

A DEGREE REDUCTION METHOD FOR AN EFFICIENT QUBO FORMULATION FOR THE GRAPH COLORING PROBLEM

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ABSTRACT. We introduce a new degree reduction method for homogeneous symmetric polynomials on binary variables that generalizes the conventional degree reduction methods on monomials introduced by Freedman and Ishikawa. We also design an degree reduction algorithm for general polynomials on binary variables, simulated on the graph coloring problem for random graphs, and compared the results with the conventional methods. The simulated results show that our new method produces reduced quadratic polynomials that contains less variables than the reduced quadratic polynomials produced by the conventional methods.

1. INTRODUCTION

A graph is a 1-dimensional object that consists of vertices and edges. Two vertices are called adjacent if they are connected by an edge, and a graph is called simple if there is neither a loop nor multiple edges that joins adjacent vertices. A vertex coloring is an assignment of “colors” to vertices in a simple graph in a way that no two adjacent vertices are assigned by the same color. The chromatic number of a simple graph is the minimum number of colors that a vertex coloring of the graph exists. The graph coloring problem is a problem that concerns about finding the chromatic number and the existence of a vertex colorings with a certain number of colors. It applies to a range problems such as scheduling [1], register allocation in compilers [3], and frequency assignment in wireless communications [8]. The graph coloring problem is NP-hard, meaning that there is no known polynomial-time algorithm that solves the problem unless $P=NP$ [2, 5].

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For graphs with large numbers of vertices and edges, finding a solution to the graph coloring problem may require lots of computational time and resources. To circumvent this, one can use a quantum annealing machine, such as D-Wave's quantum annealer, which relies on the quantum tunneling effect [4, 6]. A quantum annealing system can solve optimization problems whose objective functions are formulated as polynomials of binary variables, when there is no constraining equations. The number of qubits in a quantum annealing machine limits the number of binary variables that the objective function can have. Although there are few algorithms, such as minor-embedding, that breaks down a large problem into a set of smaller problems that a quantum annealing machine can handle [12], it is highly desired to formulate the original objective function with as few variables as possible.

An optimization problem that the objective function is given as a polynomial of degree two with binary variables and no constraining equation is called QUBO (quadratic unconstrained binary optimization) [13, 14]. D-Wave's quantum annealer can find a solution of QUBO, i.e. it can find the global minimum of a quadratic polynomial of binary variables. However, many of discrete optimization problems, such as K-SAT and graph coloring problems, are formulated with the objective functions as polynomials of the degree higher than two [10]. Thus one needs to reformulate the objective functions as quadratic polynomials by using degree reduction methods [11].

Let p be a polynomial that consists of n binary variables x_0, \dots, x_{n-1} . A **degree reduction method** is a method of finding a polynomial q of the degree less than the degree of p that consists of binary variables x_0, \dots, x_{n-1} and extra variables w_0, \dots, w_{d-1} , called **auxiliary variables**, that attains the same values of p for any given values for x_0, \dots, x_{n-1} . More precisely, we will say that the polynomial $q(x_0, \dots, x_{n-1}, w_0, \dots, w_{d-1})$ is **reduced** from $p(x_0, \dots, x_{n-1})$ if $\deg q < \deg p$ and

$$(1.1) \quad p(x_0, \dots, x_{n-1}) = \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} q(x_0, \dots, x_{n-1}, w_0, \dots, w_{d-1})$$

for any binary values for x_0, \dots, x_{n-1} .

The objective polynomial for the graph coloring problem is formulated as follows. Let V and E be the sets of vertices and edges in the graph G . Suppose that all the colors are $0, \dots, 2^m - 1$ for some $m \geq 1$, and the color of the vertex $v \in V$ is represented by the binary representation $[x_{v,0} \dots x_{v,m-1}]_{(2)}$. Given two adjacent

vertices v and w , we define the polynomial $P_{v,w}$ as

$$(1.2) \quad P_{v,w} = \prod_{k=0}^{m-1} (x_{v,k}x_{w,k} + (1 - x_{v,k})(1 - x_{w,k})).$$

The value of $P_{v,w}$ is 0 if and only if $x_{v,k} \neq x_{w,k}$ for some $k = 0, \dots, m-1$, i.e. when the colors of two vertices v, w are different. We define the polynomial Q_G as

$$(1.3) \quad Q_G = \sum_{(v,w) \in E} P_{v,w}.$$

The polynomial Q_G is the objective function for the graph coloring problem on G . The minimum value of Q_G is 0 and it is attained if and only if when the graph G is properly colored, i.e. the coloring on G satisfies the criteria of the vertex coloring. With sufficiently large $m > 0$, the solution to $Q_G = 0$ always exists, while the real question is how small the m could be in order to have such solution.

When m is small, $Q_G = 0$ may not be attainable. Even though, finding the solution for the global minimum of Q_G could be necessary, because it gives the optimal vertex coloring of the graph in the sense that it minimizes the number of conflicts, i.e. pairs of adjacent vertices that are colored with the same color.

The degree of the Q_G is greater than two, except when there are only two colors in the color set. Thus, in general, we need degree reduction methods to formulate the graph coloring problem as QUBO. There are degree reduction methods that reduce monomials of degree greater than 2 to a quadratic polynomial. Freedman's method [7] applies to the monomials whose coefficients are negative:

$$(1.4) \quad - \prod_{j=0}^{d-1} x_j = \min_{w=0,1} w \left((d-1) - \sum_{j=0}^{d-1} x_j \right),$$

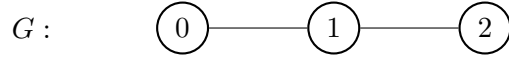
Ishikawa's method [9] applies to the monomials whose coefficients are positive, and it has two distinct formulae depending on whether the degree of the monomial is even or odd:

$$(1.5) \quad \prod_{j=0}^{2d+1} x_j = \sum_{0 \leq i < j \leq 2d+2} x_i x_j + \min_{\substack{w_i=0,1 \\ i=0, \dots, d-1}} \left[\sum_{i=0}^{d-1} w_i \left((4i+3) - 2 \sum_{j=0}^{2d+1} x_j \right) \right],$$

$$(1.6) \quad \prod_{j=0}^{2d} x_j = \sum_{0 \leq i < j \leq 2d} x_i x_j + \min_{\substack{w_i=0,1 \\ i=0, \dots, d-1}} \left[\sum_{i=0}^{d-2} w_i \left((4i+3) - 2 \sum_{j=0}^{2d} x_j \right) \right]$$

$$+ w_{d-1} \left[(2d-1) - \sum_{j=0}^{2d} x_j \right].$$

From now on, we will call these degree reduction methods as the **monomial reduction methods**. As an example, let us formulate the objective polynomial of the graph G below, and apply the monomial reduction methods.



