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Spectral graph theory of the Hypercube

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THESIS

SPECTRAL GRAPH THEORY OF THE HYPERCUBE

by

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December 2008

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In Graph Theory, every graph can be expressed in terms of certain real, symmetric matrices derived from the graph, most notably the adjacency or Laplacian matrices. Spectral Graph Theory focuses on the set of eigenvalues and eigenvectors, called the *spectrum*, of these matrices and provides several interesting areas of study. One of these is the *inverse eigenvalue problem* of a graph, which tries to determine information about the possible eigenvalues of the real symmetric matrices whose pattern of nonzero entries is determined by a given graph. A second area is the *energy* of a graph, defined to be the sum of the absolute values of the eigenvalues of the adjacency matrix of that graph.

Here we explore these two areas for the hypercube Q_n, which is formed recursively by taking the Cartesian product of Q_{n-1} with the complete graph on two vertices, K_2. We analyze and compare several key ideas from the inverse eigenvalue problem for Q_n, including the maximum multiplicity of possible eigenvalues, the minimum rank of possible matrices, and the number of paths that occur both as induced subgraphs and after deleting certain vertices. We conclude by deriving several equations for the energy of Q_n.

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SPECTRAL GRAPH THEORY OF THE HYPERCUBE

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Submitted in partial fulfillment of the
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I. INTRODUCTION

A. PURPOSE

The hypercube, denoted Q_n, is a graph of remarkable properties and numerous applications in coding, computer science, and other areas of mathematics. In this paper, we analyze Q_n from the point of view of spectral graph theory. Specifically, in Chapter I, we derive the adjacency and Laplacian matrices for Q_n. Once we have constructed these matrices, we show what their associated eigenvalues are, along with their multiplicities, as well as derive the associated eigenvectors. In Chapter II, we consider the inverse eigenvalue problem (IEP) for the hypercube. In spectral graph theory, the usual focus is on obtaining information about a graph from the associated matrices. In the IEP, almost the opposite is done. Here, we seek to determine information about the possible spectra of the matrices whose pattern of non-zero entries is described by a given graph, in this case, the hypercube. A great deal of work has been done on this problem with respect to numerous other types of graphs, most notably trees [1], but little has been done with Q_n. During this analysis, we focus on four main concepts: the maximum multiplicity of eigenvalues, the minimum rank of a certain associated set of matrices, the path cover number for Q_n, and the path vertex-deletion number for Q_n. We provide an upper bound for the minimum rank of graph Cartesian products of graphs and also show that for Q_n, $n > 2$, the maximum multiplicity of an eigenvalue is greater than the path cover number which is greater than the path vertex–deletion number. Finally, in Chapter III, we discuss the concept of the energy of a graph and derive several equations for determining the energy of Q_n.

B. GRAPH THEORY

Here we define some of the fundamental concepts and definitions of graph theory that we use in this paper; for terminology not defined here, refer to a standard graph theory text such as Chartrand & Zhang's *Introduction to Graph Theory* [2].

Formally, a graph G = (V(G), E(G)) consists of a finite nonempty set V(G) of *vertices* and a set E(G) of two-element subsets of V(G) called *edges*. A graph is a *directed graph* (or diagraph) when the two-element subsets of the set E(G) are ordered pairs, and the graph is *undirected* otherwise. Two vertices are *adjacent* if they are joined by a single edge. For undirected graphs, the *degree* of a vertex is the number of edges incident to that vertex. For directed graphs, the degree at each vertex is the number edges oriented toward that vertex, called the *in-degree*, minus the number of edges oriented away from that vertex, called the *out-degree*. A graph is called *regular* if the degree of every vertex is the same. A *walk* in a graph is defined as a sequence of vertices such that the consecutive vertices in the sequence are adjacent. A *trail* is a walk in which no edge is traversed more than once and a *path* is a walk such that no vertices are repeated. We denote a graph consisting of only one path by P_n, where n is the number of vertices. If a graph contains a path between every pair of vertices, the graph is *connected*, otherwise the graph is *disconnected*. The *distance* between two vertices is defined as the shortest path between those vertices and we define the *diameter* of a connected graph to be the greatest distance between any two vertices. A trail of three or more vertices containing repeated vertices is called a *circuit*. We define a *cycle* to be a circuit in which no vertex repeats except that the first vertex equals the last. A *complete graph*, denoted K_n where n is the number of vertices, is one in which every vertex is connected to every other vertex in the graph. A graph H is called a *subgraph* of graph G if G contains all the vertices and edges of H. H is called an *induced subgraph* of G if, for whichever vertices of G that H contains, H also contains the same edges incident to those vertices as G. If either V(H) is a proper subset of V(G) or E(H) is a proper subset of E(G), then H is a *proper subgraph* of G. A connected subgraph that is not a proper subgraph of any other connected subgraph is called a *component*. An *automorphism* of a graph G is defined as a mapping of the vertices of G onto themselves while maintaining vertex adjacency. A *vertex-transitive* graph is a graph G such that, given any two vertices a and b of G, there is an automorphism f: V(G) →V(G) such that f(a) = b.

C. MATRIX THEORY

Matrix theory, generally considered a sub-branch of linear algebra, is the branch of mathematics that studies matrices, which are collections of numbers arranged into a fixed number of rows and columns. Throughout this thesis, we use several fundamental concepts from matrix theory; for definitions of these concepts, please refer to any standard linear algebra text such as Leon's *Linear Algebra With Applications* [3]. Specifically, we use such concepts as square matrices, symmetric matrices, the set of eigenvalues of a matrix (also called the spectrum), and the associated eigenvectors.

D. SPECTRAL GRAPH THEORY

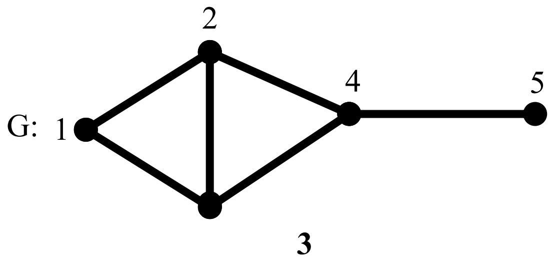
Spectral graph theory is where graph theory and matrix theory meet. Given a graph G, spectral graph theory is the study of the spectrum of the *adjacency matrix* of G, denoted as Spec(G), as well as the study of the spectra of the *incidence* and *Laplacian matrices*. We now define these matrices.

1. Adjacency Matrices

The adjacency matrix A_G of an undirected graph G with n vertices is the $n \times n$ symmetric matrix $A_G = [a_{i,j}]$, where

$$a_{i,j} = \begin{cases} 1, & \text{if } (i,j) \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

In other words, if two vertices are adjacent, then the corresponding entry in the associated matrix is a one, and the corresponding entries for all non-adjacent vertices as well as the main diagonal of the matrix are all zeros. Figure 1 shows an example of a graph and its associated adjacency matrix.



$$A_G = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Figure 1. Graph G with Associated Adjacency Matrix A_G.

