

Properties of the Binary Hypercube and Middle Level Graphs

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Abstract This paper takes a look at various properties of binary hypercubes and middle level graphs, a particular subgraph of the binary hypercube. The intention is to shed some light on the middle level conjecture by discovering patterns within the subgraphs and the known Hamiltonian cycles for those graphs. The problem is closely related to determining Hamiltonicity of graphs and is also closely tied to Gray code cycles and binary sequences.

Keywords Middle Level Conjecture, Hypercubes, Hamiltonicity, Queue Gray Code

1. Introduction

A hypercube, sometimes referred to as a n -cube, is the graphical representation of the edges and vertices in a single volumetric unit in any dimension n . It is well known that these graphs are Hamiltonian. The question of whether particular subgraphs of the hypercube are Hamiltonian is less clear.

First proposed in the 1980's by Ivan Havel, the Middle Level Conjecture, under the name "The Revolving Door Conjecture"[1] remains an open problem in mathematics unanimously thought to be true. The conjecture states that for every odd n -dimensional hypercube for $n \geq 3$, there exists a Hamiltonian cycle in the graph of the middle layers of the hypercube. The difficulty in solving the problem is undoubtedly due in part to the unclear nature of Hamiltonian cycles in general, for there is no known method to prove the existence of a Hamiltonian cycle in a graph. There are a few strategies which can be used to disprove the existence of such cycles [2], but the middle level graph, as little effort will show, fails on these accounts. As of 2006, with the aid of technology, M_{35} and M_{37} were the largest graphs of this nature to be proved to contain Hamiltonian cycles [5, 9].

This paper takes a look at various properties of the hypercube and the middle level graph as well as the use of Gray codes to develop some of these properties. Finally, this paper will look into how queue Gray codes can be used to search for paths and cycles within middle level graphs and the results of queue Gray code and antipodal tests on known Hamiltonian paths within various middle level

graphs.

2. Definitions and Notations

Definition 1 (Hypercube)

A hypercube is the graphical representation of the edges and vertices in a single volumetric unit in any dimension n . For the purpose of this paper it should be noted that all hypercubes refer to binary n -dimensional graphs. These graphs are denoted by Q_n , where n is the dimension (Fig. 1).

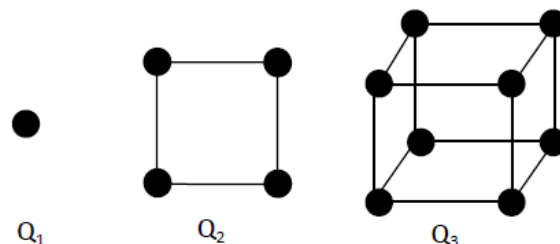


Figure 1. Hypercubes of the first, second and third dimension

Definition 2 (Hamiltonian Path)

In a graph G a path that contains every vertex of G once is referred to as a Hamiltonian Path [2].

Definition 3 (Hamiltonian Cycle)

In a graph G , a cycle c of G , which contains every vertex of G once, is said to be a Hamiltonian cycle, and for this reason, G is called a Hamiltonian graph[2].

Definition 4 (Vertex Levels of a Hypercube)

When mapped to a coordinate axis, each vertex of a hypercube, Q_n , can be assigned a binary string of length n . The i^{th} level of the hypercube refers to the set of vertices of Q_n which contain i ones in their vertex string (Fig. 2).

Definition 5 (Middle Level Graph)

The middle layer graph, denoted M_n , is a subgraph of Q_n containing the vertices in levels $\lfloor \frac{n}{2} \rfloor$ and $\lceil \frac{n}{2} \rceil$ (Fig. 2).

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Definition 6 (Word or String)

The terms word and string are used interchangeably to refer to a binary number consisting of a sequence of zeros and ones.