Let the colors at the vertices 0, 1, 2 be denoted by $[x_1x_0]_{(2)}$, $[x_3x_2]_{(2)}$, $[x_5x_4]_{(2)}$, respectively. Then objective function Q_G is

$$\begin{aligned}
 (1.7) \quad Q_G &= (x_1x_3 + (1-x_1)(1-x_3))(x_0x_2 + (1-x_0)(1-x_2)) \\
 &\quad + (x_3x_5 + (1-x_3)(1-x_5))(x_2x_4 + (1-x_2)(1-x_4)) \\
 &= 2 - x_0 - x_1 - 2x_2 - 2x_3 - x_4 - x_5 + x_0x_1 + 2x_0x_2 + x_0x_3 \\
 &\quad + x_1x_2 + 2x_1x_3 + 2x_2x_3 + 2x_2x_4 + x_2x_5 + x_3x_4 + 2x_3x_5 \\
 &\quad - 2x_0x_1x_2 - 2x_0x_1x_3 - 2x_0x_2x_3 - 2x_1x_2x_3 \\
 &\quad - 2x_2x_3x_4 - 2x_2x_3x_5 - 2x_2x_4x_5 - 2x_3x_4x_5 \\
 &\quad + 4x_0x_1x_2x_3 + 4x_2x_3x_4x_5
 \end{aligned}$$

Let us apply Freedman's methods (c.f. Equations (1.4)) to all monomials of the degree 3:

$$\begin{aligned}
 -2x_0x_1x_2 &= 2x_0x_1 + 2x_0x_2 + 2x_1x_2 + 2 \min_{w_0=0,1} [3w_0 - x_0w_0 - x_1w_0 - x_2w_0] \\
 -2x_0x_1x_3 &= 2x_0x_1 + 2x_0x_3 + 2x_1x_3 + 2 \min_{w_1=0,1} [3w_1 - x_0w_1 - x_1w_1 - x_3w_1] \\
 -2x_0x_2x_3 &= 2x_0x_2 + 2x_0x_3 + 2x_2x_3 + 2 \min_{w_2=0,1} [3w_2 - x_0w_2 - x_2w_2 - x_3w_2] \\
 -2x_1x_2x_3 &= 2x_1x_2 + 2x_1x_3 + 2x_2x_3 + 2 \min_{w_3=0,1} [3w_3 - x_1w_3 - x_2w_3 - x_3w_3] \\
 -2x_2x_3x_4 &= 2x_2x_3 + 2x_2x_4 + 2x_3x_4 + 2 \min_{w_4=0,1} [3w_4 - x_2w_4 - x_3w_4 - x_4w_4] \\
 -2x_2x_3x_5 &= 2x_2x_3 + 2x_2x_5 + 2x_3x_5 + 2 \min_{w_5=0,1} [3w_5 - x_2w_5 - x_3w_5 - x_5w_5] \\
 -2x_2x_4x_5 &= 2x_2x_4 + 2x_2x_5 + 2x_4x_5 + 2 \min_{w_6=0,1} [3w_6 - x_2w_6 - x_4w_6 - x_5w_6] \\
 -2x_3x_4x_5 &= 2x_3x_4 + 2x_3x_5 + 2x_4x_5 + 2 \min_{w_7=0,1} [3w_7 - x_3w_7 - x_4w_7 - x_5w_7]
 \end{aligned}$$

Let us apply Ishikawa's method (c.f Equation (1.5)) to all monomials of the degree 4:

$$\begin{aligned}
4x_0x_1x_2x_3 &= 4x_0x_1 + 4x_0x_2 + 4x_0x_3 + 4x_1x_2 + 4x_1x_3 + 4x_2x_3 \\
&\quad + 4 \min_{w_8=0,1} [3w_8 - 2x_0w_8 - 2x_1w_8 - 2x_2w_8 - 2x_3w_8] \\
4x_2x_3x_4x_5 &= 4x_2x_3 + 4x_2x_4 + 4x_2x_5 + 4x_3x_4 + 4x_3x_5 + 4x_4x_5 \\
&\quad + 4 \min_{w_9=0,1} [3w_9 - 2x_2w_9 - 2x_3w_9 - 2x_4w_9 - 2x_5w_9]
\end{aligned}$$

Thus Q_G is reduced to the following polynomial:

$$\begin{aligned}
Q_G &= 2 - x_0 - x_1 - 2x_2 - 2x_3 - x_4 - x_5 + 4w_0 + 4w_1 + 4w_2 + 4w_3 + 4w_4 \\
&\quad + 4w_5 + 4w_6 + 4w_7 + 12w_8 + 12w_9 + 5x_0x_1 + 6x_0x_2 + 5x_0x_3 + 5x_1x_2 \\
&\quad + 6x_1x_3 + 10x_2x_3 + 6x_2x_4 + 5x_2x_5 + 5x_3x_4 + 6x_3x_5 + 5x_4x_5 \\
&\quad + \min_{\substack{w_i=0,1 \\ i=0,\dots,9}} \left[\begin{array}{l} -2x_0w_0 - 2x_1w_0 - 2x_2w_0 - 2x_0w_1 - 2x_1w_1 - 2x_3w_1 - 2x_0w_2 \\ -2x_2w_2 - 2x_3w_2 - 2x_1w_3 - 2x_2w_3 - 2x_3w_3 - 2x_2w_4 - 2x_3w_4 \\ -2x_4w_4 - 2x_2w_5 - 2x_3w_5 - 2x_5w_5 - 2x_2w_6 - 2x_4w_6 - 2x_5w_6 \\ -2x_3w_7 - 2x_4w_7 - 2x_5w_7 - 8x_1w_8 - 8x_2w_8 - 8x_3w_8 - 8x_2w_9 \\ -8x_3w_9 - 8x_4w_9 - 8x_5w_9 \end{array} \right]
\end{aligned}$$

Note that 10 auxiliary variables are produced, and they even outnumber the original variables. This situation only gets worse when the number of vertices or edges increases. For example, the objective polynomial Q_G for the complete graph $G = K_8$ with eight colors ($m = 3$) consists of 24 binary variables and has 1429 distinct monomials. The monomial degree reduction on Q_G produces 1156 new auxiliary variables and there are total 5849 distinct monomials in the reduced quadratic polynomial (c.f. Table 3 in §5).

Meanwhile, the objective function for the graph coloring problem may contain some homogeneous symmetric polynomials. For example, Q_G in Equation (1.7) contains the following homogeneous symmetric polynomial

$$(1.8) \quad -2P_4^{(3)}(x_0, x_1, x_2, x_3) = -2(x_0x_1x_2 + x_0x_1x_3 + x_0x_2x_3 + x_1x_2x_3).$$

Higher the connectivity of the graph G is, larger the homogeneous symmetric polynomial that the objective function Q_G contains.

The values of this symmetric polynomial only depend on the number of 1's in the binary variables. For example, if $l = x_0 + \dots + x_3$, then $P_4^{(3)}(x_0, \dots, x_3) = 0$ for $l < 3$, and $P_4^{(3)}(x_0, \dots, x_3) = \binom{l}{3}$ for $3 \leq l \leq 4$. We can easily observe that this simple rule applies to all homogeneous symmetric polynomials of binary variables.

Let $S_n^{(m)}$ be the set of all subsets in $S_n = \{0, \dots, n-1\}$ whose cardinality is m . We will denote $P_n^{(m)}(x_0, \dots, x_{n-1})$ as the homogeneous symmetric polynomial of degree m on n variables x_0, \dots, x_{n-1} :

$$(1.9) \quad P_n^{(m)}(x_0, \dots, x_{n-1}) = \sum_{\{i_0, \dots, i_{m-1}\} \in S_n^{(m)}} x_{i_0} \cdots x_{i_{m-1}}.$$

Then, we have

$$(1.10) \quad P_n^{(m)}(x_0, \dots, x_{n-1}) = \begin{cases} 0 & \text{if } \sum_{j=0}^{n-1} x_j < m \\ \binom{l}{m} & \text{if } l = \sum_{j=0}^{n-1} x_j \geq m \end{cases}$$

In this paper, we propose a new degree reduction method called the **symmetric reduction method** that reduces $P_n^{(m)}$ to a quadratic polynomial. It produces less number of auxiliary variables than the monomial reduction on the objective polynomials for the graph coloring problem. In §2, we state main theorems 2.1, 2.2 on the formulae of the reduced polynomials of the symmetric polynomials with positive and negative coefficients. In §3, 4, we prove these theorems. In §5, we describe algorithms 1, 2 that implement the symmetric methods for applications. In the same section, we present the results on testing these algorithms on random and complete graphs with various vertex sizes. We compared the efficiency of the symmetric reduction method with the conventional reduction methods by comparing the numbers of variables and monomials of reduced polynomials obtained by two methods.