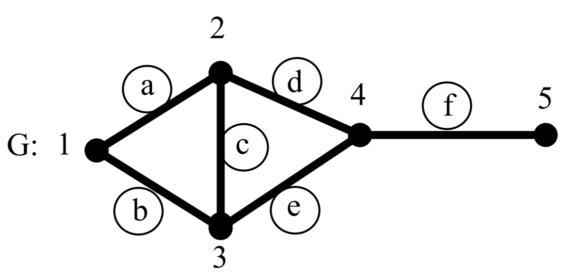
2. Incidence Matrices

a. For Undirected Graphs

The incidence matrix B_G of an undirected graph G with *n* vertices and *m* edges is the *n* x *m* matrix $B_G = [b_{i,j}]$, where

$$b_{i,j} = \begin{cases} 1, & \text{if } v_i \text{ is incident with } e_j \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, in addition to labeling the vertices, we must also label the edges. Then, once the labeling is complete, we develop a matrix where the rows represent the vertices and the columns represent the edges. If an edge is incident to a vertex in the graph, then there is a one in the corresponding entry of the matrix, otherwise the entry is zero. Figure 2 shows the graph from the previous example, but this time with its associated incidence matrix.



$$B_G = \begin{array}{c} \\ \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \\ \mathbf{4} \\ \mathbf{5} \end{array} \begin{array}{c} \begin{array}{cccccc} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} & \mathbf{f} \end{array} \\ \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

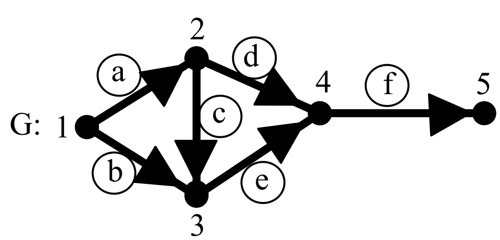
Figure 2. Graph G with Associated Incidence Matrix B_G.

b. For Directed Graphs

The incidence matrix D_G of an directed graph G with *n* vertices and *m* edges is the *n* x *m* matrix $D_G = [d_{i,j}]$, where

$$d_{i,j} = \begin{cases} 1, & \text{if } e_j \text{ points towards } v_i \\ -1, & \text{if } e_j \text{ points away from } v_i \\ 0, & \text{otherwise.} \end{cases}$$

Figure 3 shows an orientation of the graph in the previous two examples and its associated incidence matrix.



$$D_G = \begin{array}{c} \\ \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \\ \mathbf{4} \\ \mathbf{5} \end{array} \begin{array}{c} \begin{array}{cccccc} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} & \mathbf{f} \end{array} \\ \begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

Figure 3. Directed Graph D with Associated Incidence Matrix D_G.

3. Laplacian Matrices

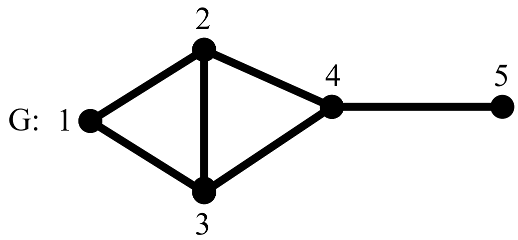
The Laplacian Matrix of a graph G, denoted L_G, can be obtained in several ways.

a. Directly from the Definition

The Laplacian matrix L_G of a graph G with *n* vertices and *m* edges is defined to be the *n* x *n* symmetric matrix $L_G = [l_{i,j}]$, where

$$l_{i,j} = \begin{cases} -1 & \text{if } (i,j) \in E(G), \\ \text{degree of } v_i & \text{if } i = j, \\ 0 & \text{otherwise} \end{cases} \quad [4].$$

Figure 4 shows the same graph as in the previous examples, but now with its Laplacian Matrix.



$$L_G = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & -`1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \end{array}$$

Figure 4. Graph G with Associated Laplacian Matrix L_G.

b. From the Adjacency Matrix

Equivalently, the Laplacian Matrix can be formed by taking $L_G = \Delta - A_G$, where Δ is a diagonal matrix with the entries on the diagonal equal the degree of the corresponding vertex.

$$L_G = \Delta - A_G = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & -`1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}.$$

c. From the Directed Incidence Matrix

The Laplacian Matrix can also be found by multiplying the directed incidence matrix by its transpose. In other words, $L_G = (D_G)(D_G)^T$.

$$L_G = \begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & -`1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}.$$

E. CARTESIAN PRODUCTS OF GRAPHS

For two graphs G and H, the Cartesian product G x H has vertex set V(G x H) = V(G) x V(H), that is, every vertex of G x H is an ordered pair (u,v), where $u \in$ V(G) and $v \in$ V(H). Two distinct vertices (u,v) and (x,y) are adjacent in G x H if either:

1. $u = x$ and $vy \in$ E(H), or
2. $v = y$ and $ux \in$ E(G).

Figure 5 is an example of the Cartesian product of two graphs.

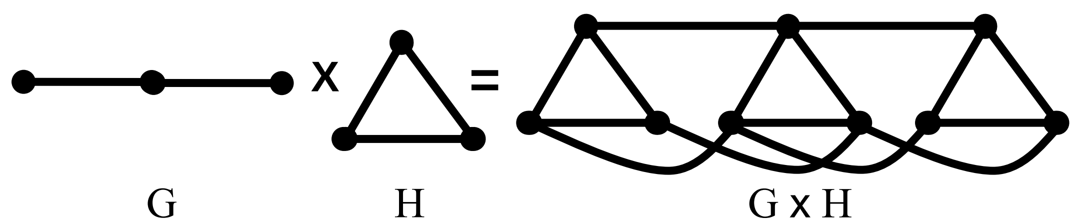


Figure 5. Cartesian Product of Graphs G and H

There are several properties and theorems in Spectral Graph Theory based on Cartesian products that will prove useful later in the paper; these will be introduced when needed. Using this notion of graph Cartesian products, we now arrive at the graph that is the focal point of this paper, the hypercube Q_n.

F. HYPERCUBES

1. Formally Defined

We define Q_1 to be K_2 and, for $n \geq 2$, define Q_n by $Q_n = Q_{n-1} \times K_2$ [2]. The hypercube Q_n may also be defined non-recursively as the graph whose vertex set V_n consists of the 2^n n-tuples with coordinates 0 or 1, where two vertices are adjacent whenever their respective vectors differ in exactly one coordinate. The hypercube Q_n for n = 1, 2, and 3 are shown in Figure 6.

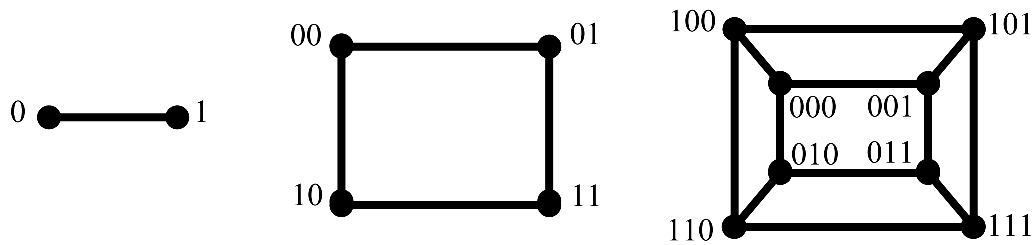


Figure 6. Hypercubes Q_1, Q_2, and Q_3.

2. Basic Properties of the Hypercube

Here we note three basic properties of the hypercube that will be useful later.

a. Regularity

Hypercubes are regular graphs and the degree of each vertex of Q_n is equal to n. As seen in Figure 6, the degrees of Q_1, Q_2, and Q_3 are 1, 2, and 3 respectively.

b. Bipartiteness

Hypercubes are also bipartite, i.e. the vertex set of the graph can be partitioned into two subsets, where, within each set no vertices are adjacent. Furthermore, for the hypercube, the cardinalities of these sets are equal, so exactly half of the vertices are in each bipartite set. Therefore, each set has 2^{n-1} vertices. In Figure 7, Q_3 is drawn in two ways, the second emphasizing the bipartition.

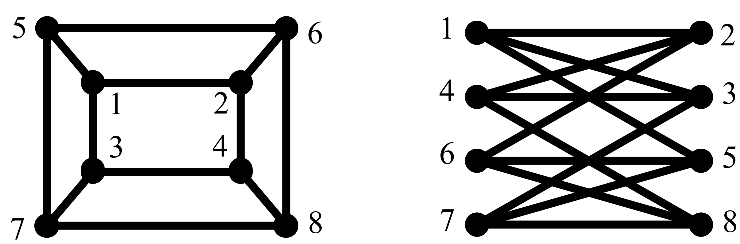


Figure 7. Q_3 Drawn Showing Bipartite Structure.

c. Vertex Transitivity

Hypercubes are vertex-transitive graphs, i.e. given any two vertices in Q_n, there is an automorphism mapping one vertex to the other while maintaining vertex adjacency.