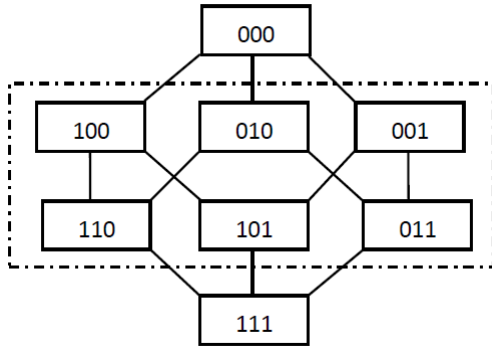


Figure 2. A layered Q_3 graph with M_3 outlined in the center

3. Gray Code

Tightly coupled with the notion of binary counting is that of Gray Code. Gray code is a binary counting system in which consecutive numbers differ by a single bit. Where the binary counting system, like the decimal counting system, places the value of a bit or number on the digit's position, Gray code does not. Rather, Gray code is produced by applying the exclusive-or operation to consecutive bits of the equivalent binary number (Table. 1)[3].

Table 1. Decimal Binary Gray Comparison

Decimal	Binary	Gray
0	0000	0000
1	0001	0001
2	0010	0011
3	0011	0010
4	0100	0110
5	0101	0111
6	0110	0101
7	0111	0100
8	1000	1100

3.1. Cyclic Gray Code

A finite Gray code sequence is called cyclic if the transition between the last word of the sequence and the first is a single bit exchange; that is the first and last strings differ by a single binary digit. Thus, a Gray code cycle consisting of words of length n contains all the 2^n possible bit string combinations [4].

Cyclic Gray code can be inductively produced through reflected binary code. The trivial case is when words have a length of one. Clearly, the two words in the Gray code sequence form a cycle. If the word length n , is two, a cyclic Gray code can be produced by concatenating the cycle for $n - 1$, and its reflection and appending a zero bit to the left side of the unreflected words and a one bit to the left of the reflected words (Fig. 3). The result is a sequence of 2^n words of length n where the first and the last differ by a

single bit. Continuing, in this manner inductively, a cyclic Gray code sequence can be produced for all words of length n .

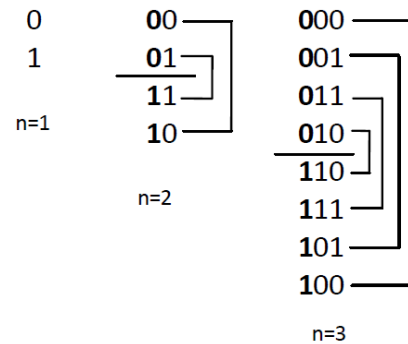


Figure 3. Recursive construction of Gray Codes for $n = 1, 2, 3$

3.2. Queue Gray Code

Queue Gray code adds an additional constraint to that of standard Gray code. In a queue Gray code every consecutive word is produced from the previous by removing the most significant bit, shifting the remaining bits one position to the left, and appending a new least significant bit (Fig. 4). Figure 6 shows several examples of queue Gray code sequences. It becomes clear then, that particular substrings become illegal in queue Gray code.

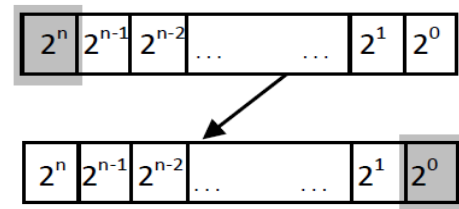


Figure 4. Queue Gray Code Bit Shift between Consecutive Words

Consider the substring '101' of a word. Shifting these bits one digit to the left will create a consecutive queue Gray code word which differs from the previous by at least two bits. This however, breaks the most basic law for Gray code. Thus, no word which contains the substring '101' can produce a consecutive queue Gray code word. Similarly, it can be shown that the substring '010' is also illegal.

Further, it is impossible to legally create either illegal substring. In order to create a word containing one, the previous consecutive word must have the two least significant bits differ; '01' or '10'. To create the illegal form, both these bit must change. Again, this violates Gray code. It follows then that no queue Gray code sequence containing words of length greater than three will contain any word containing either substring '010' or '101'.