2. THE MAIN RESULTS

Let us re-define a binomial coefficient symbol $\binom{n}{m}$ as follows: for any two non-negative integers n and m ,

$$(2.1) \quad \binom{n}{m} = \begin{cases} \frac{n!}{m!(n-m)!} & \text{if } m \leq n \\ 0 & \text{if } m > n \end{cases}.$$

Here we state our two main theorems.

Theorem 2.1. Let $n \geq m > 2$ and define $L = \binom{n-2}{m-2}$, $d = \left\lfloor \frac{n-1}{2} \right\rfloor$. For each $0 \leq i \leq d-1$, let us define

$$(2.2) \quad a_i = (4i+3) \binom{n-2}{m-2} - (m-1) \left(\binom{2i+3}{m} - \binom{2i+1}{m} \right),$$

$$(2.3) \quad b_i = \binom{2i+2}{m-1} - \binom{2i}{m-1} - 2 \binom{n-2}{m-2}.$$

Then the following equality holds:

$$(2.4) \quad P_n^{(m)}(\mathbf{x}) = L \sum_{0 \leq i < j \leq n-1} x_i x_j + \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} \left[\sum_{i=0}^{d-1} w_i \left(a_i + b_i \sum_{j=0}^{n-1} x_j \right) \right].$$

Theorem 2.2. Let $n \geq m > 2$ and define $d = \left\lfloor \frac{n-m+2}{2} \right\rfloor$. If $n-m = 2d-1$, then for each $0 \leq i \leq d-1$,

$$(2.5) \quad a_i = (m-1) \left(\binom{m+2i+1}{m} - \binom{m+2i-1}{m} \right),$$

$$(2.6) \quad b_i = -\binom{m+2i}{m-1} + \binom{m+2i-2}{m-1} \text{ for } 0 \leq i \leq d-1.$$

If $n-m = 2d-2$, then Equations (2.5), (2.6) hold for $0 \leq i \leq d-2$ and let

$$(2.7) \quad a_{d-1} = (m-1) \binom{n-1}{m-1}, \quad b_{d-1} = -\binom{n-2}{m-2}.$$

Then the following equality holds:

$$(2.8) \quad -P_n^{(m)}(\mathbf{x}) = \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} \sum_{i=0}^{d-1} w_i \left(a_i + b_i \sum_{j=0}^{n-1} x_j \right).$$

Before we present the proofs for Theorems 2.1, 2.2, let us explain the underlying ideas with examples.

Example 2.3. First, let us explain Theorem 2.1 with $P_5^{(3)}(\mathbf{x})$. Our goal is to find a quadratic polynomial Q that attains the same value of $P_5^{(3)}(\mathbf{x})$ consists of variables x_0, \dots, x_4 together with d auxiliary variables w_0, \dots, w_{d-1} . The only possible formula for Q is

$$(2.9) \quad Q = \sum_{0 \leq i < j \leq 4} L_{ij} x_i x_j + \sum_{j=0}^4 c_j x_j + \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} \left[\sum_{i=0}^{d-1} w_i \left(a_i + \sum_{j=0}^4 b_{i,j} x_j \right) \right].$$

In fact, this could be the general form of any reduced polynomial if it had a constant term. We omitted the constant term here, since we know that the minimum $P_5^{(3)}(\mathbf{x})$

is 0 (and the same for $P_n^{(m)}(\mathbf{x})$ in general). Just for now, let us assume that $b_{i,j} = b_i$, $L_{i,j} = L$, and $c_i = 0$. This means that $b_{i,j}$ will depend on the index of the auxiliary variables, $L_{i,j}$ is a constant, and Q does not have any linear terms on x_j 's.

$l(\mathbf{x})$	$P_5^{(3)}(\mathbf{x})$	$\sum_{i<j} x_i x_j$	A_l	$\min_{w_0=0,1} w_0(7-5l(\mathbf{x}))$	$\min_{w_1=0,1} w_1(3-l(\mathbf{x}))$
0	0	0	0	0	0
1	0	0	0	0	0
2	0	1	-3	-3	0
3	1	3	-8	-8	0
4	4	6	-14	-13	-1
5	10	10	-20	-18	-2

Table 1. The sequence A_l (c.f. Equation (2.10)) when $L = 3$ and the arithmetic progressions that sums up to A_l .

Let $l = l(\mathbf{x}) = x_0 + \dots + x_4$ and define the sequence A_l by

$$(2.10) \quad A_l = P_5^{(3)}(\mathbf{x}) - L \sum_{0 \leq i < j \leq 4} x_i x_j.$$

The second and third columns of Table 1 show the values for $P_5^{(3)}(\mathbf{x})$ and $\sum_{0 \leq i, j \leq 4} x_i x_j$ for $l = 0, \dots, 5$. If we choose $L = 3$, then the sequence A_l becomes a decreasing sequence of non-positive integers (the fourth column of Table 1). In fact, $L = 3$ is the minimum integer that makes the sequence A_l as a decreasing sequence. The first two non-zero numbers in A_l are $-3, -8$ at $l = 2, 3$ respectively, and they follows the arithmetic progression $7 - 5l$. Let us subtract $\min_{w_0=0,1} w_0(7 - 5l)$ (the fifth column of Table 1) from A_l for each l . Then we get a sequence that has only two negatives $-1, -2$ at $l = 4, 5$ respectively, where all other values are 0 (the sixth column of Table 1). This sequence is the same as $\min_{w_1=0,1} w_1(3 - l)$. Thus we obtain the following identity:

$$(2.11) \quad P_5^{(3)}(\mathbf{x}) = 3 \sum_{0 \leq i < j \leq 4} x_i x_j + \min_{w_0, w_1=0,1} \left[w_0(7 - 5 \sum_{j=0}^4 x_j) + w_1(3 - \sum_{j=0}^4 x_j) \right].$$

It is worth noticing that we reduced the polynomial $P_5^{(3)}(\mathbf{x})$ with only two auxiliary variables w_0 and w_1 , whereas the monomial reductions would produce 10 auxiliary variables, one for each monomial (c.f. Equation (1.6)).

$l(\mathbf{x})$	B_l	$\min_{w_0=0,1} w_0(8 - 3l(\mathbf{x}))$	$\min_{w_1=0,1} w_1(12 - 3l(\mathbf{x}))$
0	0	0	0
1	0	0	0
2	0	0	0
3	-1	-1	0
4	-4	-4	0
5	-10	-7	-3

Table 2. The values of B_l in Equation (2.12) and the arithmetic progressions that sums up to B_l .

