Compressed Quadratization of Higher Order Binary Optimization Problems

Full paper: https://arxiv.org/abs/2001.00658

Avradip Mandal, Arnab Roy, Sarvagya Upadhyay and Hayato Ushijima-Mwesigwa

Fujitsu Laboratories of America, Inc

FUJITSU

shaping tomorrow with you

Motivation

- Quantum Annealers and other quantum-inspired hardware optimizers take Quadratic Unconstrained Binary Optimization (QUBO) problem as input

- QUBO minimization captures all problems in NP

- However, some naturally occurring problems are higher order

- Examples are molecule synthesis and SAT formulations of some optimization problems

HOBO

- A HOBO problem is a discrete optimization problem that aims to minimize a polynomial over binary variables

$$\text{minimize: } q(x) = q(x_1, x_2, \ldots, x_n)$$

where either $x \in \{0,1\}^n$ (Boolean) or $x \in \{-1,+1\}^n$ (Ising)

- For HOBO, one can assume without loss of generality that there are no constraints. An example of a HOBO:

$$\text{minimize: } 4x_1 + 2x_2 + 3x_1x_3 + 5x_1x_2x_3 + x_1x_4x_5 + x_2x_3x_5x_6$$

- Computationally the class of such problems are intractable

Why study both Ising and Boolean space?

- Binary optimization problems can be represented in Ising space and Boolean space
  - Interchangeable using the affine transformation $y = 1 - 2x$, where $x \in \{0,1\}$ and $y \in \{-1,1\}$
  - Converting HOBO to QUBO in Boolean space is widely studied
- Why care about HOBO to QUBO conversion in Ising space?
  - Ising space is ubiquitous in many fields: quantum chemistry, quantum physics, computer science, combinatorics, etc.
  - A sparse HOBO in Ising space can lead to dense HOBO in Boolean space; this in turn will require more auxiliary variables to convert in to a QUBO in Boolean space. For example:

$$\prod_{i=1}^{n} x_i = \prod_{i=1}^{n} (1 - 2y_i)$$

  - LHS will require way less auxiliary variable than RHS

Techniques for HOBO → QUBO

Monomial reduction

- Degree reduction by adding auxiliary variables and constraints

Optimizing order of reduction

- Several different reduction sequences are possible

Pruning

- Exploiting the coefficient distribution of some practical problems

Monomial reduction over Boolean space

- Consider the following HOBO over Boolean variables

$$x_1x_2x_3x_4 + x_1x_2(1 - x_4)$$

- First step: Set $y_1 = x_1x_2$ and $y_2 = x_3x_4$. Problem reduces to a quadratic constrained binary optimization (QCBO). Objective function becomes

$$y_1y_2 + y_1(1 - x_4)$$

- Second step: Enforce the constraints $y_1 = x_1x_2$ and $y_2 = x_3x_4$ in the objective function using polynomials such that
  - If constraint is satisfied, contribution to objective function is 0
  - If constraint is not satisfied, contribution to objective function is positive
  - The polynomials introduced have constant, linear or quadratic terms

- Rosenberg polynomial: The following simple polynomial does the trick!

$$p(y_1, x_1, x_2) = 3y_1 + x_1x_2 - 2y_1x_1 - 2y_1x_2$$

Monomial reduction over Ising space

- Consider the following HOBO, but over Ising variables

$$x_1 x_2 x_3 x_4 + x_1 x_2 (1 - x_4)$$

- First step: Set $y_1 = x_1 x_2$ and $y_2 = x_3 x_4$. Problem reduces to a quadratic constrained binary optimization (QCBO). Objective function becomes

$$y_1 y_2 + y_1 (1 - x_4)$$

- Second step: Enforce the constraints $y_1 = x_1 x_2$ and $y_2 = x_3 x_4$ in the objective function using polynomials such that
  - If constraint is satisfied, contribution to objective function is 0
  - If constraint is not satisfied, contribution to objective function is positive
  - The polynomials introduced have constant, linear or quadratic terms

- Can we find an analogue of the Rosenberg polynomial in Ising space?

$$p(y_1, x_1, x_2) = ?$$

Impossibility with 1 auxiliary variable

- The goal is to come up with a quadratic polynomial $p(x_1, x_2, y)$ which attains minimum value only when the target auxiliary variable y equals $x_1 x_2$

- We express these conditions logically and then translate into a linear optimization problem
  - When $y = x_1 x_2$, we should have $p(x_1, x_2, y) = 0$
  - When $y \neq x_1 x_2$, we should have $p(x_1, x_2, y) > 0$

- Unfortunately, it turns out that just having y as an auxiliary variable leads to an infeasible system of inequalities

2 auxiliary variables work!

