil \log_2(n - c) \rceil$ auxiliary variables.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

For $n = 4$ and $c = 2$, we have $m = 1$, and

$$(b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4) - 3(b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4) + 6b_1 b_2 b_3 b_4 \quad (113)$$

$$\rightarrow \binom{1 - b_1 - b_2 - b_3 - b_4 + 3b_{a_1}}{2} \quad (114)$$

using the alternate form below.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \binom{(c-1) - \sum_i b_i - \sum_i^{m-1} 2^i b_{a_i} + (1 + 2^m) b_{a_m}}{2} \quad (115)$$

Bibliography

- 2018, original paper (Theorem 2): [?] and (Theorem 7): [?].

F. SFR-BCR-5 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

For an n -variable symmetric function that is the sum of all variables $f(b_1, b_2, \dots, b_n) = f(\sum b_i)$, with some large value of $\lambda > \max(f)$, such that $f(|c|) = 0$ for $c > n$, using $\lceil \sqrt{n+1} \rceil$ auxiliary variables, we have:

$$f(\sum b_i) \rightarrow \sum_{i,j}^m f((i-1)(m+1) + (j-1)) b_{a_i} b_{a_{c+j}} + \lambda \left(\left(1 - \sum_i^m b_{a_i} \right)^2 + \left(1 - \sum_i^m b_{a_{c+i}} \right)^2 + \left(\sum_i b_i - \left((m+1) \sum_i^m (i-1) y_{a_i} + \sum_i^m (i-1) b_{a_{c+i}} \right) \right)^2 + \left(\sum_i b_i - \left((m+1) \sum_i^m (i-1) y_{a_i} + \sum_i^m (i-1) b_{a_{c+i}} \right) \right)^2 \right) \quad (116)$$

Cost

- $m = \lceil \sqrt{n+1} \rceil$ auxiliary variables.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1b_2 + b_2b_3 + 2b_1b_4 - 4b_2b_4 \quad (117)$$

$$= -3b_1\bar{b}_2 - \bar{b}_2b_3 - 2b_1\bar{b}_4 - \bar{b}_2\bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (118)$$

The first expression is highly non-submodular while the second is entirely submodular.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \left(\frac{1}{2} \left((c-1) - \sum_i b_i - (2(n-c) - 2^{m-1} + 1) b_{a_m} - \sum_i^{m-1} 2^{i-1} b_{a_i} \right) \right) \quad (119)$$

Bibliography

- 2018, original paper (Theorem 9): [?] (contains a typo which was corrected in Theorem 6 of [?]).

G. SFR-BCR-6 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

For an n -variable symmetric function that is a function of a *weighted* sum of all variables $f(b_1, b_2, \dots, b_n) = f(\sum w_i b_i)$, for some large value of $\lambda > \max(f)$, and $\max(f(\sum w_i b_i)) < (m+1)^2$:

$$f(\sum w_i b_i) \rightarrow \sum_{ij}^m \alpha_{ij} b_{a_i} b_{a_{m+i}} + \lambda \left(1 + \left(\sum_i w_i b_i - (m-1) \sum_i b_{a_i} + \sum_i^m b_{a_{c+i}} \right)^2 + \sum_i^{m-1} (1 - b_{a_i}) b_{a_{i+1}} + \sum_i^{m-1} (1 - b_{a_{i+m}}) b_{a_{i+m+1}} \right) \quad (120)$$

where:

$$\sum_i^\alpha \sum_j^\beta \alpha_{ij} = f(\alpha(m+1) + \beta) \quad (121)$$

Cost

- $2m$ auxiliary variables, where $m > \sqrt{\max(f(\sum w_i b_i))} - 1$.
- $n^2 + m^2$ non-submodular quadratic terms (all possible quadratic terms involving only non-auxiliary or only auxiliary variables).
- m non-submodular linear terms (all possible linear terms involving auxiliaries).

Pros

- Small number of auxiliary terms

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms.

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (122)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (123)$$

The first expression is highly non-submodular while the second is entirely submodular.

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow \left(\frac{1}{2} \left((c-1) - \sum_i b_i - (2(n-c) - 2^{m-1} + 1) b_{a_m} - \sum_i^{m-1} 2^{i-1} b_{a_i} \right) \right) \quad (124)$$

Bibliography

- 2018, original paper (Theorem 10): [?].

H. SFR-ABCG-2 (Anthony, Boros, Crama, Gruber, 2014)

Summary

For any n -variable, k -local function that is non-zero only if $\sum b_i = 2m - 1$, we call it the "partity function" and it can be quadratized as follows:

$$f(b_1, b_2, \dots, b_n) \rightarrow \sum_i b_i + 2 \sum_{ij} b_i b_j + 4 \sum_{2i-1}^{n-1} b_{a_i} \left(2i - 1 - \sum_j b_j \right). \quad (125)$$

Cost

- $m = 2\lfloor n/2 \rfloor$ auxiliary variables.
- $\lfloor 1.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (126)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (127)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2014, original paper (Theorem 4.6): [? ?].

I. SFR-ABCG-3 (Anthony, Boros, Crama, Gruber, 2014)

Summary

The complement of the parity function can be quadratized as follow:

$$f(b_1, b_2, \dots, b_n) \rightarrow 1 + 2 \sum_{i,j} b_i b_j - \sum_i b_i + 4 \sum_{2i}^{n-1} b_{a_i} \left(i - \sum_j^n b_j \right) \quad (128)$$

Cost

- $m = 2 \lfloor \frac{n-1}{2} \rfloor$ auxiliary variables.
- $\lfloor 0.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.
- Fewer non-submodular linear terms than in the analogous quadratization for its complement (the parity function).

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries, and all n linear terms involving only the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (129)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (130)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2014, original paper (Theorem 4.6): [? ?].

J. SFR-BCR-7 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

For a symmetric function such that $f(|c|) = 0$ for $c > n$, then with $\max(\lceil \log(c) \rceil, \lceil \log(n - c) \rceil)$ auxiliary variables, we have:

$$f(b_1, b_2, \dots, b_n) \rightarrow 1 + 2 \sum_{i,j} b_i b_j - \sum_i b_i + 4 \sum_{2i}^{n-1} b_{a_i} \left(i - \sum_j^n b_j \right) \quad (131)$$

Cost

- $\max(\lceil \log(c) \rceil, \lceil \log(n - c) \rceil)$ auxiliary variables.
- $\lfloor 0.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.
- Fewer non-submodular linear terms than in the analogous quadratization for its complement (the parity function).

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries, and all n linear terms involving only the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1b_2 + b_2b_3 + 2b_1b_4 - 4b_2b_4 \quad (132)$$

$$= -3b_1\bar{b}_2 - \bar{b}_2b_3 - 2b_1\bar{b}_4 - \bar{b}_2\bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (133)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2018, original paper (Theorem 7): [?].

K. SFR-BCR-8 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

For the at least k-out-of-n function $f_{\geq k}$, using $\max(\lceil \log(c) \rceil, \lceil \log(n-c) \rceil)$ auxiliary variables, we have:

$$\begin{aligned} f(b_1, b_2, \dots, b_n) \rightarrow & \alpha + \alpha^b \sum_i b_i + \alpha_1^{b_a,1} \sum_i^{m-1} b_{a_i} + \alpha_2^{b_a,2} b_{a_m} + \alpha^{bb} \sum_{ij} b_i b_j + \alpha_1^{bb_a,1} \sum_i^{m-1} \sum_j^{m-1} b_i b_{a_j} \\ & + \alpha_2^{bb_a,2} \sum_i b_i b_{a_m} + \alpha_1^{b_a b_a,1} \sum_{ij}^{m-1} b_{a_i} b_{a_j} + \alpha_2^{b_a b_a,2} \sum_i^{m-1} b_{a_i} b_{a_m}, \end{aligned} \quad (134)$$

where:

$$\begin{pmatrix} \alpha & \alpha^{bb} \\ \alpha^b & \alpha_1^{bb_a} \\ \alpha_1^{b_a} & \alpha_2^{bb_a} \\ \alpha_2^{b_a} & \alpha_1^{b_a b_a} \\ \cdot & \alpha_2^{b_a b_a} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(c^2 + 3c + 4) & \frac{1}{2} \\ -\frac{1}{2}(2c + 3) & -2^i \\ (c + 2)2^{i-1} & -(1 + 2^m) \\ \frac{1}{2}((1 + 2^m)(2^m - 2c - 2) - 2) & 2^{i+j-1} \\ \cdot & -(1 + 2^m)2^i \end{pmatrix}. \quad (135)$$

Cost

- $\max(\lceil \log(c) \rceil, \lceil \log(n-c) \rceil)$ auxiliary variables.
- $\lfloor 0.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.
- Fewer non-submodular linear terms than in the analogous quadratization for its complement (the parity function).

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries, and all n linear terms involving only the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (136)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (137)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2018, original paper (Theorem 8): [?].

L. SFR-BCR-9 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

For a non-concave symmetric function such that $f(x) = r(X)$ for $n \geq 3$, then with m auxiliary variables where $m \geq \log(n) - 1$, we have:

$$f(b_1, b_2, \dots, b_n) \rightarrow \alpha \sum_{i,j} b_i b_j + \beta \sum_i b_i + \sum_i \sum_j^m \gamma_j b_i b_{a_j} + \sum_{i,j}^m \delta_{ij} b_{a_i} b_{a_j} + \sum_{j=1}^m \epsilon_j b_{a_j} + \phi \quad (138)$$

Cost

- A minimum of $\log(n) - 1$ auxiliary variables.

Pros

- Logarithmic number of auxiliary variables

Cons

- Only works for a special class of functions

Example

Bibliography

- Original paper (Theorem 3 / Lemma 2): [?].

M. SFR-ABCG-4 (Anthony, Boros, Crama, Gruber, 2016)

Summary

For an arbitrary y-linear quadratization of the parity function, with m auxiliary variables where $m > \sqrt{\frac{n}{4} - 1}$, we have:

$$f(b_1, b_2, \dots, b_n) \rightarrow q(b_1, b_2, \dots, b_n) + \sum_i^m a_i(b_1, b_2, \dots, b_n) b_{a_i} \quad (139)$$

where $q(b)$, and $a(b)$ are any arbitrary quadratic, and linear function respectively.

Cost

- Greater than $\sqrt{\frac{n}{4} - 1}$ auxiliary variables.

Pros

Cons

Example

For $n = 4$ and $m = 1$

$$b_1 b_2 b_3 b_4 \rightarrow b_1 b_2 + b_a(b_3 - 1) \quad (140)$$

Alternate Forms

$$f(b_1, b_2, \dots, b_n) \rightarrow q(b_1, b_2, \dots, b_n) + \sum_i^m (\ell_i(b_1, b_2, \dots, b_n) - \alpha_i) b_{a_i} \quad (141)$$

Bibliography

- 2014, original paper Definition 1.1, and Theorem 5.6: [?].

N. PFR-BCR-1 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

The parity function for even n can be quadratized with:

$$f(b_1, b_2, \dots, b_n) \rightarrow 1 + 2 \sum_{i,j} b_i b_j - \sum_i b_i + 4 \sum_{2i}^{n-1} b_{a_i} \left(i - \sum_j^n b_j \right) \quad (142)$$

Cost

- $\lceil \log^{n/2} \rceil$ auxiliary variables.
- $\lfloor 0.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.
- Fewer non-submodular linear terms than in the analogous quadratization for its complement (the parity function).

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries, and all n linear terms involving only the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (143)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (144)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2018, original paper (Theorem 11): [?] .

O. PFR-BCR-2 (Boros, Crama, Rodríguez-Heck, 2018)

Summary

The parity function for odd n can be quadratized with:

$$f(b_1, b_2, \dots, b_n) \rightarrow 1 + 2 \sum_{i,j} b_i b_j - \sum_i b_i + 4 \sum_{2i}^{n-1} b_{a_i} \left(i - \sum_j b_j \right) \quad (145)$$

Cost

- $\lceil \log^{n/2} \rceil$ auxiliary variables.
- $\lfloor 0.5n \rfloor$ non-submodular linear terms.
- n^2 non-submodular quadratic terms.

Pros

- Smaller number of auxiliary variables than the most naive methods.
- Fewer non-submodular linear terms than in the analogous quadratization for its complement (the parity function).

Cons

- Only works for a special class of functions
- Introduces many linear and even more quadratic non-submodular terms (everything is non-submodular except for $0.5n^2$ quadratic terms involving the auxiliaries with the non-auxiliaries, and all n linear terms involving only the non-auxiliaries).
- non-submodular terms can be rather large compared to the submodular terms (about $4n$ times as big).