Example 2.4. Next, let us explain Theorem 2.2 with the example of $-P_5^{(3)}(\mathbf{x})$. Let us define a sequence B_l as

$$(2.12) \quad B_l = -P_5^{(3)}(\mathbf{x}).$$

The sequence B_l is already a decreasing sequence of non-positive numbers, and its numbers are shown in the second column of Table 2. Let us observe the first two non-positives $-1, -4$ at $l = 3, 4$ respectively. The arithmetic progression that matches with these numbers is $8 - 3l$. We subtract the sequence $\min_{w_0=0,1} w_0(8 - 3l)$ from B_l to obtain a sequence of zeros except -3 at $l = 5$. Then we take the last two non-positive integers $0, -3$ at $l = 4, 5$ respectively, and use the arithmetic progression $12 - 3l$ to match these numbers. In this way, we get the following reduction:

$$(2.13) \quad -P_5^{(3)}(\mathbf{x}) = \min_{w_0, w_1=0,1} \left[w_0(8 - 3 \sum_{j=0}^4 x_j) + w_1(12 - 3 \sum_{j=0}^4 x_j) \right]$$

Again, we reduced the polynomial $-P_5^{(3)}(\mathbf{x})$ with only two auxiliary variables whereas the monomial reductions would produce 10 auxiliary variables (c.f. Equation (1.6))

Remark 2.5. Before we proceed to the next sections, let us point out some important facts.

- (1) In the sequence $A_l = P_n^{(m)}(\mathbf{x}) - L \cdot l(\mathbf{x})$, the constant L is set as minimum as possible to make A_l a non-positive decreasing sequence. There are $n - 1$ negatives in A_l , so we need $\lfloor (n - 1)/2 \rfloor$ auxiliary variables in the reduced polynomial of $P_n^{(m)}(\mathbf{x})$.
- (2) In the sequence $B_l = -P_n^{(m)}(\mathbf{x})$, there are $n - m + 2$ negatives. Thus, we need $\lfloor (n - m + 2)/2 \rfloor$ auxiliary variables in the reduced polynomials of $-P_n^{(m)}(\mathbf{x})$.
- (3) Ishikawa's formulae in Equations (1.5), (1.6) are the special cases of Theorem 2.1 when $n = m$. If $n = 2d + 2$, then for all $0 \leq i \leq d - 1$, we have

$2i + 3 \leq 2d + 1 < n = m$ and $2i + 2 \leq 2d < m - 1$, so Equations (2.2), (2.3) become

$$(2.14) \quad a_i = (4i + 3), \quad b_i = -2.$$

If $n = 2d + 1$, then Equation (2.14) hold for all $0 \leq i \leq d - 2$, and

$$a_{d-1} = (4d - 1) - (n - 1) = 2d - 1 \quad b_{d-1} = 1 - 2 = -1,$$

which coincides with Ishikawa's formula in Equations (1.5), (1.6). Freedman's formula in Equation (1.4) is a direct consequence of Theorem 2.2 when $n = m$: there is only one pair of coefficients a_0, b_0 , which are

$$a_0 = n - 1, \quad b_0 = -1.$$

Thus, we can say that Theorems 2.1, 2.2 are the generalizations of Ishikawa's and Freedman's methods.

3. PROOF OF THEOREM 2.1

The original binomial coefficients satisfies the following property: for $0 \leq s < r$,

$$(3.1) \quad \binom{r}{s} + \binom{r}{s+1} = \binom{r+1}{s+1}.$$

With the new definition of binomial coefficients in Equation (2.1), the same property holds for all $r, s \geq 0$: if $s = r$, both sides of Equation (3.1) are 1; if $s \geq r + 1$, both sides of Equation (3.1) are 0. We will use Equation (3.1) often in the subsequent calculations.

Let us fix the variables as x_0, \dots, x_{n-1} and omit the notation $\mathbf{x} = (x_0, \dots, x_{n-1})$ whenever there is no ambiguity. Let us define the sequence A_l as follows:

$$(3.2) \quad A_l = P_n^{(m)} - L \sum_{0 \leq i < j \leq n-1} x_i x_j.$$

Our first task is to find a value L so that the sequence A_l satisfies the following two properties:

P1 A_l is a decreasing finite sequence of non-positive integers for $0 \leq l \leq n$;

P2 the difference between two consecutive numbers in A_l is also decreasing, i.e.

$$(3.3) \quad (A_{n-i} - A_{n-i-1}) \leq (A_{n-i-1} - A_{n-i-2}) \text{ for all } 0 \leq i \leq n - 2.$$

For each $0 \leq i \leq n-2$, Equation (3.2) gives a triple of consecutive numbers in A_l :

$$(3.4) \quad A_{n-i-2} = \binom{n-i-2}{m} - L \binom{n-i-2}{2},$$

$$(3.5) \quad A_{n-i-1} = \binom{n-i-1}{m} - L \binom{n-i-1}{2},$$

$$(3.6) \quad A_{n-i} = \binom{n-i}{m} - L \binom{n-i}{2}.$$

We can re-write the inequality (3.3) as

$$\begin{aligned} & \left(\binom{n-i}{m} - \binom{n-i-1}{m} \right) - \left(\binom{n-i-1}{m} - \binom{n-i-2}{m} \right) \\ & - L \left(\left(\binom{n-i}{2} - \binom{n-i-1}{2} \right) - \left(\binom{n-i-1}{2} - \binom{n-i-2}{2} \right) \right) \leq 0. \end{aligned}$$

Thus we have

$$\begin{aligned} & \left(\binom{n-i-1}{m-1} - \binom{n-i-2}{m-1} \right) - L \left(\binom{n-i-1}{1} - \binom{n-i-2}{1} \right) \\ & = \binom{n-i-2}{m-2} - L \leq 0. \end{aligned}$$

The number of negatives in the sequence A_l determines the numbers of auxiliary variables in the reduced polynomial (c.f. Examples 2.3, 2.4 and Remark 2.5). Thus L should be chosen as minimum as possible so that A_l has the least number of negatives. Therefore,

$$(3.7) \quad L = \binom{n-2}{m-2}.$$

With this L , all A_l 's are also non-positive (i.e. A_l satisfies **P1**).

Next, we want to find the coefficients a_j, b_j that satisfy

$$(3.8) \quad A_l = P_n^{(m)} - L \binom{l}{2} = \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} \left[\sum_{i=0}^{d-1} w_i (a_i + b_i l) \right].$$

There are $n-1$ negative integers in A_l at $l = 2, \dots, n$. We need to split the cases for n where n is odd or n is even.

3.1. The odd case Suppose that $n = 2d+1$ for some d . Then there are $2d$ negatives in A_l and we want d arithmetic progressions in Equation (3.8) subsequently appear as follows:

$$(3.9) \quad \binom{2}{m} - \binom{n-2}{m-2} \binom{2}{2} = a_0 + 2b_0,$$

$$(3.10) \quad \binom{3}{m} - \binom{n-2}{m-2} \binom{3}{2} = a_0 + 3b_0, \quad (w_0 = 1, w_k = 0 \text{ for } 1 \leq k \leq d-1)$$

$$(3.11) \quad \binom{4}{m} - \binom{n-2}{m-2} \binom{4}{2} = (a_0 + 4b_0) + (a_1 + 4b_1),$$

$$(3.12) \quad \binom{5}{m} - \binom{n-2}{m-2} \binom{5}{2} = (a_0 + 5b_0) + (a_1 + 5b_1),$$

$$(w_0 = w_1 = 1, w_k = 0 \text{ for } 2 \leq k \leq d-1)$$

⋮

$$(3.13) \quad \binom{n-1}{m} - \binom{n-2}{m-2} \binom{n-1}{2} = \sum_{k=0}^{d-1} (a_k + (n-1)b_k),$$

$$(3.14) \quad \binom{n}{m} - \binom{n-2}{m-2} \binom{n}{2} = \sum_{k=0}^{d-1} (a_k + nb_k). \quad (w_0 = \cdots = w_{d-1} = 1)$$

That is, for each $0 \leq i \leq d-1$,

$$(3.15) \quad \binom{2i+2}{m} - \binom{n-2}{m-2} \binom{2i+2}{2} = \sum_{k=0}^i (a_k + (2i+2)b_k),$$

$$(3.16) \quad \binom{2i+3}{m} - \binom{n-2}{m-2} \binom{2i+3}{2} = \sum_{k=0}^i (a_k + (2i+3)b_k).$$

This is possible because the sequence A_l satisfies the inequality (3.3): the differences $A_{l+1} - A_l$ are getting smaller (as negatives) as l increases. We equate A_l on the left hand-side of Equation (3.8) by introducing new arithmetic progressions of negative common differences on the right hand-side.