- With 2 variables, we have a fair degree of choice. We add an extra "dummy" variable d

- Now we want to express the following two conditions:
  - When y equals x_1x_2, then for **some choice of** d, we should have
    $$p(x_1, x_2, y, d) = 0$$
  - When y doesn't equal x_1x_2, then for **all choices of** d, we should have
    $$p(x_1, x_2, y, d) > 0$$
  - We obtain the following after solving this in an ILP solver:
    $$p(x_1, x_2, y, d) = 4 + x_1 + x_2 - y - 2d + x_1x_2 - x_1y - x_2y - 2x_1d - 2x_2d + 2yd$$

Reduction order

- Consider the following polynomial:

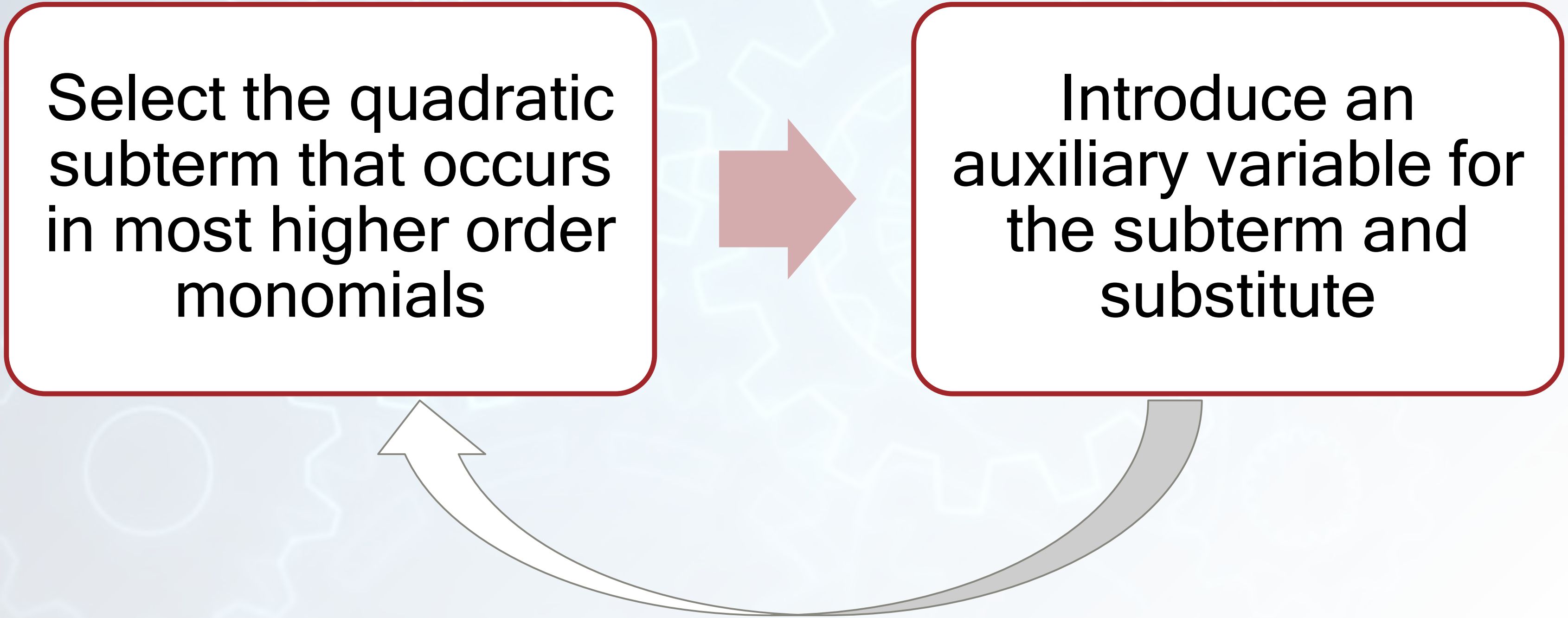
$$x_1 x_2 x_3 + x_2 x_3 x_4$$

- If we reduce first by $y_1 = x_1 x_2$ then we get $y_1 x_3 + x_2 x_3 x_4$
  - Next we reduce $y_2 = x_2 x_3$ and arrive at $y_1 x_3 + y_2 x_4$
  - This required two auxiliary variable

- If we reduce first by $y_1 = x_2 x_3$ then we get $x_1 y_1 + y_1 x_4$
  - This required one auxiliary variable!

- Order matters!

Reduction order: first strategy



Reduction order: second strategy

Select the quadratic subterm that occurs in most higher order monomials, weighted by the monomial degree

Introduce an auxiliary variable for the subterm and substitute

Pruning HOBO

- We came across natural problems where the distribution of coefficients trails off pretty sharply