Example

By bit-flipping b_2 and b_4 , i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1 b_2 + b_2 b_3 + 2b_1 b_4 - 4b_2 b_4 \quad (146)$$

$$= -3b_1 \bar{b}_2 - \bar{b}_2 b_3 - 2b_1 \bar{b}_4 - \bar{b}_2 \bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \quad (147)$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography

- 2018, original paper (Theorem 11): [?] .

P. Lower bounds for SFRs (Anthony, Boros, Crama, Gruber, 2014)

- There exist symmetric functions on n variables for which no quadratization can be done without at least $\Omega(\sqrt{n})$ auxiliary variables (Theorem 5.3 from [? ?]).
- There exist symmetric functions on n variables for which no quadratization linear in the auxiliaries can be done without at least $\Omega\left(\frac{n}{\log_2(n)}\right)$ auxiliary variables (Theorem 5.5 from [? ?]).
- The parity function on n variables cannot be quadratized without quadratic terms involving the auxiliary variables, unless there is at least $\sqrt{n/4 - 1} + 1 = \Omega(\sqrt{n})$ auxiliary variables (Theorem 5.6 from [? ?]).
- Theorem 5 of [?] gives an even tighter bound of $\lceil \log(n) \rceil - 1$ for the minimum number of auxiliary variables for the parity function.
- Corollary 5 of [?] gives $m \geq \log(1/2 - \mu) + \log(n) - 1$.

Q. Lower bounds for positive monomials (Boros, Crama, Rodríguez-Heck, 2018)

- A positive monomial with n variables cannot be quadratized with fewer than $\lceil \log(n) \rceil - 1$ auxiliary variables, unless there is some extra deduction we can make about the optimization problem, as in for example deduc-reduc (Corollary 1 from [? ?]).
- ALCN (at least c out of n) and ECN (exact c out of n) functions also cannot be quadratized with fewer than $\lceil \log(n) \rceil - 1$ auxiliary variables (Corollaries 2 and 3 from [? ?]).
- ECN (exact c out of n) functions also cannot be quadratized with fewer than $\max(\lceil \log(c) \rceil, \lceil \log(n - c) \rceil) - 1$ auxiliary variables (Corollaries 2 and 3 from [? ?]).

R. Lower bounds for ZUCs (Boros, Crama, Rodríguez-Heck, 2018)

- There exist ZUC (zero until c) functions such that every quadratization must involve at least $\Omega(2^{n/2})$ auxiliary variables, no matter what the value of c (Theorem 2 from [?]). This is true for almost all ZUC functions because the set of ZUCs requiring fewer auxiliary variables has Lebesgue measure zero.
- For any $c \geq 0$, the number of auxiliary variables is $m \geq \lceil \log(c) \rceil - 1$ (Theorem 3 of [?]).

S. Lower bounds for d -sublinear functions (Boros, Crama, Rodríguez-Heck, 2018)

- The number of auxiliary variables m is such that $2^{m+1} \geq \frac{\beta(q_1)}{2} - d + 1$ (Theorem 12 from [?]).
- For any $c \geq 0$, the number of auxiliary variables is $m \geq \lceil \log(c) \rceil - 1$ (Theorem 3 of [?]).

V. METHODS THAT QUADRATIZE MULTIPLE TERMS WITH THE SAME AUXILIARIES (CASE 2: ARBITRARY FUNCTIONS)

A. Reduction by Substitution (Rosenberg 1975)

Summary

Pick a variable pair (b_i, b_j) and substitute $b_i b_j$ with a new auxiliary variable $b_{a_{ij}}$. Enforce equality in the ground states by adding some scalar multiple of the penalty $P = b_i b_j - 2b_i b_{a_{ij}} - 2b_j b_{a_{ij}} + 3b_{a_{ij}}$ or similar. Since $P > 0$ if and only if $b_{a_{ij}} \neq b_i b_j$, the minimum of the new $(k-1)$ -local function will satisfy $b_{a_{ij}} = b_i b_j$, which means that at the minimum, we have precisely the original function. Repeat $(k-2)$ times for each k -local term and the resulting function will be 2-local. For an arbitrary cubic term we have:

$$b_i b_j b_k \rightarrow b_a b_k + b_i b_j - 2b_i b_a - 2b_j b_a + 3b_a. \quad (148)$$

Cost

- 1 auxiliary variable per reduction.
- At most kt auxiliary variables for a k -local objective function of t terms, but usually fewer.

Pros

- Variable can be used across the entire objective function, reducing many terms at once.
- Very easy to implement.
- Reproduces not only the ground state, but the full spectrum.

Cons

- Inefficient for single terms as it introduces many auxiliary variables compared to Ishikawa reduction, for example.
- Introduces quadratic terms with large positive coefficients, making them highly non-submodular.
- Determining optimal substitutions can be expensive.

Example

We pick a pair, for example b_1, b_2 and apply Eq. (148):

$$b_1 b_2 b_3 + b_1 b_2 b_4 \mapsto b_3 b_a + b_4 b_a + 2b_1 b_2 - 4b_1 b_a - 4b_2 b_a + 6b_a. \quad (149)$$

Bibliography

- Original paper: [?]
- Re-discovered in the context of diagonal quantum Hamiltonians: [?].
- Used in: [? ?].

B. FGBZ Reduction for Negative Terms (Fix-Gruber-Boros-Zabih, 2011)

Summary

We consider a set C of variables which can occur in multiple terms throughout the objective function. Each application ‘rips out’ this common component from each term [? ?].

$$-\sum_H \alpha_H \prod_{j \in H} b_j \rightarrow \sum_H \alpha_H \left(1 - \prod_{j \in C} b_j - \prod_{j \in H \setminus C} b_j \right) b_a \quad (150)$$

Cost

- One auxiliary variable per application.
- In combination with **II A**, it can reduce t negative terms of degree k in n variables using $n + t(k - 2)$ auxiliary variables in the worst case.

Pros

- Can reduce the connectivity of an objective function, as it breaks interactions between variables.

Cons

- Cannot reduce the degree of the original function if $|C| \leq 1$, and cannot quadratize anything for the other values of $|C|$ (but it can reduce their degree).

Example

First let $C = b_1 b_2$ and we can get:

$$-b_1 b_2 b_3 - b_1 b_2 b_4 \mapsto (1 - b_1 b_2 - b_3) b_{a_1} + (1 - b_1 b_2 - b_4) b_{a_1} \quad (151)$$

$$= 2b_{a_1} - b_3 b_{a_1} - b_4 b_{a_1} - 2b_1 b_2 b_{a_1} \quad (152)$$

now we can use **II A**:

$$-2b_1 b_2 b_{a_1} \mapsto 2(2 - b_1 - b_2 - b_{a_1}) b_{a_2} \quad (153)$$

$$= 4b_{a_2} - 2b_1 b_{a_2} - 2b_2 b_{a_2} - 2b_{a_1} b_{a_2}. \quad (154)$$

Bibliography

- Original paper and application to image denoising: [?].
- The example given here can be done with only one auxiliary variable using the theorem proved by Dattani and Chau.

C. FGBZ Reduction for Positive Terms (Fix-Gruber-Boros-Zabih, 2011)

Summary

We consider a set C of variables which can occur in multiple terms throughout the objective function. Each application ‘rips out’ this common component from each term [? ?]:

$$\sum_H \alpha_H \prod_{j \in H} b_j \rightarrow \sum_H \alpha_H b_a \prod_{j \in C} b_j + \sum_H \alpha_H (1 - b_a) \prod_{j \in H \setminus C} b_j. \quad (155)$$

Cost

- One auxiliary variable per application.
- In combination with II A, it can reduce t positive terms of degree k in n variables using $n + t(k - 1)$ auxiliary variables in the worst case.

Pros

- It is a ‘perfect’ transformation, meaning that after minimizing over b_a , the original degree- k function is recovered.
- Can reduce the connectivity of an objective function, as it breaks interactions between variables.

Cons

- If $|C| = 1$ the first sum will result in a quadratic but the second sum will have degree k . If $|C| = k - 1$ the second sum will be quadratic but the first term will have degree k . For any other value of $|C|$, both sums will be super-quadratic, but the part of the second sum involving b_a will be negative and therefore can be quadratized easily.

Example

With $C = b_1$ we can get:

$$b_1 b_2 b_3 + b_1 b_2 b_4 \rightarrow 2b_{a_1} b_1 + (1 - b_{a_1}) b_2 b_3 + (1 - b_{a_1}) b_2 b_4 \quad (156)$$

$$= 2b_{a_1} b_1 + b_2 b_3 + b_2 b_4 - b_{a_1} b_2 b_3 - b_{a_1} b_2 b_4 \quad (157)$$

now we can use II A to quadratize the two negative cubic terms:

$$-b_{a_1} b_2 b_3 - b_{a_1} b_2 b_4 \mapsto 2b_{a_2} - b_{a_1} b_{a_2} - b_{a_2} b_2 - b_{a_2} b_3 + 2b_{a_2} - b_{a_1} b_{a_2} - b_{a_2} b_2 - b_{a_2} b_4 \quad (158)$$

$$= 4b_{a_2} - 2b_{a_1} b_{a_2} - 2b_{a_2} b_2 - b_{a_2} b_3 - b_{a_2} b_4. \quad (159)$$

Bibliography

- Original paper and application to image denoising: [?].
- The example given here can be done with only one auxiliary variable using the theorem proved by Dattani and Chau.

D. Pairwise Covers (Anthony-Boros-Crama-Gruber, 2017)

Summary

Let S be a set of monomials, where $\mathcal{H} \subseteq S$ for each $H \in \mathcal{H}$ and each H has a weight α_H . \mathcal{H} is a pairwise cover of the function. We can partition each term of the objective function into a product of two monomials $A(S), B(S)$, which will be replaced by auxiliary variables. Each application replaces original monomials with selected auxiliary variables [?]:

$$\sum_{S \in \mathcal{F}} \alpha_S \prod_{j \in S} b_j = \min_{b_a} \sum_{S \in \mathcal{F}} \alpha_S \prod_{H \in R(S)} b_H + \sum_{H \in \mathcal{H}} |\alpha_H| \left(b_H \left(2|H| - 1 - 2 \sum_{j \in H} b_j \right) + \prod_{j \in H} b_j \right) \quad (160)$$

Cost

- One auxiliary variable per replaced monomial.
- Using at most $|\mathcal{H}|$ auxiliary variables.

Pros

- Can quadratize complex objective functions directly
- Can reduce the connectivity of an objective function, as it breaks interactions between variables.

Cons

- Determining optimal substitutions can be expensive.
- It can lead to a large number of quadratic terms and auxiliary variables in the quadratization result.

Example

We choose $b_{a_1} = b_1 b_3$, $b_{a_2} = b_2 b_4$:

$$5b_1 b_2 b_3 b_4 + 4b_1 b_2 b_4 - 3b_1 b_3 - 2b_2 b_3 b_4 \mapsto 5b_{a_1} b_{a_2} + 4b_1 b_{a_2} - 3b_{a_1} - 2b_3 b_{a_2} + \quad (161)$$

$$8(b_{a_1}(3 - 2b_1 - 2b_3) + b_1 b_3) + 11(b_{a_2}(3 - 2b_2 - 2b_4) + b_2 b_4) \quad (162)$$

Bibliography

- Theorem 4 of: [?].

E. Flag Based SAT Mapping

Summary

This method uses gadgets to produce separate 3-SAT clauses which allow variables which ‘flag’ the state of pairs of other variables.

Cost

- 24 auxiliary variables to quadratize $z_1 z_2 z_3$.

Pros

- Very general and therefore conducive to proofs.

Cons

- Extremely inefficient in terms of number of auxiliary variables.