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II. THE MATRICES AND SPECTRA OF HYPERCUBES

A. THE ADJACENCY MATRIX OF Q_n

By inspection of Figure 6, we can see that Q_1 has the following adjacency matrix:

$$A_{Q_1} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

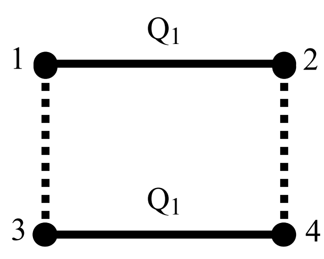
and that Q_2 has the following adjacency matrix:

$$A_{Q_2} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

Now, if we look at A_{Q_2} in terms of 2 x 2 blocks, we see that

$$A_{Q_2} = \left[\begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array}\right] = \begin{bmatrix} A_{Q_1} & I \\ I & A_{Q_1} \end{bmatrix}$$ where I is a 2 x 2 identity matrix. We can see why this happens by considering the fact that Q_n is the Cartesian product of Q_{n-1} and K_2, $n \geq 2$. Consider Figure 8.

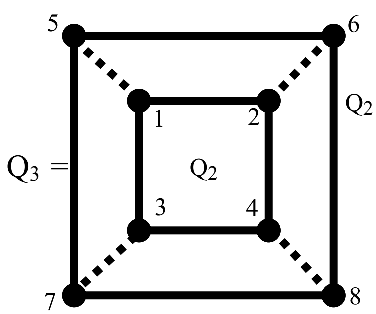
$Q_2 =$



$$A_{Q_2} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \left[\begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array}\right] \end{array}$$

Figure 8. $Q_2 = Q_1 \times K_2$ and Associated Adjacency Matrix A_{Q_2}.

When forming Q_2 from the Cartesian product $Q_1 \times K_2$, we take a second copy of Q_1, then adjoin each vertex in the second copy with its corresponding vertex in the first copy. The previous example shows this by adjoining vertex 1 to vertex 3 and vertex 2 to vertex 4. Likewise, when building the matrix for Q_3, we can see in Figure 9 that taking the two copies of Q_2 yields the upper left and lower right blocks of A_{Q3} and adjoining the appropriate corresponding vertices yields the identity matrices in the upper right and lower left blocks.



$$A_{Q_3} = \begin{array}{c|cccc|cccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 3 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 4 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ \hline 5 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 6 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 7 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 8 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{array} = \left[\begin{array}{c|c} A_{Q_2} & I \\ \hline I & A_{Q_2} \end{array}\right]$$

Figure 9. $Q_3 = Q_2 \times K_2$ and Associated Adjacency Matrix A_{Q_3}.

We can now see that the adjacency matrices for hypercubes can be built recursively with $A_{Q_n} = \begin{bmatrix} A_{Q_{n-1}} & I \\ I & A_{Q_{n-1}} \end{bmatrix}$, where I is the $2^{n-1} \times 2^{n-1}$ identity matrix [5]. In passing, we can see that this recursive structure of the adjacency matrix generalizes for any graph formed by the Cartesian product with K_2. For example, if $G = H \times K_2$, then $A_G = \begin{bmatrix} A_H & I \\ I & A_H \end{bmatrix}$.

B. THE LAPLACIAN MATRIX OF Q_n

As noted earlier, one way to construct the Laplacian matrix of a graph is to use the fact that $L_G = \Delta_G - A_G$. First, start with n = 1 to find L_{Q1}:

$$L_{Q_1} = \Delta_{Q_1} - A_{Q_1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

Now we find $L_{Q2,}$ and subsequently L_{Qn}, by examining the matrices in blocks.

$$L_{Q_2} = \Delta_{Q_2} - A_{Q_2} = \left[\begin{array}{cc|cc} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ \hline 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{array}\right] - \left[\begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array}\right] = \left[\begin{array}{cc|cc} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ \hline -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{array}\right]$$

$$= \begin{bmatrix} 2\cdot I & 0 \\ 0 & 2\cdot I \end{bmatrix} - \begin{bmatrix} A_{Q_1} & I \\ I & A_{Q_1} \end{bmatrix} = \begin{bmatrix} 2\cdot I - A_{Q_1} & -I \\ -I & 2\cdot I - A_{Q_1} \end{bmatrix}$$

In general,

$$L_{Q_n} = \Delta_{Q_n} - A_{Q_n} = \begin{bmatrix} n\cdot I & 0 \\ 0 & n\cdot I \end{bmatrix} - \begin{bmatrix} A_{Q_{n-1}} & I \\ I & A_{Q_{n-1}} \end{bmatrix} = \begin{bmatrix} n\cdot I - A_{Q_{n-1}} & -I \\ -I & n\cdot I - A_{Q_{n-1}} \end{bmatrix}.$$

Since Q_n is regular of degree n, then $\Delta_{Q_n} = n\cdot I$ and so

$$L_{Q_n} = \Delta_{Q_n} - A_{Q_n} = n\cdot I - A_{Q_n}.$$

It follows for Q_{n-1} that:

$$L_{Q_{n-1}} = (n-1)\cdot I - A_{Q_{n-1}}$$

$$= n\cdot I - I - A_{Q_{n-1}}, \text{ so}$$

$$L_{Q_{n-1}} + I = n\cdot I - A_{Q_{n-1}}.$$

Therefore, we can recursively define the Laplacian matrix of the hypercube by:

$$L_{Q_n} = \begin{bmatrix} L_{Q_{n-1}} + I & -I \\ -I & L_{Q_{n-1}} + I \end{bmatrix}.$$

C. THE EIGENVALUES OF Q_n

Now that we have properly defined the adjacency and Laplacian matrices for the hypercube, we can now analyze the eigenvalues of those matrices.

1. Eigenvalues of the Adjacency Matrix of Q_n

First, we present the eigenvalues and note the multiplicities for the adjacency matrices of Q_1 thru Q_4 followed by our observations for the eigenvalues of Q_n in Table 1 which can be verified in [6]:

n	**Eigenvalues**	**Multiplicity**
1	–1, 1	1, 1
2	–2, 0, 2	1, 2, 1
3	–3, –1, 1, 3	1, 3, 3, 1
4	–4, –2, 0, 2, 4	1, 4, 6, 4, 1
…	…	…
k	$-k, -k+2, -k+4, \ldots$ $k-4, k-2, k$	$\binom{k}{0}, \binom{k}{1}, \binom{k}{2}, \ldots \binom{k}{k-1}, \binom{k}{k}$

Table 1. Eigenvalues of the Adjacency Matrix of the Hypercube.

Because Q_n is the Cartesian product $Q_{n-1} \times K_2$, we can use [7] to note the following basic theorem about the eigenvalues of Cartesian products to derive the eigenvalues for Q_n.

Theorem 1: Let G and H be graphs with eigenvalues $\lambda_1, \ldots, \lambda_m$ and $\mu_1, \ldots, \mu_n$, respectively. The m·n eigenvalues of the Cartesian product G x H are the sums $\lambda_i + \mu_j$, for $1 \leq i \leq m$ and $1 \leq j \leq n$.

For a graph G and its associated adjacency matrix A, we will use the notation Spec(G) interchangeably with Spec(A), both representing the multiset of eigenvalues $\{\lambda_1, \lambda_2, \ldots\}$ of A. Since $K_2 = Q_1$, we can see from Table 1 that Spec(K_2) = {–1, 1}. Therefore, if we construct $Q_3 = Q_2 \times K_2$,

$$\text{Spec}(Q_3) = \{-2-1, 0-1, 0-1, 2-1, -2+1, 0+1, 0+1, 2+1\}$$
$$= \{-3, -1, -1, 1, -1, 1, 1, 3\}.$$

As observed in Table 1, the multiplicities of the eigenvalues are identical to rows of Pascal's triangle. The following theorem notes that the multiplicities for the ordered eigenvalues of the adjacency matrix of the hypercube are the binomial coefficients:

Theorem 2: If we order the n + 1 distinct eigenvalues of Q_n as $\lambda_0 \le \lambda_1 \le \ldots \le \lambda_n$, the multiplicity of λ_k is $\binom{n}{k}$, where $0 \le k \le n$ [8].