It can similarly be shown that '1001', '0110', and any substring which does not partition the 1s and 0s to the left and right side of the word is illegal.

Proof

Here we prove the case when the first and last bits are 1 and there exists at least one 0 bit in the middle. The proof for the opposite case is similar.

Suppose a word contains a substring as described above. Let the zero bit be the a^{th} bit in the string. The first ones bit immediately to left of a in the b^{th} bit of the substring, and the first ones bit immediately to the right of a be in the c^{th} bit of the substring.

In the next consecutive word, all the bits of the substring will be shifted one bit to the left. Consider this new word. In the b^{th} position there will be a zero and in the $(c - 1)^{st}$ position there will be a one. Since the previous consecutive word contained a one and a zero respectively in these positions, two bits have changed between words (Fig. 5). Thus, the shift is not a Gray code shift: a contradiction.

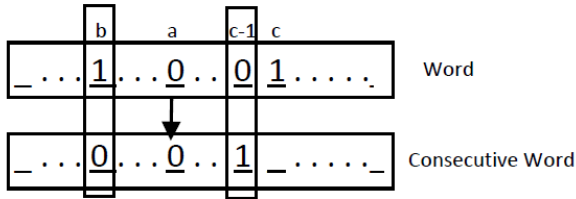


Figure 5. Queue Gray Code Illegal Substring Form

From the illegal substrings it follows that every word in a queue Gray code sequence must have the zeros and ones partitioned; that is all the zeros are on the left side of the word and the ones on the right or vice versa. This gives an upper bound of $2n$. A queue Gray code sequence, in fact a cycle, can systematically be generated (Fig. 6). From here it is clear that $2n$ is an exact upper bound for the length of a queue Gray code path.

4. Properties of the Hypercube

Given that the hypercube represents a single volumetric unit in any dimension, it follows that the length of each edge is 1 unit and that all edges which meet at a vertex are perpendicular to each other. It also follows that each vertex can be assigned a unique binary string of length n if the hypercube is placed at the origin of the coordinate systems. Each vertex string corresponds to the coordinate location of the vertex resulting in a unique binary word. The number of vertices is equivalent to the number of possible binary strings of length n : 2^n . The degree of each vertex is the dimension n and adjacent vertices differ by a single bit.

4.1. A Layered Graph

It is helpful to construct the graph of a hypercube as a layered structure. Specifically, the vertices can be grouped based on the number of ones which appear in their corresponding string; the 0^{th} layer containing no ones and the n^{th} layer containing only ones (Fig. 7).

It is apparent that edges only exist between consecutive vertex layers of the graph and not between edges of the same layer. This follows from the fact that edges only exist between vertices which differ by one bit; that is, one endpoint of an edge will contain one more one than the other. Thus, the layered graph will only contain edges between

consecutive layers. It is readily apparent then that the graph of a hypercube is also bipartite.

	00	000	0000	00000
	01	001	0001	00001
	11	011	0011	00011
	01	111	0111	00111
n=2		110	1111	01111
		100	1110	11111
		n=3	1100	11110
			1000	11100
			n=4	11000
				10000
				n=5
Length:	4	6	8	10

Figure 6. Queue Gray Code Cycles

The number of vertices in each layer is simply a combination of the number of ones and the dimension of the graph. The i^{th} vertex layer of a hypercube contains $\binom{n}{i}$ vertices and between vertex layers i and $i + 1$ there exists an edge layer containing $\binom{n}{i}(n - i)$ or equivalently $\binom{n}{i+1}(i + 1)$ edges.