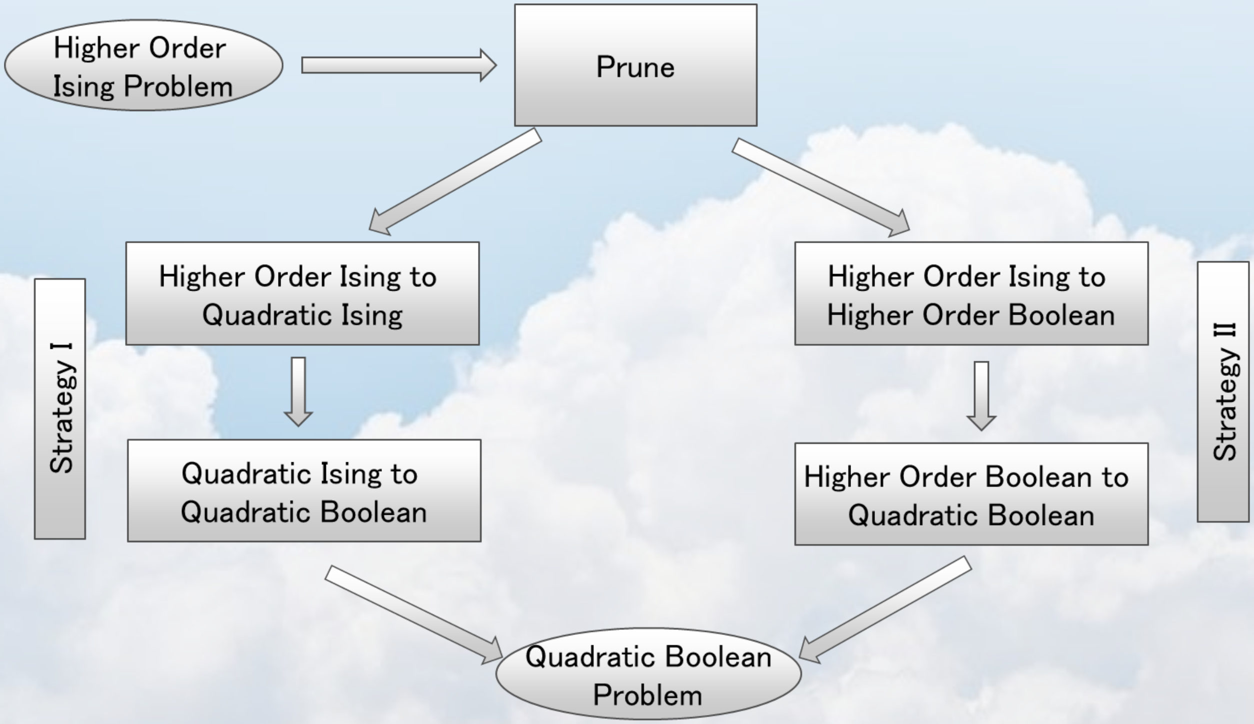
- If we can ignore a significant fraction of the low coefficient terms, then the effect compounds HOBO→QUBO conversion

- The challenge is to control the error introduced vis-à-vis the threshold allowed for eliminating monomials

Pruning HOBO

- Input: HOBO instance and error bound (as fraction of real optimal)
- Step 1: Find a lower bound of the absolute value of the minimum
  - Evaluate the polynomial with random (or educated guesses).
  - If the minimum of the random evaluation is negative, then absolute value of that is a valid lower bound
  - However, if it is positive we might have to relax and solve a continuous optimization problem.
- Step 2: Establish the error tolerance
  - Error tolerance = (lower bound of absolute minimum) x (error bound)
- Step 3: Drop terms with small absolute coefficients
  - Sort the terms in increasing order (considering the absolute value)
  - Delete initial terms until sum of absolute value of the coefficients reach the error tolerance.
- Claim: Optimal solution of the pruned HOBO is within error bound of the optimal solution of the original HOBO

Summing up


Higher Order Ising Problem
Prune
Higher Order Ising to Quadratic Ising
Quadratic Ising to Quadratic Boolean
Strategy I
Higher Order Ising to Higher Order Boolean
Higher Order Boolean to Quadratic Boolean
Strategy II
Quadratic Boolean Problem

Results on Synthetic Dataset

Dataset	Variables	Terms in Degree													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
D20A	15	15	105	60	53	49	49	48	37	20	23	12	4	-	-
D20B	14	14	91	60	55	38	31	10	5	6	-	-	-	-	-
D20C	15	15	105	62	47	52	33	46	49	26	22	26	17	7	1
D30A	17	17	136	98	61	50	30	28	22	23	6	3	1	2	-
D30B	18	18	153	130	66	50	41	35	14	12	4	2	-	-	-
D30C	20	20	190	114	65	58	50	44	24	23	7	-	2	-	-

Table 1: Distribution of number of monomials of different degrees in the dataset

Dataset	Ising, Algo 1		Ising, Algo 2		Boolean, Algo 1		Boolean, Algo 2	
	variables	terms	variables	terms	variables	terms	variables	terms
D20A	561	2581	585	2685	597	26025	583	25983
D20B	274	1290	278	1307	303	4273	314	4306
D20C	621	2857	629	2888	730	33429	1035	34344
D30A	545	2493	541	2489	1034	31189	1003	31096
D30B	512	2405	526	2466	751	15397	800	15544
D30C	706	3230	716	3269	1478	28103	1414	27911

Table 2: Experimental Results

shaping tomorrow with you