Example

To create a system which maps $b_1 b_2 b_3$, we use the following gadget (note that this is given in terms of z in the original work and translated to b here):

$$H_1(b_1, b_2, b_3) = 2 \sum_{i=1}^3 b_i b_{a_i} + 2 \sum_{i<j}^3 b_{a_i} b_{a_j} - 4 \sum_{i=1}^3 b_{a_i} - 2 \sum_{i=1}^3 b_i + \frac{23}{2}. \quad (163)$$

Implementing αH_1 , creates a situation where b_3 is a ‘flag’ for b_1 and b_2 in other words b_3 is constrained to be 1 in the low energy manifold if $b_1 = 0$ and $b_2 = 0$. It follows from the universality of 3 – SAT that these ‘flag’ clauses can be combined to map any spin Hamiltonian. To do this, we also need anti-ferromagnetic couplings to express the ‘negated’ variable, to do this, we define,

$$H_2(b_1, b_{-1}) = 2 b_1 b_{-1} - b_i - b_{-1} + 1. \quad (164)$$

As an explicit example, consider reproducing the spectrum of $z_1 z_2 z_3 = (2 b_1 - 1)(2 b_2 - 1)(2 b_3 - 1)$. In this case we need to assign a higher energy to the $(1, 1, 1)$, $(0, 0, 1)$, $(0, 1, 0)$, and $(1, 0, 0)$ states. A flag ($b_{a_{4,1}}$) which is forced into a higher energy state if these conditions are satisfied can be constructed from two instances of H_1 and an auxilliary qubit, combining these leads to

$$z_1 z_2 z_3 \rightarrow \alpha \left(\sum_{i=1}^3 H_2(b_i, b_{-i}) + \sum_{i=1}^{2^3} H_2(b_{a_i}, b_{-a_i}) + H_2(b_{a_{4,1}}, b_{a_{4,2}}) + H_1(b_{a_{1,1}}, b_{a_{1,2}}, b_{-a_1}) + H_1(b_{a_1}, b_{a_{1,3}}, b_{a_{4,1}}) + \right. \quad (165)$$

$$\left. H_1(b_1, b_2, b_{-a_2}) + H_1(b_{a_2}, b_3, b_{a_{4,2}}) + H_1(b_1, b_2, b_{-a_3}) + H_1(b_{a_3}, b_{a_{1,3}}, b_{a_{4,1}}) + H_1(b_{a_{1,1}}, b_{a_{1,2}}, b_{-a_4}) + \right. \quad (166)$$

$$\left. H_1(b_{a_4}, b_3, b_{a_{4,2}}) + H_1(b_1, b_{a_{1,2}}, b_{-a_5}) + H_1(b_{a_5}, b_3, b_{a_{4,1}}) + H_1(b_{a_{1,1}}, b_2, b_{-a_6}) + H_1(b_{a_6}, b_{a_{1,3}}, b_{a_{4,2}}) + \right. \quad (167)$$

$$\left. H_1(b_1, b_2, b_{-a_7}) + H_1(b_{a_7}, b_{a_{1,3}}, b_{a_{4,1}}) + H_1(b_{a_{1,1}}, b_{a_{1,2}}, b_{-a_8}) + H_1(b_{a_8}, b_3, b_{a_{4,2}}) \right) - 2 b_{a_{4,1}} + 1. \quad (168)$$

Each of the next four lines assigns a value to the flag variable $b_{a_{4,1}}$ for a state and $b_{a_{4,2}}$, for instance the leftmost two terms of the second line enforce that $b_{a_{4,1}} = 0$ if $(b_1, b_2, b_3) = (0, 0, 0)$, while the right two terms enforce that $b_{a_{4,1}} = 1$ if $(b_1, b_2, b_3) = (1, 1, 1)$. Because there are $2^3 = 8$ possible bitstrings for (b_1, b_2, b_3) , and each term to enforce a flag state requires two instances of H_1 (and two auxilliary variables), a total of 16 instances are required as well as 16 auxilliary variables.

Bibliography

- Paper showing the universality of the Ising spin models: [?].

F. Lower bounds for arbitrary functions (Anthony, Boros, Crama, Gruber, 2015)

- There exist functions on n variables for which no quadratization can be done without at least $\frac{2^{n/2}}{8} = \Omega(\sqrt{n})$ auxiliary variables (Theorem 5.3 from [?]).
- There exist symmetric functions on n variables for which no quadratization linear in the auxiliaries can be done without at least $\Omega\left(\frac{2^n}{n}\right)$ auxiliary variables (Theorem 5.5 from [?]).

VI. STRATEGIES FOR COMBINING METHODS

A. SCM-BCR (Boros, Crama, and Rodríguez-Heck, 2018)

Summary

Split a k -local monomial with odd k into a $(k - 1)$ -local term (with even degree) and a new odd k -local term which has negative coefficient:

$$b_1 b_2 \cdots b_k \rightarrow \prod_{i=1}^{k-1} b_i - \prod_{i=1}^{k-1} b_i (1 - b_k) \quad (169)$$

We can use any of the PTR methods for even k on the first term, and we can use any of the NTR methods on the second term. Can be generalized to split into different-degree factors when seeking an "optimum" quadratization. Can be generalized into more splits.

Cost

- Depends on the methods used for the PTR and NTR procedures.

Pros

- Very flexible.

Cons

- First turns one term into two terms, so might not be preferred when we wish to minimize the number of terms.

Bibliography

- Original paper: [?].

B. Decomposition into symmetric and anti-symmetric parts

Summary

Split a any function f into a symmetric part and anti-symmetric part:

$$f(b_1, b_2, \dots, b_n) = f_{\text{symmetric}} + f_{\text{anti-symmetric}}, \quad (170)$$

$$f_{\text{symmetric}} \equiv \frac{1}{2} (f(b_1, b_2, \dots, b_n) + f(1 - b_1, 1 - b_2, \dots, 1 - b_n)) \quad (171)$$

$$f_{\text{anti-symmetric}} \equiv \frac{1}{2} (f(b_1, b_2, \dots, b_n) - f(1 - b_1, 1 - b_2, \dots, 1 - b_n)) \quad (172)$$

We can now use any of the methods described only for symmetric functions, on the symmetric part, and use the (perhaps less powerful) general methods on the anti-symmetric part.

Cost

- Depends on the methods used.

Pros

- Allows non-symmetric functions to benefit from techniques designed only for symmetric functions.

Cons

- May result in more terms than simply quadratizing the non-symmetric function directly.

Bibliography

- Discussed in: [?].

Part II

Hamiltonians quadratic in z and linear in x (Transverse Field Ising Hamiltonians)

The Ising Hamiltonian with a transverse field in the x direction is possible to implement in hardware:

$$H = \sum_i \left(\alpha_i^{(z)} z_i + \alpha_i^{(x)} x_i \right) + \sum_{ij} \left(\alpha_{ij}^{(zz)} z_i z_j \right). \quad (173)$$

C. ZZZ-TI-CBBK: Transverse Ising from ZZZ, by Cao, Babbush, Biamonte, and Kais (2015)

There is only one reduction in the literature for reducing a Hamiltonian term to the transverse Ising Hamiltonian, and it works on 3-local zzz terms, by introducing an auxiliary qubit with label a :

$$\alpha z_i z_j z_k \rightarrow \alpha^I + \alpha_i^z z_i + \alpha_j^z z_j + \alpha_k^z z_k + \alpha_a^z z_a + \alpha_a^x x_a + \alpha_{ia}^{zz} z_i z_a + \alpha_{ja}^{zz} z_j z_a + \alpha_{ka}^{zz} z_k z_a + \alpha_{ij}^{zz} z_i z_j + \alpha_{ik}^{zz} z_i z_k + \alpha_{jk}^{zz} z_j z_k \quad (174)$$

$$\begin{aligned} \alpha^I &= \frac{1}{2} \left(\Delta + \left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} + 6 \left(\frac{\alpha}{6} \right)^{4/5} \Delta^{1/5} \right) \\ \alpha_i^z &= \alpha_j^z = \alpha_k^z = -\frac{1}{2} \left(\left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) - \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \right) \\ \alpha_a^z &= -\frac{1}{2} \left(\Delta - \left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} \right) \\ \alpha_a^x &= \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \\ \alpha_{ia}^{zz} &= \alpha_{ja}^{zz} = \alpha_{ka}^{zz} = -\frac{1}{2} \left(\left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) + \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \right) \\ \alpha_{ij}^{zz} &= \alpha_{ik}^{zz} = \alpha_{jk}^{zz} = 2 \left(\frac{\alpha}{6} \right)^{4/5} \Delta^{1/5} \end{aligned}$$

Including all coefficients and factorizing, we get:

$$\alpha z_i z_j z_k \rightarrow \left(\Delta + \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} (z_i + z_j + z_k) \right) \left(\frac{1 - z_a}{2} \right) + \left(\left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \right) x_a \quad (175)$$

$$+ \left(\left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} - \left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) (z_i + z_j + z_k) \right) \left(\frac{1 + z_a}{2} \right) \quad (176)$$

$$+ \left(\left(\frac{\alpha}{6} \right)^{4/5} \Delta^{1/5} \right) (3 + 2z_i z_j + 2z_i z_k + 2z_j z_k) \quad (177)$$

The low-lying spectrum (eigenvalues *and* eigenvectors) of the right side of Eq. (174) will match those of the left side to within a spectral error of ϵ as long as $\Delta = \mathcal{O}(\epsilon^{-5})$.

Cost

- 1 auxiliary qubit
- 8 auxiliary terms not proportional to $\mathbb{1}$.

Bibliography

- Original paper (Eq. 53-54): [?] .

Part III

General Quantum Hamiltonians

VII. NON-PERTURBATIVE GADGETS

A. NP-OY (Ocko & Yoshida, 2011)

Summary

For the 8-body Hamiltonian:

$$H_{8\text{-body}} = -J \sum_{ij} (X_{i,j,3} X_{i,j+1,2} X_{i,j,4} X_{i,j+1,4} X_{i+1,j,1} X_{i+1,j+1,1} X_{i+1,j,3} X_{i+1,j+1,2} + \\ Z_{i,j,1} Z_{i,j,2} Z_{i,j,3} Z_{i,j,4} + Z_{i-1,j,4} Z_{i,j,1} + Z_{i,j,2} Z_{i,j-1,3} + Z_{i,j,4} Z_{i+1,j,1} + Z_{i,j,3} Z_{i,j+1,2}), \quad (178)$$

we define auxiliary qubits labeled by a_{ijk} , two auxiliaries for each pair ij : labeled a_{ij1} and a_{ij2} . Then the 8-body Hamiltonian has the same low-lying eigenspace as the 4-body Hamiltonian:

$$H_{4\text{-body}} = \sum_{ij} J (-Z_{i,j,1} Z_{i,j,2} Z_{i,j,3} Z_{i,j,4} - Z_{i,j-1,4} Z_{i,j,1} - Z_{i,j,2} Z_{i,j-1,3} - Z_{i,j,4} Z_{i+1,j,1} - Z_{i,j,3} Z_{i,j+1,2} + \\ (1 - Z_{a_{ij1}} + Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}}) (Z_{a_{i,j+1,1}} + Z_{a_{i,j+1,2}} + Z_{a_{i,j+1,1}} Z_{a_{i,j+1,2}} - 1) + \\ (1 + Z_{a_{ij1}} - Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}}) (1 - Z_{a_{i+1,j,1}} - Z_{a_{i+1,j,2}} - Z_{a_{i+1,j,1}} Z_{a_{i+1,j,2}})) - \\ \frac{U}{2} (Z_{a_{ij1}} + Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}} - 1) - \\ \frac{t}{2} ((X_{a_{ij2}} + Z_{a_{ij1}} X_{a_{ij2}}) X_{i,j,3} X_{i,j,4} + (X_{a_{ij1}} X_{a_{ij2}} + Y_{a_{ij1}} Y_{a_{ij2}}) X_{i,j+1,2} X_{i,j+1,4} + \\ (X_{a_{ij2}} - Z_{a_{ij1}} X_{a_{ij2}}) X_{i+1,j+1,1} X_{i+1,j+1,2} + (X_{a_{ij1}} X_{a_{ij2}} - Y_{a_{ij1}} Y_{a_{ij2}}) X_{i+1,j,1} X_{i+1,j,3})). \quad (179)$$

Now by defining the following ququits (spin-3/2 particles, or 4-level systems):

$$S_{ijk i' j' k'}^{zz} = Z_{ijk} Z_{i' j' k'} \quad (180)$$

$$S_{a_{ij}1}^{zz} = (1 - Z_{a_{ij1}} + Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}}) \quad (181)$$

$$S_{a_{ij}2}^{zz} = (Z_{a_{ij1}} + Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}} - 1) \quad (182)$$

$$S_{a_{ij}3}^{zz} = (1 + Z_{a_{ij1}} - Z_{a_{ij2}} + Z_{a_{ij1}} Z_{a_{ij2}}) \quad (183)$$

$$S_{a_{ij}1}^{xz} = (X_{a_{ij2}} + Z_{a_{ij1}} X_{a_{ij2}}) \quad (184)$$

$$S_{a_{ij}2}^{xz} = (X_{a_{ij2}} - Z_{a_{ij1}} X_{a_{ij2}}) \quad (185)$$

$$S_{ijk i' j' k'}^{xx} = X_{ijk} X_{i' j' k'} \quad (186)$$

$$S_{a_{ij}1}^{xy} = (X_{a_{ij1}} X_{a_{ij2}} + Y_{a_{ij1}} Y_{a_{ij2}}) \quad (187)$$

$$S_{a_{ij}2}^{xy} = (X_{a_{ij1}} X_{a_{ij2}} - Y_{a_{ij1}} Y_{a_{ij2}}) \quad (188)$$

NP-OY (Ocko & Yoshida, 2011) [Continued]

We can write the 4-body Hamiltonian on qubits as a 2-body Hamiltonian on ququits:

$$H_{2\text{-body}} = \sum_{ij} \left(J \left(-s_{ij1ij2}^{zz} s_{ij3ij4}^{zz} - s_{ij-1,4ij1}^{zz} - s_{ij2ij-1,3}^{zz} - s_{ij4i+1j1}^{zz} - s_{ij3ij+1,2}^{zz} + s_{a_{ij}1}^{zz} s_{a_{ij+1}2}^{zz} - s_{a_{ij}3}^{zz} s_{a_{i+1j}3}^{zz} \right) \right. \\ \left. - \frac{U}{2} s_{a_{ij},2}^{zz} - \frac{t}{2} \left(s_{a_{ij}1}^{xz} s_{ij3ij4}^{xx} + s_{a_{ij}1}^{xy} s_{ij+1,2ij+1,4}^{xx} + s_{a_{ij}2}^{xz} s_{i+1,j+1,i+1,j+1,2}^{xx} + s_{a_{ij}2}^{xy} s_{i+1,j1,i+1,j3}^{xx} \right) \right). \quad (189)$$

The low-lying eigenspace of $H_{2\text{-body}}$ is *exactly* the same as for $H_{4\text{-local}}$.