To find the formulae of b_i , we subtract Equations (3.15) from Equation (3.16) to get

$$(3.17) \quad \begin{aligned} \sum_{k=0}^i b_k &= \binom{2i+3}{m} - \binom{2i+2}{m} - \binom{n-2}{m-2} \left(\binom{2i+3}{2} - \binom{2i+2}{2} \right) \\ &= \binom{2i+2}{m-1} - \binom{n-2}{m-2} ((2i+3)(i+1) - (i+1)(2i+1)) \\ &= \binom{2i+2}{m-1} - 2(i+1) \binom{n-2}{m-2} \end{aligned}$$

Thus for $0 \leq i \leq d-1$,

$$\begin{aligned}
(3.18) \quad b_i &= \left(\binom{2i+2}{m-1} - 2(i+1) \binom{n-2}{m-2} \right) - \left(\binom{2i}{m-1} - 2i \binom{n-2}{m-2} \right) \\
&= \binom{2i+2}{m-1} - \binom{2i}{m-1} - 2 \binom{n-2}{m-2}.
\end{aligned}$$

To find the formula of a_i , we add Equations (3.15), (3.16) to get

$$\begin{aligned}
2 \sum_{k=0}^i a_k + (4i+5) \sum_{k=0}^i b_k &= \binom{2i+2}{m} + \binom{2i+3}{m} \\
&\quad - ((2i+3)(i+1) + (i+1)(2i+1)) \binom{n-2}{m-2}
\end{aligned}$$

Applying Equation (3.17), we get

$$\begin{aligned}
(3.19) \quad \sum_{k=0}^i a_k &= \frac{1}{2} \left(\binom{2i+3}{m} + \binom{2i+2}{m} - 4(i+1)^2 \binom{n-2}{m-2} \right. \\
&\quad \left. - (4i+5) \left(\binom{2i+2}{m-1} - 2(i+1) \binom{n-2}{m-2} \right) \right) \\
&= \frac{1}{2} \left(\binom{2i+3}{m} + \binom{2i+2}{m} - (4i+5) \binom{2i+2}{m-1} \right. \\
&\quad \left. + ((4i+5)(2(i+1)) - 4(i+1)^2) \binom{n-2}{m-2} \right) \\
&= \frac{1}{2} \left(\binom{2i+3}{m} + \left(\binom{2i+2}{m} + \binom{2i+2}{m-1} \right) - 2(2i+3) \binom{2i+2}{m-1} \right. \\
&\quad \left. + 2(2i^2 + 5i + 3) \binom{n-2}{m-2} \right) \\
&= (i+1)(2i+3) \binom{n-2}{m-2} - (m-1) \binom{2i+3}{m},
\end{aligned}$$

$$\begin{aligned}
(3.20) \quad a_i &= ((i+1)(2i+3) - i(2i+1)) \binom{n-2}{m-2} \\
&\quad - (m-1) \left(\binom{2i+3}{m} - \binom{2i+1}{m} \right) \\
&= (4i+3) \binom{n-2}{m-2} - (m-1) \left(\binom{2i+3}{m} - \binom{2i+1}{m} \right)
\end{aligned}$$

3.2. The even case Suppose that $n = 2d + 2$. We have $2d - 1$ negatives in the sequence A_l for starting from $l = 2$. We can write the first few equations of Equation

(3.8) exactly as Equations (3.9) – (3.12). However, the last three equations will be

$$(3.21) \quad \binom{n-2}{m} - \binom{n-2}{m-2} \binom{n-2}{2} = \sum_{k=0}^{d-1} (a_k + (n-2)b_k),$$

$$(3.22) \quad \binom{n-1}{m} - \binom{n-2}{m-2} \binom{n-1}{2} = \sum_{k=0}^{d-1} (a_k + (n-1)b_k),$$

$$(3.23) \quad \binom{n}{m} - \binom{n-2}{m-2} \binom{n}{2} = \sum_{k=0}^{d-1} (a_k + nb_k) \quad (w_0 = \cdots = w_{d-1} = 1).$$

This happens because the triple A_{n-2}, A_{n-1}, A_n are always an arithmetic progression with a common difference:

$$\begin{aligned} A_{n-1} - A_{n-2} &= \left(\binom{n-2}{m} - \binom{n-2}{m-2} \binom{n-1}{2} \right) - \left(\binom{n-2}{m} - \binom{n-2}{m-2} \binom{n-2}{2} \right) \\ &= \left(\binom{n-1}{m} - \binom{n-2}{m} \right) - \binom{n-2}{m-2} \left(\binom{n-1}{2} - \binom{n-2}{2} \right) \\ &= \binom{n-2}{m-1} - (n-2) \binom{n-2}{m-2} \\ &= \binom{n-2}{m-1} + \binom{n-2}{m-2} - (n-1) \binom{n-2}{m-2} \\ &= \binom{n-1}{m-1} - (m-1) \binom{n-1}{m-1} \\ &= -(m-2) \binom{n-1}{m-1}, \\ A_n - A_{n-1} &= \left(\binom{n}{m} - \binom{n-2}{m-2} \binom{n}{2} \right) - \left(\binom{n-1}{m} - \binom{n-2}{m-2} \binom{n-1}{2} \right) \\ &= \left(\binom{n}{m} - \binom{n-1}{m} \right) - \binom{n-2}{m-2} \left(\binom{n}{2} - \binom{n-1}{2} \right) \\ &= \binom{n-1}{m-1} - (n-1) \binom{n-2}{m-2} \\ &= \binom{n-1}{m-1} - (m-1) \binom{n-1}{m-1} \\ &= -(m-2) \binom{n-1}{m-1} \end{aligned}$$

Therefore, the same formulae of a_i and b_i for $0 \leq i \leq d-1$ in Equations (3.18), (3.20) hold.

4. PROOF OF THEOREM 2.2

Let us define the sequence B_l as follows:

$$(4.1) \quad B_l = -P_n^{(m)}$$

The sequence B_l satisfies the properties **P1**, **P2** in the previous section: first, each B_l is obviously non-positive. Second, if $n \geq m + 2$, then for each $0 \leq i \leq n - m - 2$, the triple of consecutive numbers $B_{m+i}, B_{m+i+1}, B_{m+i+2}$ satisfies

$$\begin{aligned} & (B_{m+i+2} - B_{m+i+1}) - (B_{m+i+1} - B_{m+i}) \\ &= -\binom{m+i+2}{m} + \binom{m+i+1}{m} - \left(-\binom{m+i+1}{m} + \binom{m+i}{m} \right) \\ &= -\binom{m+i+1}{m-1} + \binom{m+i}{m-1} = -\binom{m+i}{m-2} < 0 \end{aligned}$$

The goal is to find the coefficients a_i, b_i satisfying

$$(4.2) \quad B_l = -\binom{l}{m} = \min_{\substack{w_i=0,1 \\ i=0,\dots,d-1}} \left[\sum_{i=0}^{d-1} w_i (a_i + b_i l) \right].$$

There are $n + 1 - m$ negative numbers in the sequence B_l for $m \leq l \leq n$. Thus we need to split the cases for n when $n - m$ is odd or even.