4.2. Hamiltonicity of Hypercubes

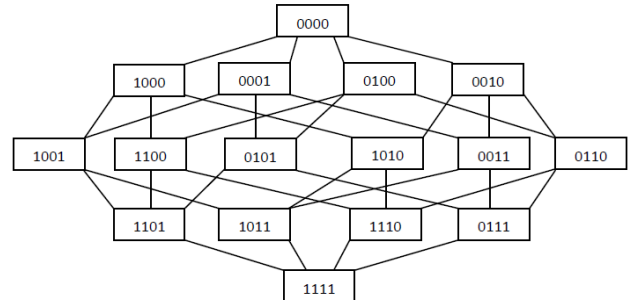


Figure 7. Layered Hypercube Graph of Q_4

A Hamiltonian path can easily be found in a Hypercube Q_n by considering the Gray code sequence of length n . Beginning at the origin, the vertex whose word is a string of n zeros, each consecutive vertex in the path is simply the consecutive Gray code word. These vertices will be adjacent because their binary strings differ by a single bit (as per the definition of Gray code). Since a Gray code sequence will exist through all 2^n possible strings, it follows that a Hamiltonian path will exist.

It can similarly be shown that the hypercube is Hamiltonian. In this case we simply consider the reflected Gray code sequences. Again, because this cyclic sequence exists and is of length 2^n , a Hamiltonian cycle will exist in Q_n .

5. The Middle Level (Layer) Graph

The middle level graph M_n is a subgraph of Q_n containing those vertices in levels $\lfloor \frac{n}{2} \rfloor$ and $\lfloor \frac{n}{2} \rfloor + 1$ and the edges between them. When n is even however, $\lfloor \frac{n}{2} \rfloor = \lfloor \frac{n}{2} \rfloor + 1$ and the subgraph contains only vertices on a single middle layer. Since no edges exist between vertices in the same vertex layer, each vertex will have a degree of zero and the graph will be completely disconnected. No Hamiltonian path or cycle could possibly exist. When n is odd, Hamiltonicity is less clear.

5.1. The Middle Level Conjecture

As there is not too much to be said about the middle layer graphs when n is even, the Middle Level Conjecture considers only graphs where the dimension is odd. As previously stated, the Middle Level Conjecture says that for every odd $n \geq 3$, M_n is Hamiltonian.

When $n = 3$, the only Hamiltonian cycle in M_3 is rather trivial as it is also an Euler path and the total number of edges is only 6 (middle level of Fig. 2). It is considerably more difficult to locate a Hamiltonian cycle in M_5 , despite the fact that the graph contains several such cycles (Fig. 9).

5.2. Edge Colouring

An approach proposed by Parkhomenko for classifying the Hamiltonian cycles in hypercubes is to classify the edges of the graph rather than to simply focus on the vertices [6]. What he proposed was to assign a weight to each of the edges based upon the axis it was parallel to. In terms of the binary string, this would be assigning a weight to an edge based on the position of the bit which changes over the edge. The weight of an edge joining two adjacent vertices which differ in the i^{th} bit, is equivalent to the weight of the i^{th} position in the string.

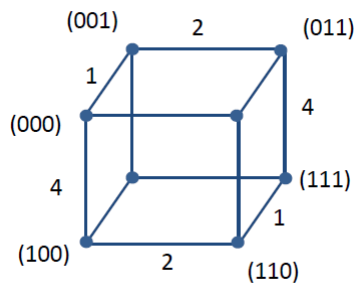


Figure 8. Edge Weights in Q_3

For example, consider that graph of a standard cube (Fig. 8). The number of axes is equal to the dimension of the cube and the length of each of the vertex words; in this case three. The x -axis is represented by the first bit in the string, the y -axis the second, and the z -axis the third. An edge that represents a change in the first bit will be parallel to the x -axis and have a weight of 2^2 . Similarly the y -axis parallel edges have a weight of 2^1 and the z -axis 2^0 . Each of the different weights can be assigned a unique colour.

What is more, in the case of M_3 the Hamiltonian path is a sequence of alternating colours $(2^0, 2^1, 2^2)$ and the graph contains the same number of edges of each colour. This is also the case with M_5 . Though there does not appear to be a clear pattern between the edge colours in the Hamiltonian cycles, there remains four edges of each colour in the cycles.

5.3. Proposition 1

Each edge level of Q_n contains an equal number of edges of each colour.