Cost

- 2 auxiliary ququits for each pair ij .
- 6 more total terms (6 terms in the 8-body version becomes 12 terms: 11 of them 2-body and 1 of them 1-body).

Pros

- Non-perturbative. No prohibitive control precision requirement.
- Only two auxiliaries required for each pair ij .
- 8-body to 2-body transformation can be accomplished in 1 step, rather than a 1B1 gadget which would take 6 steps or an SD + $(3 \rightarrow 2)$ gadget combination which would take 4 steps.

Cons

- Increase in dimension from working with only 2-level systems (spin-1/2 particles or 2×2 matrices) to working with 4-level systems (spin-3/2 particles).
- Until now, only derived for a very specific Hamiltonian form.
- This approach may become more demanding for Hamiltonians that are more than 8-local.

Bibliography

- Original paper (Eq. 1): [?].

B. NP-SJ (Subasi & Jarzynski, 2016)

Summary

Determine the k -local term, $H_{k\text{-local}}$, whose degree we wish to reduce, and factor it into two commuting factors: $H_{k'\text{-local}}H_{(k-k')\text{-local}}$, where k' can be as low as 0. Separate all terms that are at most $(k-1)$ -local into ones that commute with one of these factors (it does not matter which one, but without loss of generality we assume it to be the $(k-k')$ -local one) and ones that anti-commute with it:

$$H_{<k\text{-local}}^{\text{commuting}} + H_{<k\text{-local}}^{\text{anti-commuting}} + \alpha H_{k'\text{-local}} H_{(k-k')\text{-local}} \quad (190)$$

Introduce one auxiliary qubit labeled by a and the Hamiltonian:

$$\alpha X_a H_{k'\text{-local}} + H_{<k\text{-local}}^{\text{commuting}} + Z_a H_{<k\text{-local}}^{\text{anti-commuting}} \quad (191)$$

no longer contains $H_{k\text{-local}}$ but $H_{<k\text{-local}}^{\text{anti-commuting}}$ is now one degree higher.

Cost

- 1 auxiliary qubit to reduce k -local term to $(k' + 1)$ -local where k' can even be 0-local, meaning the k -local term is reduced to a 1-local one.
- Raises the k -locality of $H_{<k\text{-local}}^{\text{anti-commuting}}$ by 1 during each application. It can become $(> k)$ -local!

Pros

- Non-perturbative
- Can linearize a term of arbitrary degree in one step.
- Requires very few auxiliary qubits.

Cons

- Can introduce many new non-local terms as an expense for reducing only one k -local term.
- If the portion of the Hamiltonian that does not commute with the $(k-k')$ -local term has terms of degree $k-1$ (which can happen if $k'=0$) they will all become k -local, so there is no guarantee that this method reduces k -locality.
- If any terms were more than 1-local, this method will not fully quadratize the Hamiltonian (it must be combined with other methods).
- It only works when the Hamiltonian's terms of degree at most $k-1$ all either commute or anti-commute with the k -local term to be eliminated.

Example

$$4z_5 - 3x_1 + 2z_1y_2x_5 + 9x_1x_2x_3x_4 - x_1y_2z_3x_5 \rightarrow 9x_{a_1} + 4z_{a_2}z_5 - 3z_{a_3}x_1 - z_{a_3}x_{a_2} + 2x_{a_3}x_5 \quad (192)$$

Bibliography

- Original paper, and description of the choices of terms and factors used for the given example [?].

C. NP-Nagaj-1 (Nagaj, 2010)

Summary The Feynman Hamiltonian can be written as [?]:

$$\frac{1}{4} (x_1 x_2 - i y_1 x_2 + i x_1 y_2 + y_1 y_2) U_{2\text{-local}} + \frac{1}{4} (x_1 x_2 + i y_1 x_2 - i x_1 y_2 + y_1 y_2) U_{2\text{-local}}^\dagger, \quad (193)$$

where $U_{2\text{-local}}$ is an arbitrary 2-local unitary matrix that acts on qubits different from the ones labeled by "1" and "2". This Hamiltonian that is 4-local on qubits can be transformed into one that is 2-local in qubits and qutrits. Here we show the 2-local Hamiltonian for the case where $U_{2\text{-local}} = \text{CNOT} \equiv \frac{1}{2} (\mathbb{1} + z_3 + x_4 - z_3 x_4)$. We start with the specific 4-local Hamiltonian:

$$H_{4\text{-local}} = \frac{1}{4} (x_1 x_2 + y_1 y_2 + x_1 x_2 z_3 + x_1 x_2 x_4 + y_1 y_2 z_3 + y_1 y_2 x_4 - x_1 x_2 z_3 x_4 - y_1 y_2 z_3 x_4), \quad (194)$$

and after adding 4 auxiliary qubits labeled by a_1 to a_4 and 6 auxiliary qutrits labeled by a_5 to a_{10} and acted on by the Gell-Mann matrices λ_1 to λ_9 , we get the following 2-local Hamiltonian:

$$H_{2\text{-local}} = \frac{1}{2} (x_1 \lambda_{1,a_5} + y_1 \lambda_{2,a_5} + \lambda_{6,a_5} - \lambda_{6,a_5} z_3 + \lambda_{4,a_5} x_{a_1} + \lambda_{5,a_5} y_{a_1} + x_{a_1} \lambda_{1,a_6} + \quad (195)$$

$$y_{a_1} \lambda_{2,a_6} + 2\lambda_{6,a_6} x_4 + \lambda_{4,a_6} x_{a_2} + \lambda_{5,a_6} y_{a_2} + x_{a_2} \lambda_{1,a_7} + y_{a_2} \lambda_{2,a_7} + \lambda_{6,a_7} - \lambda_{6,a_7} z_3 + \quad (196)$$

$$\lambda_{4,a_7} x_2 + \lambda_{5,a_7} y_2 + x_1 \lambda_{1,a_8} + y_1 \lambda_{2,a_8} + \lambda_{6,a_8} + \lambda_{6,a_8} z_3 + \lambda_{4,a_8} x_{a_3} + \lambda_{5,a_8} y_{a_3} + \quad (197)$$

$$x_{a_3} \lambda_{1,a_9} + y_{a_3} \lambda_{2,a_9} + 2\lambda_{6,a_9} + \lambda_{4,a_9} x_{a_4} + \lambda_{5,a_9} y_{a_4} + x_{a_4} \lambda_{1,a_{10}} + y_{a_4} \lambda_{2,a_{10}} + \quad (198)$$

$$\lambda_{6,a_{10}} + \lambda_{6,a_{10}} z_3 + \lambda_{4,a_{10}} x_2 + \lambda_{5,a_{10}} y_2), \quad (199)$$

whose low-lying spectrum is equivalent to the spectrum of $H_{2\text{-local}}$.

Cost

- 6 auxiliary qutrits and 4 auxiliary qubits
- 2 quartic, 4 cubic, and 2 quadratic terms becomes 27 quadratic terms and 5 linear terms in the Pauli-GellMann basis.

Pros

- Exact (non-perturbative). No special control precision demands.
- All coefficients are equal to each other, with a value of $1/2$, except one which is equal to 1.
- With more auxiliary qubits, can be further reduced to only containing qubits.

Cons

- Involves qutrits in all 32 terms.
- Only derived (so far) for the Feynman Hamiltonian.
- High overhead in terms of number of auxiliary qubits and number of terms.

Example

The transformation presented above was for the case of $U_{2\text{-local}} = \text{CNOT} \equiv \frac{1}{2} (\mathbb{1} + z_3 + x_4 - z_3 x_4)$, but similar transformations can be derived for any arbitrary unitary matrix $U_{2\text{-local}}$.

Bibliography

- Original paper: [?].

D. NP-Nagaj-2 (Nagaj, 2012)

Summary

Similar to NP-Nagaj-1 but instead of using qutrits, we use two qubits for each qutrit, according to:

$$|0\rangle \rightarrow |00\rangle, \quad |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \quad |2\rangle \rightarrow \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \quad (200)$$

which leads to the following transformations:

$$|01\rangle\langle 10|_{ij} + h.c. \rightarrow \frac{1}{\sqrt{2}}(|01\rangle\langle 10|_{ij_1} + |01\rangle\langle 10|_{ij_2}) + h.c. \quad (201)$$

$$|02\rangle\langle 10|_{ij} + h.c. \rightarrow \frac{1}{\sqrt{2}}(|01\rangle\langle 10|_{ij_1} - |01\rangle\langle 10|_{ij_2}) + h.c. \quad (202)$$

$$|1\rangle\langle 2|_j + h.c. \rightarrow \frac{1}{2}(z_{j_1} - z_{j_2}), \quad (203)$$

and the following 2-local Hamiltonian involving only qubits:

$$\begin{aligned} H_{2\text{-local}} = & \frac{1}{4}(z_{a_5} - z_{a_6} - z_{a_5}z_3 + z_{a_6}z_3 + z_{a_9} - z_{a_{10}} - z_{a_9}z_3 + z_{a_{10}}z_3 + z_{a_{11}} - z_{a_{12}} + \\ & z_{a_{11}}z_3 - z_{a_{12}}z_3 + z_{a_{15}} - z_{a_{16}} + z_{a_{15}}z_3 - z_{a_{16}}z_3) + \frac{1}{2}(z_{a_7}x_4 - z_{a_8}x_4 + z_{a_{13}} - z_{a_{14}}) + \\ & \frac{1}{2\sqrt{2}}(x_1x_{a_5} + y_1y_{a_5} + x_1x_{a_6} + y_1y_{a_6} - x_{a_5}x_{a_1} - y_{a_5}y_{a_1} + x_{a_6}x_{a_1} + y_{a_6}y_{a_1} + \\ & x_{a_1}x_{a_7} + y_{a_1}y_{a_7} + x_{a_1}x_{a_8} + y_{a_1}y_{a_8} - x_{a_7}x_{a_2} - y_{a_7}y_{a_2} + x_{a_8}x_{a_2} + y_{a_8}y_{a_2} + x_{a_2}x_{a_9} + y_{a_2}y_{a_9} + \\ & x_{a_2}x_{a_{10}} + y_{a_2}y_{a_{10}} - x_{a_9}x_2 - y_{a_9}y_2 + x_{a_{10}}x_2 + y_{a_{10}}y_2 + x_1x_{a_{11}} + y_1y_{a_{11}} + x_1x_{a_{12}} + y_1y_{a_{12}} - \\ & x_{a_{11}}x_{a_3} - y_{a_{11}}y_{a_3} + x_{a_{12}}x_{a_3} + y_{a_{12}}y_{a_3} + x_{a_3}x_{a_{13}} + y_{a_3}y_{a_{13}} + x_{a_3}x_{a_{14}} + y_{a_3}y_{a_{14}} - x_{a_{13}}x_{a_4} - y_{a_{13}}y_{a_4} + \\ & x_{a_{14}}x_{a_4} + y_{a_{14}}y_{a_4} + x_{a_4}x_{a_{15}} + y_{a_4}y_{a_{15}} + x_{a_4}x_{a_{16}} + y_{a_4}y_{a_{16}} - x_{a_{15}}x_2 - y_{a_{15}}y_2 + x_{a_{16}}x_2 + y_{a_{16}}y_2) \end{aligned} \quad (204)$$

whose low-lying spectrum is equivalent to the spectrum of $H_{2\text{-local}}$.