4.1. The odd case Suppose that $n - m = 2d - 1$, i.e. $n - m + 1 = 2d$. Then there are d arithmetic progressions in Equation (4.2) that appears subsequently as follows:

$$(4.3) \quad -\binom{m}{m} = a_0 + mb_0,$$

$$(4.4) \quad -\binom{m+1}{m} = a_0 + (m+1)b_0, \quad (w_0 = 1, w_k = 0 \text{ for } 1 \leq k \leq d-1)$$

$$(4.5) \quad -\binom{m+2}{m} = (a_0 + (m+2)b_0) + (a_1 + (m+2)b_1),$$

$$(4.6) \quad -\binom{m+3}{m} = (a_0 + (m+3)b_0) + (a_1 + (m+3)b_1),$$

$$(w_0 = w_1 = 1, w_k = 0 \text{ for } 2 \leq k \leq d-1)$$

⋮

$$(4.7) \quad -\binom{n-1}{m} = \sum_{k=0}^{d-1} (a_k + (n-1)b_k),$$

$$(4.8) \quad -\binom{n}{m} = \sum_{k=0}^{d-1} (a_k + nb_k). \quad (w_0 = \cdots = w_{d-1} = 1)$$

For $0 \leq i \leq d-1$, we have

$$(4.9) \quad -\binom{m+2i}{m} = \sum_{k=0}^i (a_k + (m+2i)b_k),$$

$$(4.10) \quad -\binom{m+2i+1}{m} = \sum_{k=0}^i (a_k + (m+2i+1)b_k),$$

Subtracting Equation (4.9) from Equation (4.10), we get

$$(4.11) \quad \sum_{k=0}^i b_k = -\binom{m+2i+1}{m} + \binom{m+2i}{m} = -\binom{m+2i}{m-1}.$$

Therefore, for $0 \leq i \leq d-1$,

$$(4.12) \quad b_i = -\binom{m+2i}{m-1} + \binom{m+2i-2}{m-1}.$$

By adding Equations (4.9), (4.10), we get

$$(4.13) \quad 2 \sum_{k=1}^i a_k + (2m+4i+1) \sum_{k=1}^i b_k = -\binom{m+2i+1}{m} - \binom{m+2i}{m}.$$

Applying Equation (4.11), we get

$$\begin{aligned} \sum_{k=0}^i a_k &= \frac{1}{2} \left(-\binom{m+2i+1}{m} - \binom{m+2i}{m} + (2m+4i+1) \binom{m+2i}{m-1} \right) \\ &= \frac{1}{2} \left(-\left(\binom{m+2i+1}{m} + \binom{m+2i}{m} + \binom{m+2i}{m-1} \right) + 2(m+2i+1) \binom{m+2i}{m-1} \right) \\ &= -\binom{m+2i+1}{m} + (m+2i+1) \binom{m+2i}{m-1} \\ &= (m-1) \binom{m+2i+1}{m} \end{aligned}$$

Therefore,

$$(4.14) \quad a_i = (m-1) \left(\binom{m+2i+1}{m} - \binom{m+2i-1}{m} \right)$$

4.2. The even case Next, suppose that $n - m = 2d - 2$. In this case, the first few equations of Equation (4.2) are exactly same as Equations (4.3) – (4.6), but the last three equations would be

$$(4.15) \quad -\binom{n-2}{m} = \sum_{k=0}^{d-2} (a_k + (n-2)b_k),$$

$$(4.16) \quad -\binom{n-1}{m} = \sum_{k=0}^{d-2} (a_k + (n-1)b_k), \quad (w_0 = \cdots = w_{d-2} = 1)$$

$$(4.17) \quad -\binom{n}{m} = \sum_{k=0}^{d-2} (a_k + nb_k) + (a_{d-1} + nb_{d-1}). \quad (w_{d-1} = 1)$$

The last arithmetic progression $a_{d-1} + b_{d-1}l$ must satisfy $a + (n-1)b_{d-1} = 0$. This means

$$(4.18) \quad \begin{aligned} b_{d-1} &= -\binom{n}{m} + \binom{n-1}{m} - \sum_{k=0}^{d-2} b_k \\ &= -\binom{n-1}{m-1} + \binom{m+2(d-2)}{m-1} = -\binom{n-1}{m-1} + \binom{n-2}{m-1} \\ &= -\binom{n-2}{m-2}, \end{aligned}$$

$$(4.19) \quad \begin{aligned} a_{d-1} &= -(n-1)b_d = (n-1)\binom{n-2}{m-2} \\ &= (m-1)\binom{n-1}{m-1}. \end{aligned}$$

5. SIMULATED RESULTS

In this section, we introduce two algorithms, **MaxSymm** and **SymmRed**, which implement the symmetric degree reduction method based on Theorems 2.1, 2.2. **MaxSymm** is an algorithm that finds *maximal* (which will be defined shortly) symmetric polynomials in a given polynomial. **SymmRed** is an algorithm that obtains a reduced quadratic polynomial from a given polynomial of binary variables, which prioritize the degree reduction of symmetric polynomials found by **MaxSymm**. After reducing all symmetric homogeneous polynomials, **SymmRed** still uses the monomial reduction methods for reducing the remaining monomials.

We will call $P_n^{(m)}(\mathbf{x})$ for $\mathbf{x} = (x_0, \dots, x_{n-1})$ in Equation (1.10) as the **symmetric m -polynomial on \mathbf{x}** . We will say a polynomial q lies in a polynomial p if all

monomials in q are monomials in p . In this case, we will say p **contains** q . A symmetric m -polynomial q is said to be **maximal in** p if q lies in p and there is no other symmetric m -polynomial that lies in p and contains q . For example, the symmetric 3-polynomial on 5 variables $P_5^{(3)}(x_0, \dots, x_4)$ is larger than the symmetric 3-polynomial on 4 variables $P_4^{(3)}(x_0, \dots, x_3)$.

The **MaxSymm** algorithm takes two arguments, the polynomial p and the degree m . Again, this algorithm finds maximal symmetric m -polynomials that lies in p . We say a symmetric m -polynomial is **trivial** if it consists of only m variables, and the algorithm returns nil if there is no symmetric m -polynomial except trivial ones. Let us call a monomial of degree m simply as **m -monomial**. We can represent every m -monomial by a set of distinct m variables (or more simply, m indices). Generally, we can represent every symmetric m -polynomial by a set of distinct variables (or indices) whenever there is no ambiguity on the constant m . For example, the symmetric polynomial $P_5^{(3)}(x_0, \dots, x_4)$ is characterized by the set $\{x_0, x_1, x_2, x_3, x_4\}$, or more simply, $\{0, 1, 2, 3, 4\}$.