2. Eigenvalues of the Laplacian Matrix of Q_n

We can determine the Laplacian Matrices for Q_1 thru Q_4 as previously shown and, using any standard mathematics software, determine the associated eigenvalues with multiplicities which are shown in Table 2.

n	**Eigenvalues**	**Multiplicity**
1	0, 2	1, 1
2	0, 2, 4	1, 2, 1
3	0, 2, 4, 6	1, 3, 3, 1
4	0, 2, 4, 6, 8	1, 4, 6, 4, 1
…	…	…
k	0, k + 2, k + 4, . . 2k – 4, 2k – 2, 2k	$\binom{k}{0}, \binom{k}{1}, \binom{k}{2}, \ldots \binom{k}{k-1}, \binom{k}{k}$

Table 2. Eigenvalues of the Laplacian Matrix of the Hypercube.

As can be immediately observed, the eigenvalues μ_i of the Laplacian are just a shift by n from the eigenvalues λ_i of the adjacency matrix. To show why this is true, consider from basic linear algebra that if $A\mathbf{x} = \lambda\mathbf{x}$, then $(A + n \cdot I) \cdot \mathbf{x} = (\lambda + n) \cdot \mathbf{x}$. Since $L = \Delta - A = n \cdot I - A$, and because of the symmetry of the eigenvalues of A, we can see that $\mu_i = \lambda_i + n$. The following table illustrates this shift for n = 3.

Adjacency Matrix (eigenvalue = λ)	$\lambda =$	{–3,	–1,	–1,	–1,	1,	1,	1,	3}
n	n = 3								
Laplacian Matrix (eigenvalue = μ = λ + n)	$\mu =$	{0,	2,	2,	2,	4,	4,	4,	6}

Table 3. Eigenvalue Comparison of Adjacency and Laplacian Matrices for Q_3.

As shown in Table 3, since the spectrum of Laplacian matrices are just shifts from the spectrum of the adjacency matrices, each eigenvalue in the Laplacian matrix retains the same multiplicity as its corresponding eigenvalue in the adjacency matrix.

D. THE EIGENVECTORS OF Q_n

The eigenvectors of the adjacency matrix for the hypercube can also be readily determined. We once again use the fact that Q_n is the Cartesian product $Q_{n-1} \times K_2$. In general, if a graph G has an eigenvalue λ and associated eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ and if the graph H has an eigenvalue μ and associated eigenvector $\mathbf{y} = (y_1, y_2, \ldots, y_m)^T$ then the eigenvector $\mathbf{z}_{ij}$ $(1 \le i \le n,\ 1 \le j \le m)$ in the Cartesian product of G x H for eigenvalue $\lambda_i + \mu_j$ is found by $\mathbf{z}_{i,j} = \begin{bmatrix} y_{j1}\mathbf{x}_i \\ y_{j2}\mathbf{x}_i \\ \cdots \\ y_{jm}\mathbf{x}_i \end{bmatrix}$ [4], [9].

We can use this construction to derive the eigenvectors for the hypercube. Let us start by determining the eigenvectors for A_{Q_2} by taking Q_1 x K_2 where A_{Q_1} has eigenvalues λ_i and A_{K_2} has eigenvalues μ_i. The eigenvectors of A_{Q_1} are as follows:

$$\text{for } \lambda_1 = 1, \mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \text{ and for } \lambda_2 = -1, \ \mathbf{x}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

Since $Q_1 = K_2$, the eigenvectors for A_{K_2} are as follows:

$$\text{for } \mu_1 = 1, \ \mathbf{y}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \text{ and for } \mu_2 = -1, \ \mathbf{y}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

Now, we use the preceding construction to build the eigenvectors of Q_n for $n \geq 2$. For Q_2 there are $2 \cdot 2 = 4$ eigenvectors, shown in Figure 10.

$$\lambda_2+\mu_1 = 1+1 = 2 \qquad \mathbf{z}_{1,1} = \begin{bmatrix} y_1\mathbf{x}_1 \\ y_1\mathbf{x}_1 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ 1 \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\lambda_2+\mu_1 = -1+1 = 0 \qquad \mathbf{z}_{2,1} = \begin{bmatrix} y_1\mathbf{x}_2 \\ y_1\mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} \\ 1 \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix}$$

$$\lambda_1+\mu_2 = 1 - 1 = 0 \qquad \mathbf{z}_{1,2} = \begin{bmatrix} y_2\mathbf{x}_1 \\ y_2\mathbf{x}_1 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ -1 \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

$$\lambda_2 + \mu_2 = -1-1 = -2 \qquad \mathbf{z}_{2,2} = \begin{bmatrix} y_2\mathbf{x}_2 \\ y_2\mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} \\ -1 \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$$

Figure 10. Deriving the Eigenvectors for Q_2.

If we combine the eigenvectors of Q_2 into a matrix Z, where $Z = \begin{bmatrix} \mathbf{z}_{1,1} & \mathbf{z}_{2,1} & \mathbf{z}_{1,2} & \mathbf{z}_{2,2} \end{bmatrix}$, we have $Z = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$. This matrix is an example of a *Sylvester–Hadamard* Matrix. An n x n Sylvester–Hadamard matrix H_n is recursively defined by $H_n = \begin{bmatrix} H_{n-1} & H_{n-1} \\ H_{n-1} & -H_{n-1} \end{bmatrix}$ where $H_1 = [1]$. This Sylvester–Hadamard-type recursion occurs in $Q_{n-1} \times K_2$, since K_2 has eigenvectors $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$. If Q_n has eigenvectors of length 2^n, say $\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \ldots, \mathbf{z}_{2^n}$, then Q_{n+1} has eigenvectors $\begin{bmatrix} \mathbf{z}_1 \\ \mathbf{z}_1 \end{bmatrix}, \begin{bmatrix} \mathbf{z}_2 \\ \mathbf{z}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{z}_3 \\ \mathbf{z}_3 \end{bmatrix}, \ldots, \begin{bmatrix} \mathbf{z}_{2^n} \\ \mathbf{z}_{2^n} \end{bmatrix}, \begin{bmatrix} \mathbf{z}_1 \\ -\mathbf{z}_1 \end{bmatrix}, \begin{bmatrix} \mathbf{z}_2 \\ -\mathbf{z}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{z}_3 \\ -\mathbf{z}_3 \end{bmatrix}, \ldots, \begin{bmatrix} \mathbf{z}_{2^n} \\ -\mathbf{z}_{2^n} \end{bmatrix}$, all in $\mathbb{R}^{2^{n+1}}$. Thus, we can conclude that the eigenvectors for the adjacency matrix of the hypercube Q_n are given by the columns of the Sylvester–Hadamard Matrix H_n. Since the columns of Sylvester–Hadamard matrices are pairwise orthogonal, we can also conclude that the adjacency matrix for Q_n always has a complete, orthogonal set of eigenvectors. Note that for Q_1, the adjacency matrix and the Laplacian matrix both have eigenvectors $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$, and so this recursive eigenvector construction for Q_n applies to both matrices.

III. THE INVERSE EIGENVALUE PROBLEM FOR THE HYPERCUBE

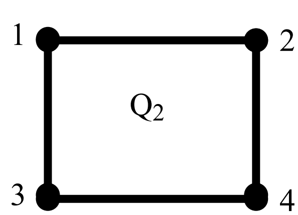
A. INTRODUCTION

In her paper, Spectral Graph Theory and The Inverse Eigenvalue Problem of a Graph [1], Hogben describes how spectral graph theory originally focused on obtaining information about the graph from examining the associated matrices (adjacency and Laplacian). The *inverse eigenvalue problem* looks at the problem the other way and tries to determine information about the possible eigenvalues of the real symmetric matrices whose pattern of nonzero entries is described by a given graph [1], [10].