Proof (Please refer to Fig. 7)

Let VLi refer to vertex level i and ELj refer to edge level j which resides between $VL(j-1)$ and VLj . Each of the j ones in VLj will refer to an edge in ELj and following the edge to $VL(j-1)$ will result in a string missing one of the ones. Recall the position of the missing one determines the colour of the edge. We also know that each vertex will contain an edge of every colour, each corresponding to the axis represented by the changing bit.

Beginning with $EL1$, $VL1$ contains exactly $\binom{n}{1}$ vertices representing each of the n possible positions of the ones bit in the word. It follows then that $EL1$ contains a single edge of each colour.

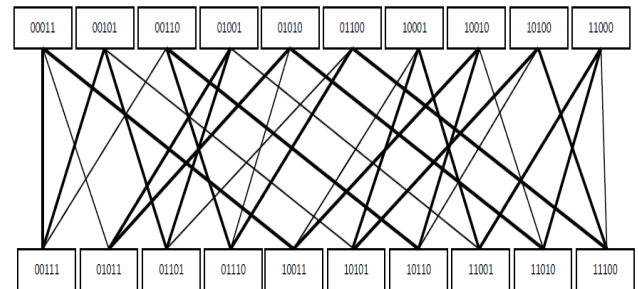


Figure 9. Hamiltonian Path in M_5

Moving down to $EL2$, $VL2$ contains exactly $\binom{n}{2}$ combinations of positions for the two ones in the words. Each of the $\binom{n}{2}$ vertices will be adjacent to a pair of uniquely coloured edges in $EL2$. By fixing one colour and choosing another from the remaining $(n-1)$ we get that there are $\binom{n-1}{1} = n-1$ edges of each colour. Looking up to $VL1$ it can be seen that an edge of each colour extends down from each of the vertices to a vertex in $VL2$ except for the vertex in $VL1$ which is adjacent to $VL0$ by an edge of that colour. The total number of edges in $EL2$ is confirmed by multiplying the number of vertices in $VL2$ by their degree in $EL2$: $n(n-1) = 2\binom{n}{2}$.

Similarly, $VL3$ contains $\binom{n}{3}$ different vertices each containing a unique set of three coloured edges in $EL3$, $\binom{n-1}{2}$ edges of each colour exist in $EL3$, and the total number of edges in $EL3$ is equal to the product of number of edges of each colour and the number of colours: $n\binom{n-1}{2}$.

The number of edges of each colour in EL_j is $\binom{n-1}{j-1}$. Therefore, there are an equal number of edges of each colour in each of the edge layers.

5.4. Proposition 2

Each Hamiltonian cycle in M_n contains an equal number of edges of each colour.

Proof

The middle level graph contains two sets of vertices; one containing $\lfloor \frac{n}{2} \rfloor$ ones and $\lfloor \frac{n}{2} \rfloor$ zeros and the other containing $\lfloor \frac{n}{2} \rfloor$ zeros and $\lfloor \frac{n}{2} \rfloor$ ones. Suppose we fix the a^{th} ($0 \leq a \leq n$) bit of a vertex in the first set to one and the a^{th} bit of a vertex in the second set to a zero. It follows then $\binom{n-1}{\lfloor \frac{n}{2} \rfloor - 1}$ strings from the first set will contain a one in the a^{th} bit position and $\binom{n-1}{\lfloor \frac{n}{2} \rfloor - 1}$ strings from the second set will contain a zero in the a^{th} bit position. Similarly, the number of strings from the first set containing a zero in a^{th} bit position is equal to the number of strings from the second set containing a one in the a^{th} position: $\binom{n-1}{\lfloor \frac{n}{2} \rfloor - 1}$. Thus, the total number of strings in the middle level containing a one in the a^{th} bit position equals the total number of strings containing a zero in that position, and there are an equal number of zeros and ones in each position.

Since the Hamiltonian cycles of the graph contain each of the vertices of the graph, the number of bit changes for each position must be the same. This implies the number of edges of each colour is the same.