Algorithm 1 MaxSymm algorithm

```

1: procedure MAXSYMM( $p, m$ ) ▷  $p$  is a polynomial,  $m \geq 3$  is a degree
2:    $A, B \leftarrow$  the set of all  $m$ -monomials in  $p$ 
3:   while  $C$  is not empty do
4:      $B, C \leftarrow C, \emptyset$ 
5:     for  $q$  in  $B$  do
6:       for  $r$  in  $A$  do
7:         if  $r \not\subseteq q$  then
8:            $s \leftarrow$  the symmetric  $m$ -polynomial on  $q \cup r$ 
9:           if  $s$  lie in  $p$  then
10:             $C \leftarrow C \cup \{s\}$ 
11:          end if
12:        end if
13:      end for
14:    end for
15:  end while
16:  return  $B$ 
17: end procedure

```

Algorithm 1 is a pseudocode of **MaxSymm** algorithm. It utilizes three sets A, B, C . The set A is the set of the all m -monomials in p , and it is the reference set so we do not change it throughout the algorithm. The set B is the set of largest symmetric m -polynomials in p polynomials that are currently found. The set C is

the set of all symmetric m -polynomials in p that are even larger than at least one in B . The algorithm starts by initializing the sets A, B, C as the set of all monomials in p . The initialization of C is only for the first iteration of the below cycle to happen. (The line numbers refers to Algorithm 1.)

- (1) Firstly, we replace the set B by C and empty the set C (Line 4). This means we transfer all information on the symmetric m -polynomials in C to B .
- (2) Secondly, we look up all pairs (q, r) of monomials in B and A (Lines 5, 6). Only when r contains an element which is not in q (Line 7), the algorithm creates the symmetric m -polynomial s on all variables in the set $q \cup r$ (Line 8). If s lies in p , we insert s in C as an element (Lines 9, 10).
- (3) The cycle aborts when there is no update on C after the full iteration of (2).

After the iteration of cycles are aborted, the algorithm returns all symmetric polynomials stored in the set B .

Example 5.1. Let us re-visit the example in Equation (1.7) to see how $\mathbf{MaxSymm}(p, 3)$ works:

$$\begin{aligned}
p = & 2 - x_0 - x_1 - 2x_2 - 2x_3 - x_4 - x_5 + x_0x_1 + 2x_0x_2 + x_0x_3 \\
& + x_1x_2 + 2x_1x_3 + 2x_2x_3 + 2x_2x_4 + x_2x_5 + x_3x_4 + 2x_3x_5 \\
& - 2x_0x_1x_2 - 2x_0x_1x_3 - 2x_0x_2x_3 - 2x_1x_2x_3 \\
& - 2x_2x_3x_4 - 2x_2x_3x_5 - 2x_2x_4x_5 - 2x_3x_4x_5 + 4x_0x_1x_2x_3 + 4x_2x_3x_4x_5
\end{aligned}$$

At the beginning of the algorithm, the sets A, B are initialized as below (variables are represented by their indices):

$$A = \{\{0, 1, 2\}, \{0, 1, 3\}, \{0, 2, 3\}, \{1, 2, 3\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 5\}, \{3, 4, 5\}\}.$$

At the first cycle, the algorithm searches all pairs of elements in the set B and A . The pair $(\{0, 1, 2\}, \{0, 1, 3\})$ produces a symmetric 3-polynomial $s = \{0, 1, 2, 3\}$ (Line 8). Since $P_4^{(3)}(x_0, x_1, x_2, x_3)$ lies in p , we update the set C as $C = \{\{0, 1, 2, 3\}\}$ (Line 10). There is no further update to the set C until the end of this cycle. Since $C \neq \emptyset$, the algorithm goes into the second cycle, which starts with $B = \{\{0, 1, 2, 3\}\}$ and $C = \emptyset$. Since there is no other symmetric polynomial in p that consists of variables more than x_0, x_1, x_2, x_3 , there is no update to the set C . The algorithm returns $\{\{0, 1, 2, 3\}\}$ and terminates.

The algorithm **SymmRed** takes a single argument, the polynomial p that requires a degree reduction. It uses the algorithm **MaxSymm** to find any maximal symmetric m -polynomials iteratively for m from 3 to $\deg p$. For each maximal symmetric polynomial found, namely s , it determines a constant a so that the m -monomials in p are maximally removed by $p - a \cdot s$. For this matter, this algorithm works properly only when the polynomial p has a discrete spectrum of coefficients. Then the symmetric m -polynomial s is reduced to quadratic polynomial by Theorems 2.1, 2.2. When the process of searching and reducing maximal symmetric polynomials are done, the algorithm applies the monomial reduction methods to the remaining monomials.

Algorithm 2 The Symmetric Reduction algorithm

```

1: procedure SYMMRED( $p$ ) ▷  $p$  is a polynomial
2:    $q \leftarrow 0$ 
3:   for  $m \leftarrow 3$  to  $\deg p$  do
4:     while  $s \leftarrow \text{MaxSymm}(p, m); s \neq 0$  do
5:        $a \leftarrow$  the most common coefficient of monomials in  $p$  and  $s$ 
6:        $p \leftarrow p - a \cdot s$ 
7:       if  $a > 0$  then
8:          $r \leftarrow$  apply Theorem 2.1 to  $s$ 
9:       else
10:         $r \leftarrow$  apply Theorem 2.2 to  $-s$ 
11:       end if
12:        $q \leftarrow q + |a| \cdot r$ 
13:     end while
14:   end for
15:    $q \leftarrow q + \text{MonoRed}(p)$  ▷ do the monomial reduction
16: end procedure

```

Algorithm 2 shows a pseudocode for **SymmRed**. The constant a (Line 5 in Algorithm 2) is determined by counting the number of occurrences of all coefficients of monomials in p that lies in s . However, the choice of a may not be unique. For example, suppose that $s = \{0, 1, 2, 3\}$, $m = 3$, and the polynomial p is

$$\begin{aligned}
 & -x_0x_1x_2 - x_0x_1x_3 + x_0x_2x_3 + x_1x_2x_3 \\
 (5.1) \quad & = \underbrace{x_0x_1x_2 + x_0x_1x_3 + x_0x_2x_3 + x_1x_2x_3}_{\text{Theorem 2.1}} - \underbrace{2x_0x_1x_2 - 2x_0x_1x_3}_{\text{monomial reduction}} \\
 (5.2) \quad & = \underbrace{-x_0x_1x_2 - x_0x_1x_3 - x_0x_2x_3 - x_1x_2x_3}_{\text{Theorem 2.2}} + \underbrace{2x_0x_2x_3 + 2x_1x_2x_3}_{\text{monomial reduction}}
 \end{aligned}$$

Since there are the same numbers of $+1$ and -1 coefficients, we can take either Equation (5.1) or (5.2). In the actual implementation of the algorithm, we took a random choice of a between candidates when this kind of situation happened.