First, we need to define which matrices qualify for the inverse eigenvalue problem of a graph. For a symmetric real n x n matrix B, the graph of B, G(B), is the graph with vertices {1, 2, . . . , n} and edge set $\{\{i,j\} \mid b_{ij} \neq 0 \text{ and } i \neq j\}$. We define S(G) to be the set of all real n x n matrices such that G(B) = G [1]. In other words, if A is the adjacency matrix for graph G, then B is an element of S(G) if B

1. Is real and symmetric,
2. Has the same off-diagonal zeros as A,
3. Has non-zeros where A has ones, and
4. Has arbitrary real numbers on its diagonal.

Figure 11 gives a simple example, using the hypercube Q_2, to illustrate what kinds of matrices qualify for the inverse eigenvalue problem.



$$A_{Q_2} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

$$B = \begin{bmatrix} a & e & f & 0 \\ e & b & 0 & g \\ f & 0 & c & h \\ 0 & g & h & d \end{bmatrix}$$

where a thru h are real numbers and e thru h are non zero

Figure 11. Matrix for the Inverse Eigenvalue Problem of Q_2.

Initially, this seems to include such a large number of matrices derived from each graph that it would be difficult to determine anything interesting about the corresponding possible eigenvalues of matrices in S(G). This may be true in many cases, but there has been a great deal of study done on the inverse eigenvalue problem of trees. Surprisingly, relatively little work has been done on graphs other than trees, including the hypercube. Hogben [1] defines four key terms that will help us make progress on the inverse eigenvalue problem of the hypercube:

1. The Maximum Multiplicity of a Graph, denoted M(G)
2. The Minimum Rank of a Graph, denoted mr(G)
3. The Path Cover Number, denoted P(G)
4. The Path Vertex–Deletion Number, denoted Δ(G)

1. Maximum Multiplicity M(G)

The algebraic multiplicity of an eigenvalue is simply the number of times that eigenvalue is repeated in the spectrum of that matrix, i.e., its multiplicity as a zero of the characteristic polynomial. The *maximum multiplicity* for the inverse eigenvalue problem denotes the maximum number of times we can find an eigenvalue repeated in the spectrum among all matrices $B \in S(G)$.

2. Minimum Rank mr(G)

Closely related to maximum multiplicity is the *minimum rank* of G, which refers to the lowest rank we can find among all matrices $B \in S(G)$. We note here that, from basic matrix theory, finding the matrix that yields the minimum rank is equivalent to finding the matrix with largest algebraic multiplicity of zero as an eigenvalue. Hogben showed the following fundamental theorem relating maximum multiplicity and minimum rank.

Theorem 3 [1]: M(G) + mr(G) = n (where n is the number of vertices of G, which is also the number of rows and columns in the adjacency matrix of G).

To explain this relationship between M(G) and mr(G), consider finding a matrix B* with eigenvalue λ, which has largest multiplicity, say x, among all eigenvalues of all matrices $B \in S(G)$. Since subtracting a constant multiple of the identity matrix only shifts the eigenvalues and does not change their multiplicities, we can now take $C = B^* - \lambda \cdot I$, where C has eigenvalue $\mu = 0$, also with multiplicity x. Because the diagonal is ignored in the inverse eigenvalue problem, $C \in S(G)$. Now, since C has the most zero eigenvalues of any matrix in S(G), we can see that C will yield the minimum rank of G.

3. Path Cover Number P(G)

The *path cover number* of G, P(G), is the minimum number of vertex-disjoint paths occurring as induced subgraphs of G that cover all the vertices of G.

4. The Path Vertex–Deletion Number Δ(G)

The *path vertex–deletion number* is given by

$$\Delta(G) = \max\{p - q \mid \text{there is a set of } q \text{ vertices whose deletion leaves } p \text{ disjoint paths}\}.$$

Johnson and Duarte [11] noted that a single vertex counts as a trivial path and that $\Delta(G)$ may also be described as max $[p - q]$ such that there are $n - q$ vertices of G that induce a subgraph of p components, each of which is a path. Hogben [1] point outs three basic theorems that involve these terms.

Theorem 4: For any graph G, $\Delta(G) \leq P(G)$.

Theorem 5: For any graph G, $\Delta(G) \leq M(G)$.

Theorem 6: For any tree T, $M(T) = P(T) = \Delta(T)$.

While Theorem 6 holds for trees, little is known about the relationship between M, P, and Δ for graphs in general, other than the results in Theorems 4 and 5. In cases where G is not a tree, Hogben shows one graph where $M(G) > P(G)$ and another graph where $P(G) > M(G)$ [1]. Also, since $M(G) + mr(G) = n$, what is the relation between mr(G) and $\Delta(G)$ or P(G)? From these, we draw the central question that inspires the work in the remainder of this chapter of the thesis: **What are $M(Q_n)$, $mr(Q_n)$, $P(Q_n)$, and $\Delta(Q_n)$, and what are the relationships between them?**

B. MINIMUM RANK FOR GRAPH CARTESIAN PRODUCTS

1. Background

In this section we look at the minimum rank of the hypercube from the standpoint that $Q_n = Q_{n-1} \times K_2$, for $n \geq 2$. First, we look at the adjacency matrix for Q_2. We have

$$A_{Q_2} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$ with $mr(Q_2) = 2$ and $Spec(Q_2) = \{-2, 0, 0, 2\}$. Now, if we look at $Q_3 = Q_2 \times K_2$, with $Spec(K_2) = \{-1, 1\}$, we can use Theorem 1 to show that

$$Spec(Q_3) = \{\lambda_i + \mu_j \mid \lambda_i \in Spec(Q_2), \mu_j \in Spec(K_2)\}.$$

$$= \{-2-1, 0-1, 0-1, 2-1, -2+1, 0+1, 0+1, 2+1\}$$

$$= \{-3, -1, -1, 1, -1, 1, 1, 3\}.$$

So now, under the inverse eigenvalue problem in looking at $B \in S(Q_3)$, if we take $B = A_{Q_2} + I$, then $Spec(B) = \{-2, 0, 0, 0, 2, 2, 2, 4\}$, and the three zero eigenvalues give that $mr(Q_3) \leq 5$. But Godsil shows that $mr(Q_3) = 4$ by proving the following theorem.

Theorem 7. $mr(Q_n) = 2^{n-1}$ for $n \geq 2$ [12].

Godsil is able to construct a matrix $B \in S(Q_3)$ of which four of the eigenvalues are zero (exactly half the eigenvalues) and so B has lower rank than the adjacency matrix of Q_3. Let us examine the matrix L_n that he develops to see how he accomplishes this. He defines $$L_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$ where $Spec(L_2) = \{-1, 1\}$. Constructing $H_3 = L_2 \times A_{K2}$, since $Spec(K_2) = \{-1, 1\}$, we see that $Spec(H_3) = \{-1-1, -1+1, 1-1, 1+1\}$

$$= \{-2, 0, 0, 2\}.$$

Next, $L_3 = \frac{1}{\sqrt{2}}\begin{bmatrix} L_2 & I \\ I & -L_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$ with Spec(L_3) = {–1, –1, 1, 1}.