Cost

- 16 auxiliary qubits.

Pros

- Exact (non-perturbative). No special control precision demands.
- Only involves qubits (as opposed to NP-Nagaj-1 which contains qutrits and NP-OY which contains ququits).

Cons

- Only derived (so far) for the Feynman Hamiltonian.
- High overhead in terms of number of auxiliary qubits and number of terms.

Example

The transformation presented above was for the case of $U_{2\text{-local}} = \text{CNOT} \equiv \frac{1}{2}(\mathbb{1} + z_3 + x_4 - z_3x_4)$, but similar transformations can be derived for any arbitrary unitary matrix $U_{2\text{-local}}$.

Bibliography

- Original paper: [?].

VIII. PERTURBATIVE ($3 \rightarrow 2$) GADGETS

The first gadgets for arbitrary Hamiltonians acting on some number of qubits, were designed to reproduce the spectrum of a 3-local Hamiltonian in the low-lying spectrum of a 2-local Hamiltonian.

A. $P(3 \rightarrow 2)$ -DC1 (Duan, Chen, 2011)

Summary

For any group of 3-local terms that can be factored into a product of three 1-local factors, we can define three auxiliary qubits (regardless of the number of qubits we have in total) labeled by a_i and make the transformation:

$$\prod_i \sum_j \alpha_{ij} S_i \rightarrow \alpha + \alpha_i^{ss} \sum_i \left(\sum_j \alpha_{ij} S_{ij} \right)^2 + \alpha_i^{sx} \sum_i \sum_j \alpha_{ij} S_{ij} X_{a_i} + \alpha^{zz} \sum_{ij} Z_{a_i} Z_{a_j} \quad (205)$$

$$\begin{pmatrix} \alpha & \alpha^{ss} \\ \alpha^{sx} & \alpha^{zz} \end{pmatrix} = \begin{pmatrix} \frac{\Delta}{8} & \frac{\Delta^{1/3}}{6} \\ -\frac{\Delta^{2/3}}{6} & -\frac{\Delta}{24} \end{pmatrix} \quad (206)$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3\text{-local}}$ to within ϵ as long as $\Delta = \Theta(\epsilon^{-3})$.

Cost

- 3 auxiliary qubits for each group of 3-local terms that can be factored into three 1-local factors.
- $\Delta = \Theta(\epsilon^{-3})$

Pros

- Very few auxiliary qubits needed

Cons

- Will not work for Hamiltonians that do not factorize appropriately.

Example

$$(x_1 + 3x_2) z_3 y_4 + z_1 x_2 \rightarrow \alpha + \alpha_{12}^{xx} (x_1 + 3x_2)^2 + \alpha_3^{zz} z_3^2 + \alpha_4^{yy} y_4^2 + \alpha^{xx} (x_1 x_{a_1} + 3x_2 x_{a_1}) \quad (207)$$

$$+ \alpha^{zx} z_3 x_{a_2} + \alpha^{yx} y_4 x_{a_3} + \alpha^{zz} (z_{a_1} z_{a_2} + z_{a_1} z_{a_3} + z_{a_2} z_{a_3}) + z_1 x_2 \quad (208)$$

Bibliography

- Original paper (Eqs. 33-36): [?]

B. $P(3 \rightarrow 2)$ -DC2 (Duan, Chen, 2011)

Summary

For any 3-local term (product of Pauli matrices s_i) in the Hamiltonian, we can define *one* auxiliary qubit labeled by a and make the transformation:

$$a \prod_i^3 s_i \rightarrow \alpha + \alpha^s s_3 + \alpha^z z_a + \alpha^{ss} (s_1 + s_2)^2 + \alpha^{sz} s_3 z_a + \alpha^{sx} (s_1 x_a + s_2 x_a) \quad (209)$$

$$\begin{pmatrix} \alpha & \alpha^s & \alpha^z \\ \alpha^{ss} & \alpha^{sz} & \alpha^{sx} \end{pmatrix} = \begin{pmatrix} \frac{\Delta}{2} & a \left(\frac{\Delta^{2/3}}{4} - 1 \right) & \frac{\Delta}{2} \\ \Delta^{1/3} & \frac{a\Delta^{2/3}}{4} & \Delta^{2/3} \end{pmatrix} \quad (210)$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3\text{-local}}$ to within ϵ as long as $\Delta = \Theta(\epsilon^{-3})$.

Cost

- 1 auxiliary qubit for each 3-local term.
- $\Delta = \Theta(\epsilon^{-3})$

Example

$$x_1 z_2 y_3 - 3x_1 x_2 y_4 + z_1 x_2 \rightarrow 2\alpha + \alpha_1^y y_3 + \alpha_2^y y_4 + \alpha^z (z_{a_1} + z_{a_2}) + \alpha_{12}^{xz} (x_1 + z_2)^2 + \alpha_{12}^{xx} (x_1 + x_2)^2 \quad (211)$$

$$+ \alpha_1^{yz} y_3 z_{a_1} + \alpha_2^{yz} y_4 z_{a_2} + \alpha^{zx} z_2 x_{a_1} + \alpha^{xx} (x_1 x_{a_1} + x_1 x_{a_2} + x_2 x_{a_2}) + z_1 x_2 \quad (212)$$

Bibliography

- Original paper (Eq. 2-5, and 19-22 which are equivalent): [?]

C. $P(3 \rightarrow 2)$ -KKR (Kempe, Kitaev, Regev, 2004)

Summary

For any 3-local term (product of commuting matrices s_i) in the Hamiltonian, we can define three auxiliary qubits labeled by a_i and make the transformation:

$$a \prod_i^3 s_i \rightarrow \alpha + \alpha^{ss} \sum_i s_i^2 + \alpha^{sx} \sum_i s_i x_{a_i} + \alpha^{zz} \sum_{i,j} z_{a_i} z_{a_j} \quad (213)$$

$$\begin{pmatrix} \alpha & \alpha^{ss} \\ \alpha^{sx} & \alpha^{zz} \end{pmatrix} = \begin{pmatrix} \frac{3\Delta}{4} & \Delta^{1/3} \\ -\Delta^{2/3} & -\frac{\Delta}{4} \end{pmatrix} \quad (214)$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3\text{-local}}$ to within ϵ as long as $\Delta = \Theta(\epsilon^{-3})$.

Notes

For a term on the right-hand-side (the quadratic Hamiltonian) such as $x_1 x_2$ or $x_2 x_{a_3}$ the choice of whether to use α^{ss} or α^{sx} may seem ambiguous since we would get xx in both cases by setting $s = x$, however the defining formula for this quadratization shows that α^{ss} is to be used when both x operators are acting on logical qubits, whereas α^{sx} is only used when one of the qubits is an auxiliary qubit.

Cost

- 3 auxiliary qubits for each 3-local term.
- $\Delta = \Theta(\epsilon^{-3})$

Example

$$z_1 x_2 - 5x_1 z_2 y_3 + 8x_1 x_2 y_4 \rightarrow z_1 x_2 + 2\alpha \mathbb{1} + \alpha^{ss} (2x_1^2 + z_2^2 + y_3^2 + x_2^2 + y_4^2) \quad (215)$$

$$+ \alpha^{sx} (x_1 x_{a_{11}} + z_2 x_{a_{12}} + y_3 x_{a_{13}} + x_1 x_{a_{21}} + x_2 x_{a_{22}} + y_4 x_{a_{23}}) \quad (216)$$

$$+ \alpha^{zz} (z_{a_{11}} z_{a_{12}} + z_{a_{11}} z_{a_{13}} + z_{a_{12}} z_{a_{13}} + z_{a_{21}} z_{a_{22}} + z_{a_{21}} z_{a_{23}} + z_{a_{22}} z_{a_{23}}) \quad (217)$$

Alternate Forms

$$-6s_1 s_2 s_3 \rightarrow \frac{3\Delta}{4} + \Delta^{1/3} (s_1^2 + s_2^2 + s_3^2) - \Delta^{2/3} (s_1 x_{a_1} + s_2 x_{a_2} + s_3 x_{a_3}) - \frac{\Delta}{4} (z_{a_1} z_{a_2} + z_{a_1} z_{a_3} + z_{a_2} z_{a_3}) \quad (218)$$

Bibliography

- Original paper on arXiv (Eq. 13): [?]]
- Journal publication two years later (Eq. 6.2): [?]]

D. P(3 → 2)-OT (Oliveira-Terhal, 2005)

Summary

For any 3-local term which is a product of 1-local matrices s_i , we can define one auxiliary qubit labeled by a and make the transformation:

$$a \prod_i^3 s_i \rightarrow \alpha + \alpha_1^s s_1^2 + \alpha_2^s s_2^2 + \alpha_3^s s_3 + \alpha_a^z z_a + \alpha_{12}^{ss} s_1 s_2 + \alpha_{13}^{ss} s_1^2 s_3 + \alpha_{23}^{ss} s_2^2 s_3 + \alpha_{3a}^{sz} s_3 z_a + \alpha_{1a}^{sx} s_1 x_a + \alpha_{2a}^{sx} s_2 x_a \quad (219)$$

$$\begin{pmatrix} \alpha & \alpha_{12}^{ss} \\ \alpha_1^s & \alpha_{13}^{ss} \\ \alpha_2^s & \alpha_{23}^{ss} \\ \alpha_3^s & \alpha_{3a}^{sz} \\ \alpha_a^z & \alpha_{1a}^{sx} \\ \text{N/A} & \alpha_{2a}^{sx} \end{pmatrix} = \begin{pmatrix} \frac{\Delta}{2} & -\Delta^{1/3} a^{2/3} \\ \frac{a^{2/3} \Delta^{1/3}}{2} & \frac{a}{2} \\ \frac{a^{2/3} \Delta^{1/3}}{2} & \frac{a}{2} \\ -\frac{a^{1/3} \Delta^{2/3}}{2} & \frac{a^{1/3} \Delta^{2/3}}{2} \\ -\frac{\Delta}{2} & -\frac{a^{1/3} \Delta^{2/3}}{\sqrt{2}} \\ \text{N/A} & \frac{a^{1/3} \Delta^{2/3}}{\sqrt{2}} \end{pmatrix} \quad (220)$$

Including all coefficients and factorizing, we get:

$$a \prod_i^3 s_i \rightarrow (\Delta - a^{1/3} \Delta^{2/3} s_3) \left(\frac{1 - z_a}{2} \right) + \frac{a^{1/3} \Delta^{2/3}}{\sqrt{2}} (s_2 - s_1) x_a \quad (221)$$

$$+ \frac{a^{2/3} \Delta^{1/3}}{2} (s_2 - s_1)^2 + \frac{a}{2} (s_1^2 + s_2^2) s_3 \quad (222)$$

A k -local Hamiltonian with a 3-local term replaced by this 2-local Hamiltonian will have an equivalent low-lying spectrum to within ϵ as long as $\Delta = \Omega(\epsilon^{-3})$.

Cost

- 1 auxiliary qubit for each 3-local term.
- $\Delta = \Omega(\epsilon^{-3})$

Example

$$3y_1 z_2 x_3 + 4z_1 x_2 y_3 - z_1 y_2 \rightarrow 2\alpha + \alpha_1^y y_1^2 + \alpha_1^z z_1^2 + \alpha_2^z z_2^2 + \alpha_2^x x_2^2 + \alpha_3^x x_3 + \alpha_3^y y_3 + \alpha_a^z (z_{a1} + z_{a2}) \quad (223)$$

$$+ \alpha_{12}^{yz} y_1 z_2 + \alpha_{12}^{zx} z_1 x_2 + \alpha_{13}^{yx} y_1^2 x_3 + \alpha_{13}^{zy} z_1^2 y_3 + \alpha_{23}^{zx} z_2^2 x_3 + \alpha_{23}^{xy} x_2^2 y_3 \quad (224)$$

$$+ \alpha_{3a}^{xz} x_3 z_{a1} + \alpha_{3a}^{yz} y_3 z_{a2} + \alpha_{1a}^{yx} y_1 x_{a1} + \alpha_{1a}^{zx} z_1 x_{a2} + \alpha_{2a}^{zx} z_2 x_{a1} + \alpha_{2a}^{xy} x_2 x_{a2} - z_1 y_2 \quad (225)$$

Bibliography

- Original paper where $\alpha = 1$: [?]. For arbitrary α see the 2005 v1 from arXiv, or [?]. Connection to improved version: [?].