Now, we present the efficiency of the symmetric reduction method. We tested **SymmRed** on the objective function Q_G in Equation (1.3) for random p -graphs G , where p is the probability of the existence of an edge between each pair of two vertices in G . We varied the number v of vertices $v = 3, 4, 5, 6, 7, 8$ and $p = 0.75, 0.80, 0.85, 0.90, 0.95$. The number of colors are set to be the minimum number of the form 2^m satisfying $v \leq 2^m$. Thus $m = \lfloor \log_2(v-1) \rfloor + 1$ number of binary digits are used for the binary representation of colors, and $n = mv$ binary variables are used in the objective function. We generated 10^4 random graphs and their objective functions for each p and v . We applied the symmetric and the monomial reduction methods, and counted the numbers of total variables and monomials in the reduced quadratic polynomials.

p	v	n	Symmetric reduction		Monomial reduction		$\frac{r_1 - n}{r_2 - n}$	N_1/N_2
			r_1	N_1	r_2	N_2		
0.75	3	6	10.31	41.72	17.20	66.97	40.00%	62.29%
	4	8	16.90	75.88	30.41	125.41	40.00%	60.50%
	5	15	145.12	795.16	327.76	1597.50	41.61%	49.78%
	6	18	212.62	1182.61	486.06	2382.62	41.58%	49.63%
	7	21	291.53	1636.67	673.41	3313.83	41.47%	49.39%
	8	24	384.38	2174.45	894.23	4413.20	41.41%	49.27%
0.80	3	6	10.63	43.49	17.87	70.04	40.00%	62.10%
	4	8	17.52	79.96	31.89	132.63	40.00%	60.28%
	5	15	153.63	845.02	348.57	1701.93	41.56%	49.65%
	6	18	224.47	1253.53	515.08	2528.39	41.54%	49.58%
	7	21	309.64	1743.23	717.00	3532.79	41.47%	49.34%
	8	24	407.97	2315.10	951.84	4702.65	41.38%	49.23%
0.85	3	6	10.98	45.53	18.64	73.59	40.00%	61.87%
	4	8	18.20	84.52	33.53	140.75	40.00%	60.05%
	5	15	162.28	895.16	369.25	1805.79	41.58%	49.57%
	6	18	237.42	1331.70	546.97	2688.59	41.48%	49.53%
	7	21	326.47	1841.98	758.43	3740.97	41.42%	49.24%
	8	24	431.16	2453.30	1007.69	4983.24	41.39%	49.23%
0.90	3	6	11.35	47.78	19.47	77.54	40.00%	61.62%
	4	8	18.82	88.81	35.07	148.39	40.00%	59.85%
	5	15	170.38	942.11	389.19	1905.94	41.52%	49.43%
	6	18	249.12	1404.09	577.36	2841.28	41.32%	49.42%

	7	21	344.49	1946.97	803.22	3966.03	41.36%	49.09%
	8	24	454.33	2594.31	1065.11	5271.75	41.33%	49.21%
0.95	3	6	11.69	49.87	20.23	81.22	40.00%	61.41%
	4	8	19.40	92.83	36.51	155.55	40.00%	59.68%
	5	15	178.64	989.51	409.39	2007.44	41.49%	49.29%
	6	18	259.17	1470.89	608.56	2998.07	40.84%	49.06%
	7	21	360.95	2041.47	844.74	4174.64	41.27%	48.90%
	8	24	474.11	2722.52	1121.66	5555.88	41.01%	49.00%
1.00	3	6	12	52	21	85	40.00%	61.18%
	4	8	20	97	38	163	40.00%	59.51%
	5	15	187	1037	430	2111	41.45%	49.12%
	6	18	264	1516	639	3151	39.61%	48.11%
	7	21	378	2137	889	4397	41.13%	48.60%
	8	24	480	2797	1180	5849	39.45%	47.82%

Table 3. The average numbers of total variables r_i and monomials N_i in the quadratic polynomials reduced from the objective function of the graph coloring problem on the random p -graphs, obtained by the symmetric reduction method ($i = 1$) and the monomial reduction methods ($i = 2$). The v is the number of vertices in the random graph and n is the number of variables in the objective function. The last two columns are ratios between averages on numbers of auxiliary variables $((r_1 - n)/(r_2 - n))$ and the total numbers of monomials N_1/N_2 .

Table 3 shows the summarized results. The r_1 and r_2 on the fourth and sixth columns of the table are the average numbers of all variables in the reduced quadratic polynomials obtained by applying the symmetric and monomial reduction methods respectively. The N_1 and N_2 on the fifth and seventh column of the table are the average numbers of all monomials in the reduced quadratic polynomials obtained by the symmetric and monomial reduction methods respectively. We take the ratio between average numbers of auxiliary variables in the reduced quadratic polynomial obtained by the symmetric and monomial reduction methods. The last rows of Table 3 shows the cases for the complete graphs.

Figure 1 shows the data points for (v, r_1) and (v, r_2) for each p . The symmetric reduction method produces only 39.45% \sim 41.61% of auxiliary variables than the monomial reduction method. The average number of monomials in the reduced polynomial obtained by the symmetric reduction method are approximately 47.82% \sim 62.29% of what produced by the monomial reduction method.

6. CONCLUSION

One of the main limitation that the current quantum annealing systems have, in solving real-world problems, is the number of qubits of the quantum annealing machines. Thus minimizing the number of variables in a QUBO formulation is essential. We showed that the symmetric reduction method can produces substantially less number of auxiliary variables than the conventional methods for the QUBO formulation of the graph coloring problem.

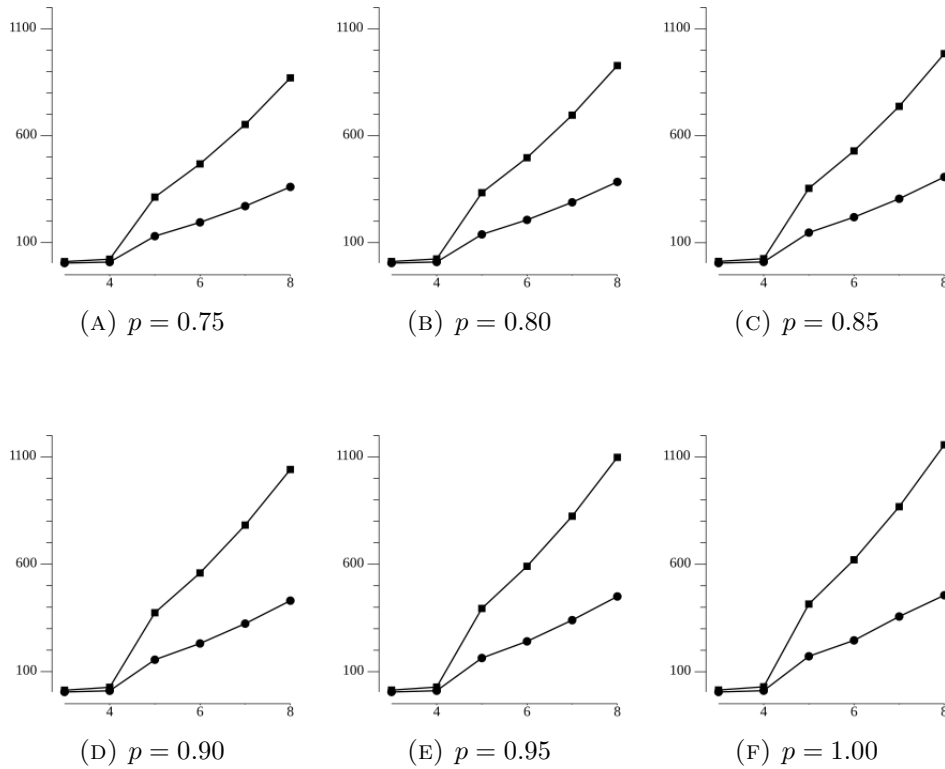


Figure 1. Plots on the average numbers of auxiliary variables in the quadratic polynomial reduced from the objective functions of the graph coloring problems on random p -graphs by the symmetric reduction method (circle-dot) and the monomial reductions (square-dots). The number of colors are set to be the number of vertices of the graph. The horizontal axis represents the number of vertices and the vertical axis represents the average numbers of auxiliary variable.

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