6. Computational Pattern Search

With code provided by Dr. Markov of Sofia University[5], Hamiltonian cycles were generated for M_5 and M_7 . The growth of the number of Hamiltonian cycles as the dimensions of the graphs increases is rather fantastic. It is clear that M_3 contains only one Hamiltonian Path, and for M_5 there are 24 Hamiltonian Cycles. For M_7 however, there are millions. All 24 paths for M_5 were generated with the provided code within a matter of seconds. After running the program for just shy of three straight days, 746692 Hamiltonian cycles were found for M_7 before the program was stopped.

Using the collected data, subsequent programs were developed to search the cycles for particular properties within. Various queue Gray code properties were searched as well as the antipodal property.

6.1. k -shift Queue Gray Code

As earlier stated, a queue Gray code sequence is a sequence of binary strings in which consecutive words differ by a single bit and are constructed by removing the most significant bit, shifting the remaining bits one digit left and,

appending a new least significant bit. Since '101' is an illegal substring, and M_5 will contain the string '10101' M_5 cannot contain a Hamiltonian path which is a queue Gray code sequence. Similarly, M_7 contains the string '1010101' and any larger middle layer graph will contain a similar illegal string.

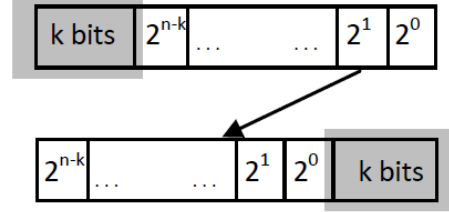


Figure 10. Generalized k -shift Queue Gray code

Consider, alternatively, what would occur if the shift was generalized. Suppose that rather than considering a bit shift of one, a shift of two or three was considered. Let k be the number of bits to be shifted, and a k -shift refer to a queue Gray code shift of k bits (Fig. 10). As earlier stated, no cycles will exist when $k = 1$. In the case where a 2-shift was considered, the program found no cycles in M_5 or M_7 containing the queue Gray code shift. This too makes sense considering a substring of '0011' will exist in at least one of the vertices' strings and this substring, if a 2-shift is applied, will fail to be a Gray code transition. Moving to a 3-shift, again no cycles were found. This is reasonable given that some vertex will contain the substring '00011'. If a 3-shift is applied to the word containing this substring then the two words will fail to be a Gray code sequence.

Given the failure on all accounts where the shift is less than or equal to $\lfloor \frac{n}{2} \rfloor$, we consider the case where any of the three shifts is acceptable. That is, between any consecutive vertex strings, a 1-shift, 2-shift, or a 3-shift is permitted. This too failed to produce any results. There was no cycle in M_5 found to contain the property and none of the produced cycles for M_7 did either. Looking closer into the case of M_5 the reason for this is evident. All of the Hamiltonian cycles in M_5 contain at least one of the following pairs of consecutive vertices (decimal): 3-19, 3-11, 7-5, or 7-6. Looking at their binary equivalents (Table 2) it is clear that all these consecutive words do not contain any k -shift for $k = 1, 2, 3$.

Table 2. Consecutive Vertices of M_5

Consecutive Words ($a - b$)	Binary Equivalent of a	Binary Equivalent of b
3-19	00011	10011
3-11	00011	01011
7-5	00111	00101
7-6	00111	00110

6.2. Antipodal Paths/Cycles

A cycle is known as antipodal if opposite nodes of the cycle are complementary bit strings. When the nodes are binary strings this simply means that opposite strings hold

zeros and ones in opposite positions and the sum of the two strings will be a string of all ones (the largest binary number possible for strings of that length). For example, consider the middle level graph in the third dimension. When each of the six binary strings are arranged evenly in a circular pattern the opposite vertices have a sum of '111'. In the positions where one of the strings has zeros, its opposite string holds ones and where this string holds zeros the other has ones (Fig. 11). This idea can easily be extended to paths by considering opposite vertices to be those separated by $\binom{n}{2} - 1$ strings, where n is the even number of strings in the sequence and each vertex is represented by string.