We can see that in forming $H_4 = L_3 \times A_{K_2}$, we have

$$\text{Spec}(H_4) = \{-1-1, -1-1, -1+1, -1+1, 1-1, 1-1, 1+1, 1+1\}$$
$$= \{-2, -2, 0, 0, 0, 0, 2, 2\}.$$

Thus, since half the eigenvalues are zero, Godsil has constructed $H_3 \in S(Q_3)$ such that $\text{mr}(H_3) = 2^{n/2}$. From looking at H_3 and H_4, we can see that Godsil's construction of $L_n = \frac{1}{\sqrt{2}}\begin{bmatrix} L_{n-1} & I \\ I & -L_{n-1} \end{bmatrix}$ for $n \geq 3$ recursively builds matrices L_n that have half their eigenvalues equal to –1 and the other half equal to +1. Now, when we take $H_n = L_n \times A_{K_2}$, we can see that

$$\text{Spec}(H_n) = \begin{cases} -2, & \text{with multiplicity } 2^{n/4} \\ 0, & \text{with multiplicity } 2^{n/2} \\ 2, & \text{with multiplicity } 2^{n/4}. \end{cases}$$

Recall from Theorem 3 that $M(Q_n) + \text{mr}(Q_n) = 2^n$ (the number of vertices of Q_n). Since $\text{mr}(Q_n) = 2^{n-1}$, we can conclude that $M(Q_n) = 2^{n-1}$ as well and so $\mathbf{M(Q_n) = mr(Q_n)}$.

2. Minimum Rank for Cartesian Products

Based on the analysis of Godsil's construction, as well as Theorem 1 and Theorem 3, we can see that the minimum rank of a matrix for the inverse eigenvalue problem of the Cartesian product of two graphs is less than or equal to the order of that matrix minus the product of the maximum multiplicity of the two graphs. Godsil certainly showed that in the case of the hypercube we can do better, but the following corollary to Theorem 3 gives an upper bound for the minimum rank of any graph Cartesian product.

Corollary 8: Let G and H be two graphs with orders m and n respectively. Then $mr(G \times H) < m \cdot n - M(G) \cdot M(H)$.

Proof: Let G be a graph of order m. If M(G) = p, then we can find $A \in S(G)$ with eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_m$ such that $\lambda_1 = \lambda_2 = \ldots = \lambda_p = 0$. Next, let H be a graph of order n. If M(H) = q, then we can find $B \in S(H)$ with eigenvalues $\mu_1, \mu_2, \ldots \mu_n$ such that $\mu_1 = \mu_2 = \ldots = \mu_q = 0$. When we form the eigenvalues of G x H we have $\lambda_1 + \mu_1 = \lambda_1 + \mu_2 = \lambda_1 + \mu_3 = \ldots = \lambda_1 + \mu_q = \lambda_2 + \mu_1 = \lambda_2 + \mu_2 = \lambda_2 + \mu_3 = \ldots = \lambda_p + \mu_q = 0$, so we have $p \cdot q$ eigenvalues guaranteed to equal to zero in G x H. Now, since $p \cdot q = M(G) \cdot M(H)$, we can conclude that the minimum rank of G x H is less than or equal to the total number of eigenvalues minus the product of the number of eigenvalues equal to zero of G and H. QED.

Here is an example of the corollary: Take a graph G with five vertices and graph H with three vertices. If Spec(G) ={–1, –2, 1, 1, 1} and Spec(H) = {–1, 0, 1}, then

$$\text{Spec}(G \times H) = \{-3, -2, -2, -1, -1, 0, 0, 0, 0, 1, 1, 1, 2, 2, 2\}.$$

We can see that there is a matrix $C \in S(G \times H)$ that has a maximum multiplicity at least four and thus $mr(G \times H) \leq 15 - 4 = 11$, and we see that the corollary is satisfied:

$$mr(G \times H) \leq 11 \leq m \cdot n - M(G) \cdot M(H) = 5 \cdot 3 - 3 \cdot 1 = 12.$$

The inequality in this corollary can be strict, as we show below for Q_n.

$$2^n = mr(Q_n \times K_2) < m \cdot n - M(Q_n) \cdot M(K_2) = 2^n \cdot 2 - 2^{n-1} \cdot 1 = 2^n (2 - \frac{1}{2}) = 2^n \left(\frac{3}{2}\right).$$

C. COMPARING $M(Q_n)$, $P(Q_n)$, AND $\Delta(Q_n)$

1. Introduction

In this section we explore the relationship between the maximum multiplicity $M(G)$, the path cover number $P(G)$, and the path vertex-deletion number $\Delta(G)$ for hypercubes. Hogben [1] points out that for any graph G we have $\Delta(G) \leq P(G)$. For trees these three quantities are equal, but little is known about their relationship on other graphs [1]. Here we analyze each of these three values for Q_n and show that $M(Q_n) > P(Q_n) > \Delta(Q_n)$ for all $n \geq 3$.

2. The Maximum Multiplicity of Q_n

As we have presented, Godsil proves that $M(Q_n) = 2^{n-1}$ for all $n \geq 1$. Here we simply list the results for n = 1 to n = 5 for subsequent comparison.

n	**$M(Q_n)$**
n = 1	1
n = 2	2
n = 3	4
n = 4	8
n = 5	16

Table 4. Maximum Multiplicity $M(Q_n)$ for $1 \leq n \leq 5$.

3. The Path Cover Number of Q_n for $1 \leq n \leq 3$

We begin our analysis by stating the obvious case: $P(Q_1) = 1$, since $Q_1 = P_2$.

Next, we can see that for both $P(Q_2)$ and $P(Q_3)$, using just one path would create an induced cycle, so $P(Q_2), P(Q_3) > 1$. Since we can cover both Q_2 and Q_3 with two paths, we can conclude that $P(Q_2) = P(Q_3) = 2$. See Figure 12. Additionally, we can see that $M(Q_n) = P(Q_n)$ for n = 1, 2.

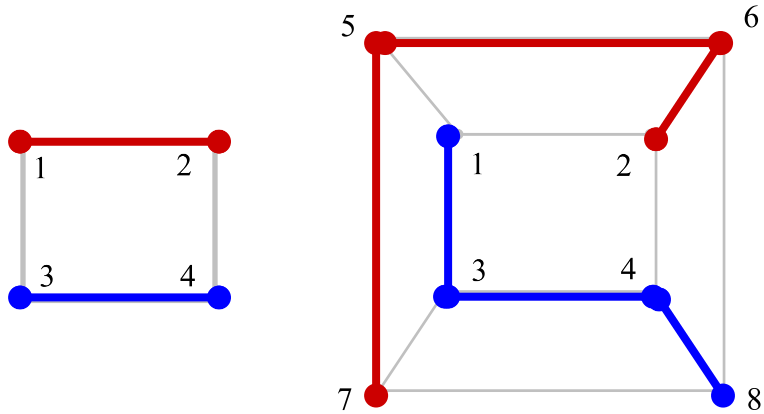


Figure 12. Path Coverings showing $P(Q_2) = P(Q_3) = 2$.

4. The Relationship Between $M(Q_n)$ and $P(Q_n)$ for $n \geq 3$

Theorem 9: If $n \geq 3$, $M(Q_n) > P(Q_n)$.

Proof: First, note that $M(Q_3) = 4 > 2 = P(Q_3)$. Now consider $Q_4 = Q_3 \times K_2$. If we simply apply the construction for $P(Q_3)$ to both copies of Q_3 in Q_4 we can see that it must be the case that $P(Q_4) \leq 4$. This is actually a loose bound; we will show later that $P(Q_4) = 3$, but $P(Q_4) \leq 4$ suffices for this proof.

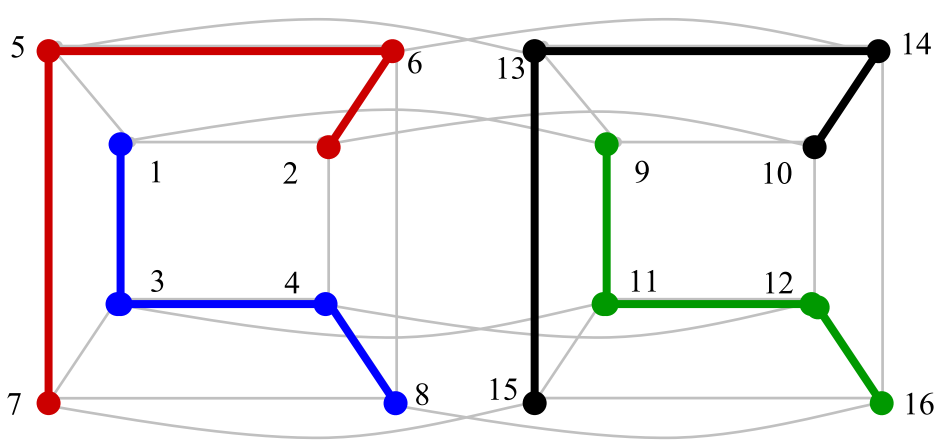


Figure 13. A Path Covering of Q_4 showing that $P(Q_4) \leq 4$.