E. P(3 → 2)-CBBK (Cao, Babbush, Biamonte, Kais, 2015)

Summary

For any 3-local term which is a product of 1-local matrices s_i , we can define one auxiliary qubit labeled by a and make the transformation:

$$a \prod_i s_i \rightarrow \alpha^I + \alpha_3^s s_3 + \alpha_a^z z_a + \alpha_{12}^{ss} s_1 s_2 + \alpha_{3a}^{sz} s_3 z_a + \alpha_{1a}^{sx} s_1 x_a + \alpha_{2a}^{sx} s_2 x_a \quad (226)$$

$$\begin{aligned} \alpha^I &= \frac{\Delta}{2} + \frac{1}{2} \left(\frac{a}{2}\right)^{2/3} \Delta^{1/2} (\text{sgn}^2(a) + 1) - \text{sgn}^2(a) \left(\frac{a}{2}\right)^{4/3} (\text{sgn}^2(a) + 1) \\ \alpha_3^s &= \frac{1}{2} \left(\frac{a}{2}\right)^{1/3} \Delta^{1/2} - \frac{a}{4} (\text{sgn}^2(a) + 1) \\ \alpha_a^z &= -\frac{\Delta}{2} + \frac{1}{2} \left(\frac{a}{2}\right)^{2/3} \Delta^{1/2} (\text{sgn}^2(a) + 1) - \text{sgn}^2(a) \left(\frac{a}{2}\right)^{4/3} (\text{sgn}^2(a) + 1) \\ \alpha_{12}^{ss} &= 2\text{sgn}(a) \left(\frac{a}{2}\right)^{2/3} \Delta^{1/2} - 4\text{sgn}(a) \left(\frac{a}{2}\right)^{4/3} \\ \alpha_{3a}^{sz} &= -\frac{1}{2} \left(\frac{a}{2}\right)^{1/3} \Delta^{1/2} - \frac{a}{4} (\text{sgn}^2(a) + 1) \\ \alpha_{1a}^{sx} &= \text{sgn}(a) \left(\frac{a}{2}\right)^{1/3} \Delta^{3/4} \\ \alpha_{2a}^{sx} &= \left(\frac{a}{2}\right)^{1/3} \Delta^{3/4} \end{aligned}$$

Including all coefficients and factorizing, we get:

$$a \prod_i s_i \rightarrow \left(\Delta + \left(\frac{a}{2}\right)^{1/3} \Delta^{1/2} s_3 \right) \left(\frac{1 - z_a}{2} \right) \quad (227)$$

$$- \frac{a^{2/3}}{2} (\text{sgn}^2(a) + 1) \left((2a)^{2/3} \text{sgn}^2(a) + a^{1/3} s_3 - \sqrt[3]{2} \Delta^{1/2} \right) \left(\frac{1 + z_a}{2} \right) \quad (228)$$

$$+ \left(\frac{a}{2}\right)^{1/3} \Delta^{3/4} (\text{sgn}(a) s_1 + s_2) x_a + \text{sgn}(a) \left(\sqrt[3]{2} a^{2/3} \Delta^{1/2} - 4 \left(\frac{a}{2}\right)^{4/3} \right) s_1 s_2 \quad (229)$$

Cost

- 1 auxiliary qubit for each 3-local term.
- $\Delta = \Theta(\epsilon^{-3})$.

Example

$$3x_1 z_2 y_3 + 2y_1 x_2 z_4 - z_1 x_2 \rightarrow \alpha_1^I + \alpha_2^I + \alpha_3^y y_3 + \alpha_4^z z_4 + \alpha_{a_1}^z z_{a_1} + \alpha_{a_2}^z z_{a_2} + \alpha_{12}^{xz} x_1 z_2 + \alpha_{12}^{yx} y_1 x_2 + \alpha_{3a_1}^{yz} y_3 z_{a_1} \quad (230)$$

$$+ \alpha_{4a_2}^{zz} z_4 z_{a_2} + \alpha_{1a_1}^{xx} x_1 x_{a_1} + \alpha_{1a_2}^{yx} y_1 x_{a_2} + \alpha_{2a_1}^{zx} z_2 x_{a_1} + \alpha_{2a_2}^{xx} x_2 x_{a_2} - z_1 x_2 \quad (231)$$

Bibliography

- Original paper (Eq. 28-29): [?].

F. $P(3 \rightarrow 2)$ -CBBK2 (Cao, Babbush, Biamonte, Kais, 2015)

Summary

Given a sum of m 3-local terms, we can define m auxiliary qubits and make the following transformation:

$$\sum_{i=1}^m a_i s_{1_i} s_{2_i} s_{3_i} \rightarrow \sum_{i=1}^m \left(\left(\Delta + \left(\frac{|a_i|}{2} \right)^{1/3} \Delta^{1/2} s_{3_i} \right) \left(\frac{1 - z_{a_i}}{2} \right) \right) \quad (232)$$

$$+ \sum_{i=1}^m \left(\left(\frac{|a_i|}{2} \right)^{1/3} \Delta^{3/4} (\text{sgn}(a_i) s_{1_i} + s_{2_i}) + \left(\frac{|a_i|}{2} \right)^{1/3} \Delta^{1/2} (\text{sgn}(a_i) s_{1_i} + s_{2_i})^2 \right) \quad (233)$$

$$+ \sum_{i=1}^m \left(- \left(\frac{|a_i|}{2} \right) (\text{sgn}^2(a_i) + 1) s_{3_i} - \left(\frac{|a_i|}{2} \right)^{4/3} (\text{sgn}(a_i) s_{1_i} + s_{2_i})^4 \right) \quad (234)$$

$$+ \sum_{i=1}^m \sum_{j=1, j \neq i}^m [-\alpha_1^{(i,j)} \text{sgn}^2(a_i) \text{sgn}^2(a_j) \left(\frac{|a_i|}{2} \right)^{2/3} \left(\frac{|a_j|}{2} \right)^{2/3}] \quad (235)$$

$$- 2\alpha_2^{(i,j)} \left(\frac{|a_i|}{2} \right)^{2/3} \left(\frac{|a_j|}{2} \right)^{2/3} (\text{sgn}^2(a_i) \text{sgn}^2(a_j) - \text{sgn}(a_i) \text{sgn}(a_j) s_{1_i} s_{1_j} s_{2_i} s_{2_j})] \quad (236)$$

$$\alpha_1^{(i,j)} = \alpha_{11}^{(i,j)} + \alpha_{12}^{(i,j)}$$

$$\alpha_{11}^{(i,j)} = \begin{cases} 1 & \text{if } \begin{cases} [s_{1_i}, s_{1_j}] \neq 0 \\ [s_{2_i}, s_{2_j}] = 0 \end{cases} \text{ or } \begin{cases} [s_{2_i}, s_{2_j}] \neq 0 \\ [s_{1_i}, s_{1_j}] = 0 \end{cases} \\ 0 & \text{otherwise} \end{cases}$$

$$\alpha_{12}^{(i,j)} = \begin{cases} 1 & [s_{1_i}, s_{2_j}] \neq 0 \text{ or } [s_{2_i}, s_{1_j}] \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\alpha_2^{(i,j)} = \begin{cases} 1 & [s_{1_i}, s_{1_j}] \neq 0 \text{ and } [s_{2_i}, s_{2_j}] \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Cost

- One auxiliary qubit for each 3-local term.
- $\Delta = \Theta(\epsilon^{-2})$

Pros

Cons

Example

$$3x_1 z_2 y_3 + 5y_1 x_2 z_4 - z_1 x_2 \rightarrow \left(\Delta + \left(\frac{3}{2} \right)^{1/3} \Delta^{1/2} y_3 \right) \left(\frac{1 - z_{a_1}}{2} \right) + \left(\frac{3}{2} \right)^{1/3} \Delta^{3/4} (x_1 + z_2) x_{a_1} + \left(\frac{3}{2} \right)^{2/3} \Delta^{1/2} (x_1 + z_2)^2 - 3y_3 \quad (237)$$

$$- \left(\frac{3}{2} \right)^{4/3} (x_1 + z_2)^4 + \left(\Delta + \left(\frac{5}{2} \right)^{1/3} \Delta^{1/2} z_4 \right) \left(\frac{1 - z_{a_2}}{2} \right) + \left(\frac{5}{2} \right)^{1/3} \Delta^{3/4} (y_1 + x_2) x_{a_2} \quad (238)$$

$$+ \left(\frac{5}{2} \right)^{2/3} \Delta^{1/2} (y_1 + x_2)^2 - 5z_4 - \left(\frac{5}{2} \right)^{4/3} (y_1 + x_2)^4 \quad (239)$$

$$- \left(2 \left(\frac{3}{2} \right)^{2/3} \left(\frac{5}{2} \right)^{2/3} - 2 \left(\frac{3}{2} \right)^{2/3} \left(\frac{5}{2} \right)^{2/3} x_1 y_1 z_2 x_2 \right) - z_1 x_2 \quad (240)$$

Bibliography

- Original paper (Eq. A2 - A9): [?].

IX. PERTURBATIVE 1-BY-1 GADGETS

A 1B1 gadget allows k -local terms to be quadratized one step at a time, where at each step the term's order is reduced by at most one. In each step, a k -local term is reduced to $(k-1)$ -local, contrary to SD (sub-division) gadgets which can reduce k -local terms to $(k/2)$ -local in one step.

A. P1B1-OT (Oliveira & Terhal, 2008)

Summary

We wish to reduce the k -local term:

$$H_{k\text{-local}} = \alpha \prod_j^k s_j. \quad (241)$$

Define one auxiliary qubit labeled by a and make the transformation:

$$H_{k\text{-local}} \rightarrow \left(\Delta - \left(\frac{\alpha}{2} \right)^{1/3} \Delta^{2/3} s_k \right) \left(\frac{1 - z_a}{2} \right) + \frac{\alpha^{1/3} \Delta^{2/3}}{\sqrt{2}} \left(s_{k-1} - \prod_j^{k-2} s_j \right) x_a \quad (242)$$

$$+ \frac{\alpha^{2/3} \Delta^{1/3}}{2} \left(s_{k-1} - \prod_j^{k-2} s_j \right)^2 + \frac{\alpha}{2} \left(\left(\prod_j^{k-2} s_j \right)^2 + s_{k-1}^2 \right) s_k \quad (243)$$

The result will be a $(k-1)$ -local Hamiltonian with the same low-lying spectrum as $H_{k\text{-local}}$ to within ϵ as long as $\Delta = \Omega(\epsilon^{-3})$.

Cost

- Only 1 auxiliary qubit.
- $\Delta = \Omega(\epsilon^{-3})$

Example

$$3y_1 z_2 x_3 x_4 y_5 \rightarrow \left(\Delta - \left(\frac{3}{2} \right)^{1/3} \Delta^{2/3} y_5 \right) \left(\frac{1 - z_a}{2} \right) + \frac{3^{1/3} \Delta^{2/3}}{\sqrt{2}} (x_4 - y_1 z_2 x_3) x_a \quad (244)$$

$$+ \frac{3^{2/3} \Delta^{1/3}}{2} (x_4 - y_1 z_2 x_3)^2 + \frac{3}{2} ((y_1 z_2 x_3)^2 + x_4^2) y_5 \quad (245)$$

Bibliography

- Described in: [?], based on: [?].

B. P1B1-CBBK (Cao, Babbush, Biamonte, Kais, 2015)

Summary

Define one auxiliary qubit labeled by a and make the transformation:

$$H_{k\text{-local}} \rightarrow \left(\Delta + \left(\frac{\alpha}{2} \right)^{1/3} \Delta^{1/2} s_k \right) \left(\frac{1 - z_a}{2} \right) + \left(\frac{\alpha}{2} \right)^{1/3} \Delta^{3/4} \left(\text{sgn}(\alpha) \prod_j^{k-2} s_j + s_{k-1} \right) x_a \quad (246)$$

$$- \frac{\alpha^{2/3}}{2} (1 + \text{sgn}^2 \alpha) \left((2\alpha)^{2/3} \text{sgn}^2 \alpha + \alpha^{1/3} s_k - \sqrt[3]{2} \Delta^{1/2} \right) \left(\frac{1 + z_a}{2} \right) \quad (247)$$

$$+ \text{sgn}(\alpha) \left(\sqrt[3]{2} \alpha^{2/3} \Delta^{1/2} - 4 \left(\frac{\alpha}{2} \right)^{4/3} \right) \prod_j^{k-1} s_j \quad (248)$$

The result is $(k-1)$ -local and its low-lying spectrum is the same as that of $H_{k\text{-local}}$ when Δ is large enough.