Table 3. Antipodal Hamiltonian Cycle in M_7

Opposite Vertices in Cycle (a,b)	String at Vertex a	String at Vertex b
1,36	0000111	1111000
2,37	1000111	0111000
3,38	1000011	0111100
4,39	1100011	0011100
5,40	0100011	1011100
6,41	0110011	1001100
7,42	0010011	1101100
8,43	1010011	0101100
9,44	1010001	0101110
10,45	1110001	0001110
11,46	0110001	1001110
12,47	0111001	1000110
13,48	0011001	1100110
14,49	1011001	0100110
15,50	1011000	0100111
16,51	1011010	0100101
17,52	1001010	0110101
18,53	1001011	0110100
19,54	1001001	0110110
20,55	1001101	0110010
21,56	1000101	0111010
22,57	1010101	0101010
23,58	1010100	0101011
24,59	1010110	0101001
25,60	1010010	0101101
26,61	1110010	0001101
27,62	1100010	0011101
28,63	1101010	0010101
29,64	1101000	0010111
30,65	1101001	0010110
31,66	1100001	0011110
32,67	1100101	0011010
33,68	1100100	0011011
34,69	1110100	0001011
35,70	1110000	0001111

As it is clear from Fig. 11, the antipodal property holds for the Hamiltonian cycle in the middle level of a 3-dimensional cube. For the middle level graphs of higher dimension where there are more Hamiltonian cycles, whether an antipodal one exists or not, is not so apparent.

We developed a program to search for this property in M_5 and M_7 . Results reveal that no Hamiltonian cycle in M_5 is antipodal. However, there were numerous, at least thousands,

of cycles in M_7 which were. One such cycle is given in Table 3 below.

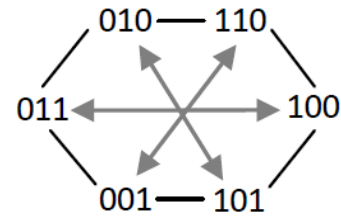


Figure 11. Antipodal Property of M_3

7. Conclusions

The difficulty in solving the middle level conjecture lies in part in the fact that patterns are difficult to find. There doesn't appear to be any clear consistent pattern among the Hamiltonian cycles of the middle level graphs. Though all such cycles will inevitably be cyclic Gray code sequences, every path within any binary hypercube will also be a Gray code sequence. However, it can be said that like the hypercube, and the middle level graph, every Hamiltonian cycle in a middle level graph will contain an equal number of edges of each colour when colouring is based on the weight of the bit being changed between the adjacent vertices. As far as queue Gray code is concerned, no patterns can be found (within the first three middle level graphs at least) as no queue Gray code cycles could be found even with a flexible bit shift. Antipodal cycles however, do exist but not consistently throughout all dimensional graphs. The elusive nature of the Hamiltonian cycle in middle level graphs makes it difficult to derive any feasible algorithmic method for their discovery.

To put this in a larger context, the study of the Middle Level Conjecture has contributed new ideas and methods to combinatorics [8]. As we already mentioned, the computational results strengthen the belief that the conjecture is true. If and when it is finally settled this will not be a breakthrough. However, the work on it during the last three decades has illuminated other areas and influenced them. One of the primary beneficiaries is the study of Gray codes. The general question here, given the hamiltonicity of the binary hypercube is to find smaller/restricted structures [12] that admit Gray codes (the middle level is one of them), and conversely find a structure in Gray codes that have certain restrictions imposed on them: the queue property, the generalized queue property or similar. To this end, we would like to mention that it is conjectured that a Hamiltonian cycle exists not only in the k -th and $(k + 1)$ -st level of the $(2k + 1)$ -dimensional hypercube, but between the k -th and $(n - k)$ -th level of the n -dimensional hypercube under the generalized notion of adjacency through $(n - 2k)$ bit flips instead of a single bit flip. Many research articles in recent years [7, 9, 10, 11, 13, 14] offer methods for finding large cycles in the middle layer and hope that these techniques can be extended towards general proof of hamiltonicity.

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