Now, if we apply the same construction again recursively using paths of length 4, we can see that $P(Q_5) \leq 8$:

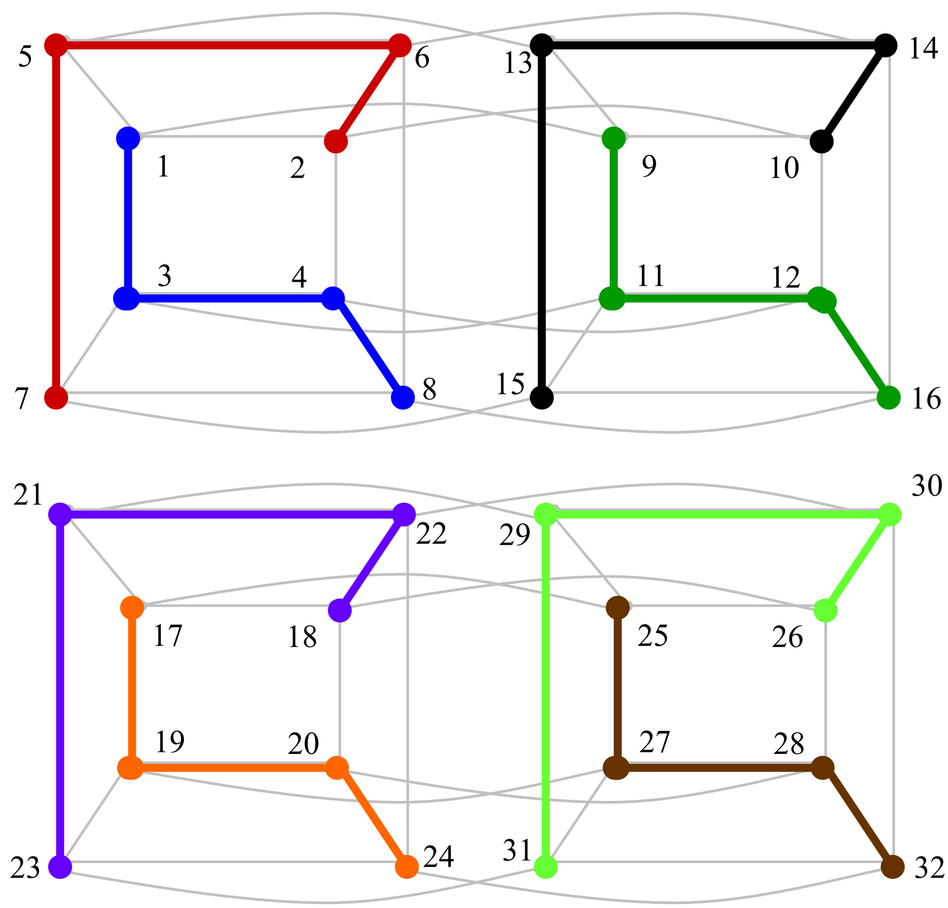


Figure 14. A Path Covering of Q_5 showing that $P(Q_5) \leq 8$.

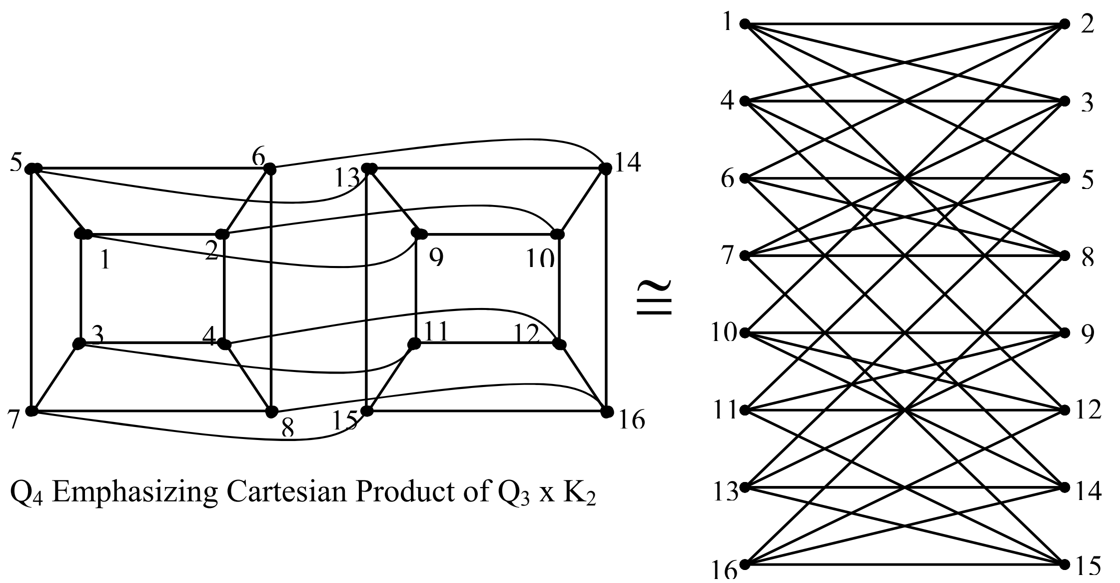
Again, as with the case of Q_4, this is a fairly loose upper bound as we will later show that $P(Q_5) = 3$. So, as we continue this recursive process for each successive Q_n, we obtain that $P(Q_n) \leq 2^{n-2}$. Since Godsil showed that $M(Q_n) = 2^{n-1}$, we can conclude that $M(Q_n) = 2^{n-1} > 2^{n-2} \geq P(Q_n)$. QED.

5. The Path Cover Number of Q_4

Developing the proper path covering for Q_4 and higher order becomes more difficult. The main issue is that, because of the large number of cycles in Q_n, as we progress along a path we soon run out of vertices that would not generate a cycle in the resulting induced subgraph and thus eliminate the path from consideration. In the previous section we showed that $P(Q_4) \leq 4$. We now show that $P(Q_4) > 2$. We proceed using a constructive, exhaustive proof that has two parts. First, we demonstrate that the longest "allowed paths" (i.e. the longest vertex disjoint paths occurring as induced subgraphs) in Q_4 are of length eight. Thus, the only way we could properly cover the 16 vertices of Q_4 in two paths is for the second path to also be of length eight. We will show in the second part of the proof that in every case, the remaining eight vertices cannot be connected by a single path.

a. The Longest Path in Q_4 is Length Eight

We exploit the fact that the hypercube is bipartite, and redraw it as shown in Figure 15.



Q_4 Emphasizing Cartesian Product of Q_3 x K_2

Q_4 Emphasizing Bipartite Structure

Figure 15. Q_4, Drawn to Show Bipartite Structure.