Cost

- Only 1 auxiliary qubit.
- $\Delta = \Omega(\epsilon^{-3})$

Example

$$3x_1 z_2 y_3 y_4 x_5 - z_1 x_3 \rightarrow \left(\Delta + \left(\frac{3}{2} \right)^{1/3} \Delta^{1/3} x_5 \right) \left(\frac{1 - z_a}{2} \right) + \left(\frac{3}{2} \right)^{1/3} \Delta^{3/4} (x_1 z_2 y_3 + y_4) x_a \quad (249)$$

$$- 3^{2/3} \left(6^{2/3} + 3^{1/3} x_5 - \sqrt[3]{2} \Delta^{1/2} \right) \left(\frac{1 + z_a}{2} \right) \quad (250)$$

$$+ \left(3^{2/3} \sqrt[3]{2} \Delta^{1/2} - 4 \left(\frac{3}{2} \right)^{4/3} \right) x_1 z_2 y_3 y_4 - z_1 x_3 \quad (251)$$

Bibliography

- Described in: [?], based on: [?].

X. PERTURBATIVE SUBDIVISION GADGETS

Instead of recursively reducing k -local to $(k-1)$ -local one reduction at a time, we can reduce k -local terms to $(k/2)$ -local terms directly for even k , or to $(k+1)/2$ -local terms directly for odd k . Since when k is odd we can add an identity operator to the k -local term to make it even, we will assume in the following that k is even, in order to avoid having to write floor and ceiling functions.

A. PSD-OT (Oliveira & Terhal, 2008)

Summary

We factor a k -local term into a product of three factors: operators H_1, H_2 acting on non-overlapping spaces, and scalar α . Then introduce an auxiliary qubit labelled by a and make the transformation:

$$H_{k\text{-local}} \rightarrow \Delta \left(\frac{1 - z_a}{2} \right) + \frac{\alpha}{2} H_1^2 + \frac{\alpha}{2} H_2^2 + \sqrt{\frac{\alpha \Delta}{2}} (-H_1 + H_2) x_a. \quad (252)$$

The resulting Hamiltonian has a degree of 1 larger than the degree of whichever factor H_1 or H_2 has a larger degree, and the low-lying spectrum is equivalent to the original one to within $\mathcal{O}(\alpha\epsilon)$ for sufficiently large Δ .

Cost

- 1 auxiliary qubit for each k -local term that can be factored into two non-overlapping subspaces, is enough to reduce the degree down to $k/2 + 1$.
- $\Delta = \frac{\alpha(\|H_{(\text{else})}\| + \Omega(\sqrt{2})\max(\|H_1\|, \|H_2\|))^6}{\epsilon^2} = \Omega(\alpha\epsilon^{-2})$.

Pros

- Potentially very few auxiliary qubits needed.

Cons

- Requires the ability to factor k -local terms into non-overlapping subspaces that are at most $(k-2)$ -local in order to reduce k -locality. This is not possible for $z_1 x_2 x_3 + z_2 z_3 x_4$, for example.
- Δ needs to be rather large.
- Cannot reduce 3-local to 2-local unless we generalize to a factor of 3 non-overlapping subspaces instead of 2. Needs to be combined with $3 \rightarrow 2$ gadgets, for example.
- A lot of work may be needed to find the optimal reduction, since each k -local term can be factored in many ways, and some of these ways may affect the ability to reduce other k -local terms.

Example

$$3x_1 z_2 y_3 z_4 x_5 y_6 \rightarrow \Delta \left(\frac{1 - z_a}{2} \right) + \frac{3}{2} (x_1 z_2 y_3)^2 + \frac{3}{2} (z_4 x_5 y_6)^2 + \sqrt{\frac{3\Delta}{2}} (-x_1 z_2 y_3 + z_4 x_5 y_6) x_a \quad (253)$$

Bibliography

- Original paper where $\alpha = 1$: [?]. For arbitrary α see the 2005 v1 from arXiv, or [?]. Connection to improved version: [?].

B. PSD-CBBK (Cao, Babbush, Biamonte, Kais 2015)

Summary

For any k -local term, we can subdivide it into a product of two $(k/2)$ -local terms:

$$H_{k\text{-local}} = \alpha H_{1,(k/2)\text{-local}} H_{2,(k/2)\text{-local}} + H_{(k-1)\text{-local}}. \quad (254)$$

Define one qubit a and make the following Hamiltonian is $(k/2)$ -local:

$$\Delta \left(\frac{1 - z_a}{2} \right) + |\alpha| \left(\frac{1 + z_a}{2} \right) + \sqrt{\frac{|\alpha| \Delta}{2}} (\text{sgn}(\alpha) H_{1,(k/2)\text{-local}} - H_{2,(k/2)\text{-local}}) x_a \quad (255)$$

The result is a $(k/2)$ -local Hamiltonian with the same low-lying spectrum as $H_{k\text{-local}}$ for large enough Δ . The disadvantage is that Δ has to be larger.

Cost

- $\Delta \geq \left(\frac{2|\alpha|}{\epsilon} + 1 \right) (|\alpha| + \epsilon + 22 \|H_{(k-1)\text{-local}}\|)$

Pros

- only one qubit to reduce k to $\lceil k/2 \rceil + 1$

Cons

- Only beneficial for $k \geq 5$.

Example

$$5x_1z_2y_3z_4x_5y_6 \rightarrow \Delta \left(\frac{1 - z_a}{2} \right) + 5 \left(\frac{1 + z_a}{2} \right) + \sqrt{\frac{5\Delta}{2}} (x_1z_2y_3 - z_4x_5y_6) x_a \quad (256)$$

Bibliography

- Original paper (Eq. 4): [?].

C. PSD-CN (Cao & Nagaj, 2014)

Summary

For a sum of terms that are k -local, with each term j written as a product $H_{1j}H_{2j}$, introduce N_{core} ‘core’ auxiliary qubits labeled by a_i and N_{direct} ‘direct’ auxiliary qubits labeled by a_{ij} for each term j . Make all core auxiliary qubits couple to all others, and make the direct auxiliary qubits couple each H_{1j} and H_{2j} to the core auxiliary qubits, as follows:

$$\sum_j a_j H_{1j} H_{2j} \rightarrow \sum_{ij} (\alpha(1 - z_{a_{ij}} z_{a_i}) + \alpha_j x_{a_{ij}} (H_{1j} - H_{2j})) + \alpha \sum_i \left(1 - z_{a_i} + \sum_j (1 - z_{a_i} z_{a_j}) \right) \quad (257)$$

If we would like the spectrum of the RHS to be close to that of the LHS, with a difference of $O(\epsilon)$, then for any $d \in (0, 1)$ we can choose

$$N_{\text{direct}} \in \Omega \left(\max \left\{ \epsilon^{-\frac{2}{d}}, \left(\frac{\|H_{\text{else}}\|^2}{2M^4 \max_j |a_j|} \right)^{\frac{1}{d}}, (M^3 \epsilon^{-2})^{\frac{1}{1-d}} \right\} \right), \quad (258)$$

$$N_{\text{core}} \in \Omega \left(M^3 N_{\text{direct}}^d \epsilon^{-1} \right), \quad (259)$$

$$\alpha_j, \alpha \in O(\epsilon). \quad (260)$$

Notes

- $+\sum_j a_j$ was not in the original paper.

Pros

- For spectral error ϵ , uses only $O(\epsilon)$ coupling between the qubits (See Equation 260).

Cons

- Uses $\text{poly}(\epsilon^{-1})$ ancilla qubits (See Equations 258 and 259).
- The construction only describes the asymptotic scaling of the parameters rather than concrete assignments of them. More work is needed for finding tight non-asymptotic error bounds in perturbative expansion.

Example

$$3x_1 y_2 z_3 y_4 \rightarrow \frac{\Delta}{2}(1 - z_{a_{11}} z_{a_1}) + \frac{\Delta}{2}(1 - z_{a_1} + 1 - z_{a_1} z_{a_1}) + \sqrt{\frac{3\Delta}{2}}(x_1 y_2 - z_3 y_4) x_{a_{11}} + 3 \quad (261)$$

Bibliography

- Original paper (Eq. 13): [?].

XI. PERTURBATIVE DIRECT GADGETS

Here we do not reduce k by one order at a time (1B1 reduction) or by $k/2$ at a time (SD reduction), but we directly reduce k -local terms to 2-local terms.

A. PD-JF (Jordan & Farhi, 2008)

Summary

Express a sum of k -local terms as a sum of products of Pauli matrices s_{ij} , and define k auxiliary qubits labelled by a_{ij} for each term i , and make the transformation:

$$\sum_i \alpha_i \prod_j^k s_{ij} \rightarrow \frac{1}{2} \sum_i \sum_{1 \leq j < l \leq k} (1 - z_{a_{ij}} z_{a_{il}}) + \epsilon \sum_i \left(\alpha_i s_{i1} x_{i1} + \sum_{j=2}^k s_{ij} x_{ij} \right) \quad (262)$$

The result is a 2-local Hamiltonian with the same low-lying spectrum to within ϵ^{k+1} for sufficiently small ϵ .

Notes

- $-\sum_i \alpha_i$ term not in original paper.

Cost

- Number of auxiliary qubits is tk for t terms.
- Unknown requirement for ϵ .

Pros

- All done in one step, so easier to implement than 1B1 and SD gadgets.

Cons

- Requires 2 more auxiliary qubits per term than 1B1-KKR.
- Unknown polynomial $f(\lambda)$

Example

$$3x_1y_2z_3 + 5y_1z_2y_4 \rightarrow \frac{1}{2}(6 - z_{a_{11}}z_{a_{12}} - z_{a_{11}}z_{a_{13}} - z_{a_{12}}z_{a_{13}} - z_{a_{21}}z_{a_{22}} - z_{a_{21}}z_{a_{23}} - z_{a_{22}}z_{a_{23}}) \quad (263)$$

$$+ \epsilon(3x_1x_{a_{11}} + y_2x_{a_{12}} + z_3x_{a_{13}} + 5y_1x_{a_{21}} + z_2x_{a_{22}} + y_4x_{a_{23}}) - 8 \quad (264)$$

Bibliography

- Original paper (Eq. 4-6): [?].

B. PD-BFBD (Brell, Flammia, Bartlett, Doherty, 2011)

Summary

The 4-body Hamiltonian:

$$H_{4\text{-local}} = - \sum_{ij} (Z_{4i+1,j} Z_{4i+2,j} Z_{4i+3,j} Z_{4i+4,j} + X_{4i+3,j} X_{4i+4,j} X_{4i+6,j} X_{4i+4,j+1}) \quad (265)$$

is transformed into the 2-body Hamiltonian:

$$H_{2\text{-local}} = - \sum_{ij} (X_{8i+4,j} X_{8i+6,j} + X_{8i+3,j+1} X_{8i+5,j+1} + Z_{8i+4,j} Z_{8i+3,j+1} + Z_{8i+6,j} Z_{8i+5,j+1} + \quad (266)$$

$$+ \lambda (X_{8i+1,j} X_{8i+3,j+1} + X_{8i+2,j} X_{8i+4,j} + X_{8i+5,j+1} X_{8i+7,j} + X_{8i+6,j} X_{8i+8,j} \quad (267)$$

$$+ Z_{8i+1,j} Z_{8i+3,j+1} + Z_{8i+2,j} Z_{8i+4,j} + Z_{8i+5,j+1} Z_{8i+7,j} + Z_{8i+6,j} Z_{8i+8,j})) \quad (268)$$

For $\lambda = \mathcal{O}(\epsilon^{-5})$, the 2-local Hamiltonian has the same low-lying spectrum as the 4-local Hamiltonian, to within an error of ϵ .

Cost

- In total, uses four times the number of qubits of the original Hamiltonian.
- Unknown requirement for λ .

Pros

- All done in one step, so easier to implement than implementing two 1B1 gadgets.
- Very symmetric

Cons

- Ordinary 1B1 or SD followed by 3→2 gadgets would require half as many total qubits.
- Many 2-local terms.
- Perturbative, as opposed to NR-OY which is similar but does not involve any λ parameter.
- Required value of λ for it to work, is presently unknown.

Bibliography

- Original paper (Eq. 3-7): [?].

C. PD-CK (Cao, Kais, 2016)

Summary

Given a sum of m k -local terms, we can define k auxiliary qubits for each k -local term and make the following transformation:

$$\sum_{i=1}^m a_i \prod_{j=1}^k s_{ij} \rightarrow \sum_i \sum_{1 \leq s < t \leq k} \frac{\Delta}{2(k-1)} (1 - z_{a_{is}} z_{a_{it}}) + \sum_i \sum_j a_i^{1/k} s_{ij} x_{ij} \quad (269)$$

The result is 2-local and its low-lying spectrum will be the same as the k -local Hamiltonian when Δ is large enough.

Cost

- k auxiliary qubits for each k -local term, for a total of km auxiliary qubits.
- $\Delta = O(\epsilon^{-k})$

Pros

Cons

Example

$$a_1 x_1 x_2 x_3 + a_2 x_2 y_4 z_5 \rightarrow \frac{\Delta}{4} (3 - z_{a_{11}} z_{a_{12}} - z_{a_{12}} z_{a_{13}} - z_{a_{11}} z_{a_{13}}) + \frac{\Delta}{4} (3 - z_{a_{21}} z_{a_{22}} - z_{a_{22}} z_{a_{23}} - z_{a_{21}} z_{a_{23}}) \quad (270)$$

$$+ a_1^{1/3} (x_1 x_{a_{11}} + x_2 x_{a_{12}} + x_3 x_{a_{13}}) + a_2^{1/3} (y_4 x_{a_{21}} + x_2 x_{a_{22}} + z_5 x_{a_{23}}) \quad (271)$$

Bibliography

- Original paper (Eq. 4-5, Example on Eq. 44-45): [?]]

Part IV

Appendix

XII. TRANSFORMATIONS FROM TERNARY TO BINARY VARIABLES

$$H_{\text{ternary}} = -\lambda(z_1 z_2 + z_1 - z_2) \quad (272)$$

In this implementation the variable $\frac{1}{2}(z_1 + z_2)$ plays the role of t , assuming λ is large and positive. For instance, when coupled to a binary variable t $z_3 \rightarrow \frac{1}{2}(z_1 + z_2) z_3$.

XIII. FURTHER EXAMPLES

Example Here we show how deductions can arise naturally from the Ramsey number problem. Consider $\mathcal{R}(4, 3)$ with $N = 4$ nodes. Consider a Hamiltonian:

$$H = (1 - z_{12})(1 - z_{13})(1 - z_{23}) + \dots + (1 - z_{23})(1 - z_{24})(1 - z_{34}) + z_{12}z_{13}z_{14}z_{23}z_{24}z_{34}. \quad (273)$$

See [?] for full details of how we arrive at this Hamiltonian.

Since we are assuming we have no 3-independent sets, we know that $(1 - z_{12})(1 - z_{13})(1 - z_{23}) = 0$, so $z_{12}z_{13}z_{23} = z_{12}z_{13} + z_{12}z_{23} + z_{13}z_{23} - z_{12} - z_{13} - z_{23} + 1$. This will be our deduction.

Using deduc-reduc we can substitute this into our 6-local term to get:

$$H = 2(1 - z_{12})(1 - z_{13})(1 - z_{23}) + \dots + (1 - z_{23})(1 - z_{24})(1 - z_{34}) + \quad (274)$$

$$z_{14}z_{24}z_{34}(z_{12}z_{13} + z_{12}z_{23} + z_{13}z_{23} - z_{12} - z_{13} - z_{23} + 1). \quad (275)$$

We could repeat this process to remove all 5- and 4-local terms without adding any auxiliary qubits. Note in this case the error terms added by deduc-reduc already appear in our Hamiltonian.

XIV. $2 \rightarrow 2$ GADGETS

This review has only focused on k -local to 2-local transformations where $k > 2$. There is also a large number of 2-local to 2-local transformations in the literature, which are used for various purposes. Some of these are listed here:

- Gadgetization of any 2-local Hamiltonian into $\{\mathbb{1}, z, x, zz, xx\}$ or $\{\mathbb{1}, z, x, zx\}$ [?]. Used for the proof that $xx + zz$ or xz is universal is enough for universal quantum computation. In other words, *any* computation can be transformed into a problem of finding the ground state of a 2-local Hamiltonian containing terms from $\{\mathbb{1}, z, x, zz, xx\}$ or from $\{\mathbb{1}, z, x, zx\}$ with real coefficients, and the ground state can be found by adiabatic quantum computing with only polynomial time and space overhead over the best alternative algorithm for the problem.
- Transformation of any 2-local Hamiltonian into $\{\mathbb{1}, z, x, zz, xx + yy\}$, without any perturbative gadgets, and only requiring the qubits to be connected in an almost 2D lattice [?].
- "Cross gadget", "fork gadget", and "triangle gadget" described in [?].
- Gadgetization of a 2-local Hamiltonian with very strong couplings, into a 2-local Hamiltonian with strengths in $\mathcal{O}(1/\text{poly}(\epsilon^{-1}, n))$, and $\text{poly}(\epsilon^{-1}, n)$ auxiliary qubits and $\text{poly}(\epsilon^{-1}, n)$ new quadratic terms. [?].
- yy creation gadget: Simulation of yy terms using $\{\mathbb{1}, z, x, zz, xx\}$, with coupling strength restriction defined according to $\Delta = \Theta(\epsilon^{-4})$ [?].

A. Minor-embedding quadratic functions for different graphs

- Minor-embedding general problems for the Chimera [?] graph [? ?].
- Minor-embedding quadratization gadgets for the Pegasus [?] graph [?].

XV. FURTHER REFERENCES

- Gadgets for pseudo-Boolean optimization problems, with reduced precision requirements: [?].
- Formalization of pseudo-Boolean gadgets in quantum language. [?].
- By adding more couplers and more auxiliary qubits, we can bring the error down arbitrarily low: [?].
- More toric code gadgets: [?].
- Parity adiabatic quantum computing (LHZ lattice): [?].
- Extensions of the LHZ scheme: [?].
- Minimizing k -local discrete functions with the help of continuous variable calculus [?].
- ORI graph which attempts to give optimal quadratizations [?].
- Survey on pseudo-Boolean optimization [?].
- Linearization of equations before they are squared [?], and its application to factoring numbers [?].
- Mentioned in [?] as an early application of quadratization: [?].
- Characterization of NTRs for cubics: [?].
- Relation between cones of nonnegative quadratic pseudo-Boolean functions and the Boolean quadric polytope [?].
- Relation between cones of nonnegative quadratic pseudo-Boolean functions and the Boolean quadric polytope [?].
- Effective non-Hermitian Hamiltonian with 3-body interactions which helps to calculate electronic structure energies closer to the complete basis set limit [?].
- Hubbard-Stratonovich transformation [? ?] is used to derive Eq. 10a, 10b, and 10c of [?], in which the exponential of a quadratic equals the trace/integral of an exponential of something linear. In the case where the number operator is written as a product of two operators, this means a 4-body operator in the exponent becomes a 2-body operator in the exponent.

XVI. CIRCUITS THAT EFFECTIVELY IMPLEMENT DEGREE- k TERMS FOR SUPERCONDUCTING QUBITS

- Presentation by Northrop Grumman about a zzz coupler [?] and associated patent [? ?].
- Presentation that included discussion about engineering multi-qubit interactions [?], presentation by the same lab about the design and experimental demonstration of a $zzzz$ coupling [?], and associated patent [? ? ?].
- Design of an effective $zzzz$ coupling without any auxiliary logical qubits [?].
- Design of a tunable zzz coupling with 2 auxiliary qubits in which all zz couplings are cancelled, and its experimental demonstration [?].

XVII. CONTRIBUTORS

Richard Tanburn

- Richard was the original creator and maintainer of the Git repository.
- Richard created the Tex commands used throughout the document, and contributed majorly to the overall layout.
- Richard wrote the original versions of the following sections: (1) Deduc-Reduc, (2) ELC Reduction, (3) Groebner Bases, (4) Split Reduction, (5) NTR-KZFD, (6) NTR-GBP, (7) PTR, (8) PTR-Ishikawa, (9) PTR-KZ, (10) PTR-GBP, (11) Bit flipping, (12) RBS, and (13) FGBZ.
- Richard also wrote the "Further Example" of Deduc-Reduc in the Appendix.

Nicholas Chancellor

- Nick made contributions to the following sections: (1) RMS (in terms of z), (2) PTR-RBL-(3 \rightarrow 2), (3) PTR-RBL-(4 \rightarrow 2), (4) SBM, (5) Flag based SAT Mapping, and to the qutrit \rightarrow qubit transformation (6).

Szilard Szalay

- Szilard re-derived Nike's transformations for the sections: (1) SFR-BCR-1, (2) SFR-BCR-2, (3) SFR-BCR-3, and (4) SFR-BCR-4 from the notation of the original paper, into the format consistent with the rest of the book. In doing so he corrected errors in Nike's work and also fixed them in the main document.

Ka Wa Yip

- Ka Wa Yip the original version of a section which was later converted by Nike into the following two sections: (1) NTR-YXKK, and (2) PTR-YXKK.

Yudong Cao

- Yudong wrote the first version of the following section: (1) PSD-CN.

Daniel Nagaj

- Daniel provided a .tex document to Nike in May 2018 which helped Nike to write the following sections: (1) NP-Nagaj-1, (2) NP-Nagaj-2. The document that Daniel provided made it easier for Nike to write these sections than the original papers.

Aritanan Gruber

- Aritanan informed us in August 2015 of what we ended up making the following sections: (1) PTR-Ishikawa.

Charles Herrmann

- Charles informed us in May 2018 of the papers which contained results which became the following sections: (1) PTR-BCR-1, (2) PTR-BCR-2, (3) PTR-BCR-3, (4) PTR-BCR-4, (5) SFR-BCR-1, (6) SFR-BCR-2, (7) SFR-BCR-3, (8) SFR-BCR-4, (9) SFR-BCR-5, (10) SFR-BCR-6.

Elisabeth Rodriguez-Heck

- Elisabeth provided us with a 2-page PDF document with valuable comments on the entire Book.
- Elisabeth also pointed us to what became the following section: (1) ABCG Reduction.

Hou Tin Chau

- Tin made the examples for the following sections: SFR-BCR-1,2,3,4.
- Tin fixed a typo in the alternative forms of the following sections: SFR-BCR-3,4.

Andreas Soteriou

- Andreas found typos on the opening page in the arXiv version which surprisingly no one else found (or pointed out), and he diligently fixed them.
- Andreas created the example involving x, y , and z presented on the opening page in the September 2019 version (I plan to have this example further improved at a later time).
- Andreas added the minimum and maximum coefficient ranges into the cost section for PTR-BCR-4.

Jacob Biamonte

- Jacob made valuable edits during a proof-reading of the book.

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- We thank Mohammad Amin of D-Wave for pointing Nike Dattani to the paper [?] on determining Ramsey numbers on the D-Wave device, which contained what we call in this review "Reduction by substitution", later found through Ishikawa's paper to be from the much older 1970s paper by Rozenberg.
- We thank Catherine McGeoch of Amherst University and D-Wave, for helpful discussions with Nike Dattani in December 2014 about how to map quadratic pseudo-Boolean optimization problems onto the chimera graph of the D-Wave hardware and for pointing us to the important references of Vicky Choi. While chimerization is very different from quadratization, understanding that roughly n^2 variables would be needed to map a quadratic function of n variables, helped Nike Dattani and Richard Tanburn to appreciate how important it is to be able to quadratize with as few variables as possible, and having this in mind throughout our studies helped inspire us in our goals towards "optimal quadratization".
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- We thank Toby Cathcart-Burn of Oxford University, who during the third year of undergraduate study, worked with Nike Dattani and Richard Tanburn and in Autumn 2015 and Winter 2016 helped us gain insights about the application of deduc-reduc and bit flipping to the problem of determining Ramsey numbers via discrete optimization, and for insights into the trade-offs between Ishikawa's symmetric reduction and reduction by substitution.
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to quadratize for D-Wave and NMR devices. He taught us that far more total (original plus auxiliary) variables can be tolerated on classical computers than on D-Wave machines or NMR systems, and approximate solutions to the optimization problems are acceptable (unlike for the factorization and Ramsey number problems in which we were interested). This gave us more insight into what trade-offs one might wish to prioritize when quadratizing optially. We also thank him for helping us in our quest to determine whether or not "deduc-reduc" was a re-discovery by Richard, Emile, and Nike, or perhaps a novel quadratization scheme.

- We thank Salil Bedkihal for informing Nike of the paper by Hirsch which uses the Hubbard-Stratonovich transformation, now mentioned in the "Further References" section.
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