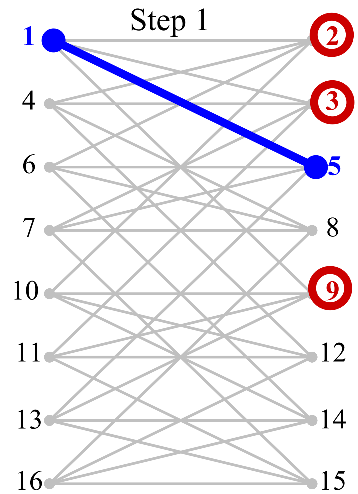
Next, to begin our path, and without loss of generality, we start at vertex 1. As we proceed along the path, once we choose each successive vertex we eliminate the other neighbors of its predecessor from later joining the path, since this would induce a cycle. For instance, if we travel from vertex 1 to 2, we eliminate the other neighbors of vertex 1, which are vertices 3, 5, and 9. We will show later in part c that in every case, as the path reaches length eight, we eliminate eight vertices as well, thus leaving no more vertices to continue the path.

b. The Remaining Eight Vertices

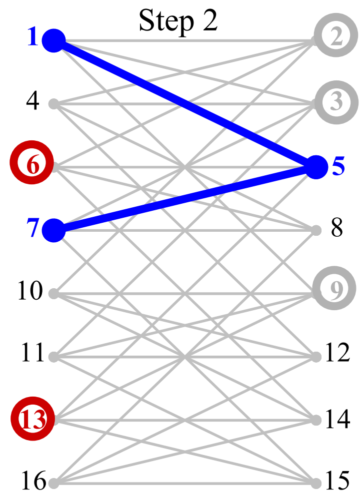
Given that the longest path in Q_4 is of length eight, since there are 16 vertices total, in order to achieve $P(Q_4) = 2$ the other path must also be of length eight. We find in every case, though, that in the set of eight remaining vertices there is at least one vertex that has three neighbors in the same set, and so that vertex would have degree three in an induced subgraph. But in a path the only possible degrees are one for the end vertices and two for all others. Therefore, the remaining eight vertices cannot form a single path.

c. Example Showing Construction for the Proof

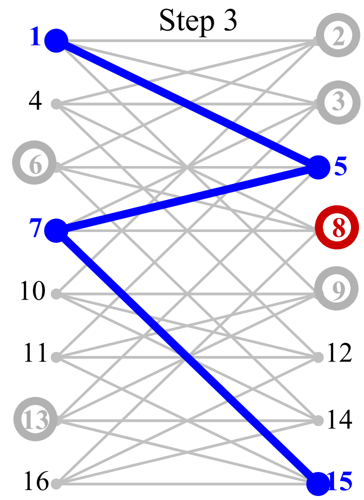
We now begin the construction of a path of length eight in Figure 16. The path is denoted in blue, and the circled red vertices are those eliminated from possible inclusion in our path due to the fact that they would create a cycle. The following figure has nine steps. The first seven steps denote the construction of a path of length eight and the last two steps show how the remaining eight vertices cannot be covered in one additional path.



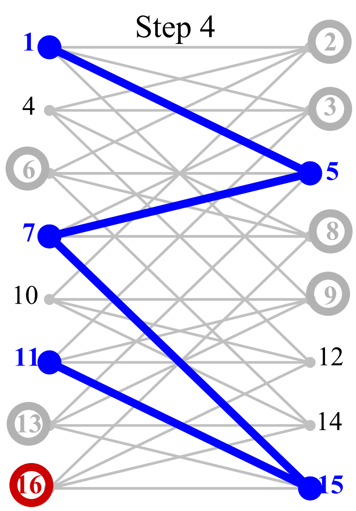
Begin by going from V_1 to V_5. Since V_1 is our starting vertex, then V_2, V_3, and V_9 cannot be vertices in our path as they will create a cycle back to V_1.



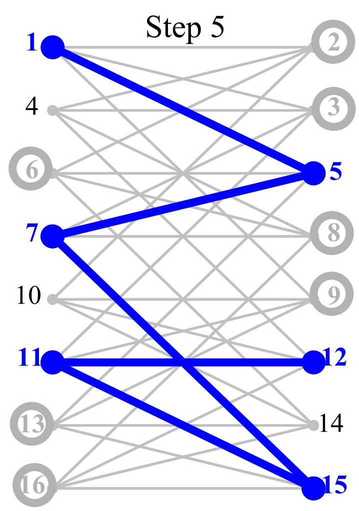
Going from V_5 to V_7 eliminates vertices V_6 and V_{13}.



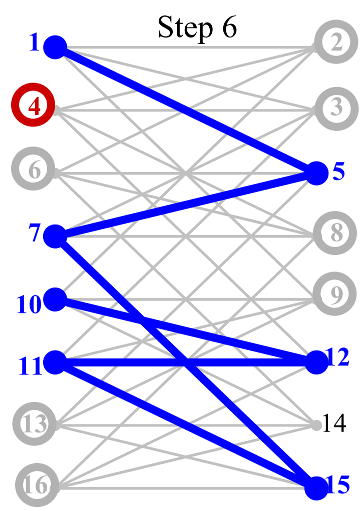
Going from V_7 to V_{15} eliminates vertex V_8.



V_{15} to V_{11} eliminates vertex V_{16}.



V_{11} to V_{12}. Here, no vertices are eliminated.



V_{12} to V_{10} eliminates vertex V_4.

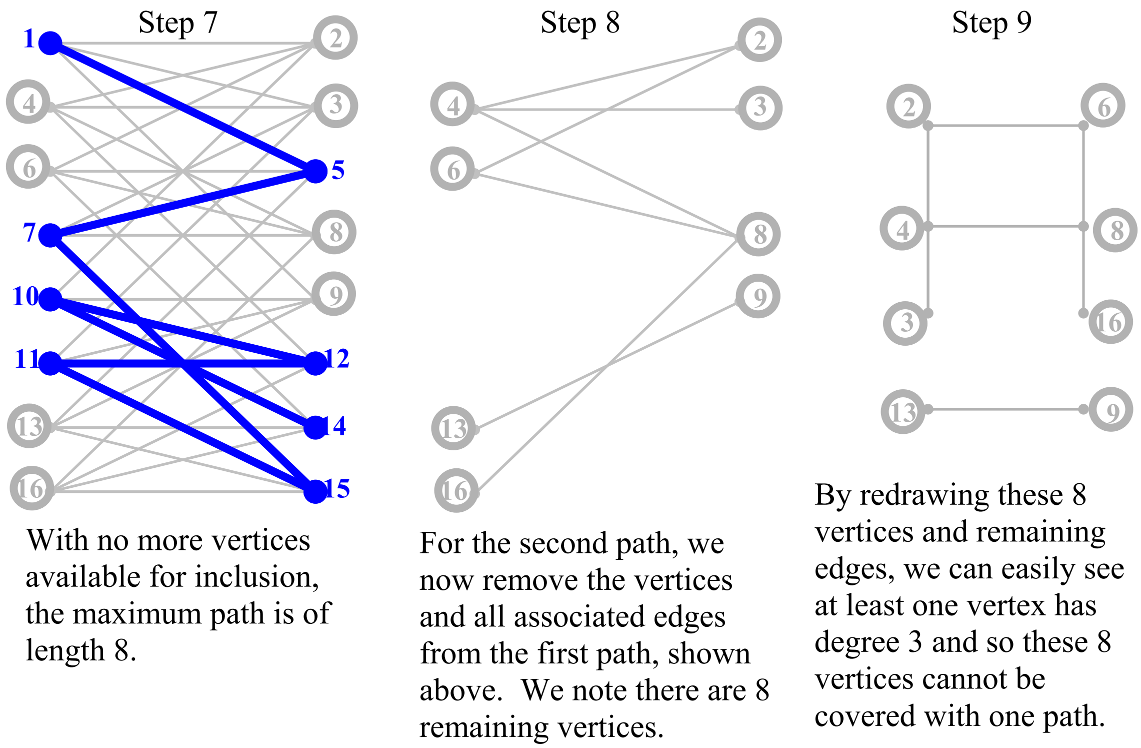


Figure 16. Constructing a Path Covering for Q_4.

d. Remaining Paths Starting at Vertex 1

The previous example shows one possible path of length eight for Q_4. If we continually repeat the process for all possible paths of length eight (starting with vertex one), we find 24 possible paths, listed in Table 5. For each path, we also denote the set of remaining vertices and from that set which vertex has three neighbors and thus causes the induced subgraph not to be a path. Because the hypercube is vertex transitive, without loss of generality, we can conclude the same result for any starting vertex.

Paths of Length 8	**Remaining Vertices**	**Vertex From Remaining Vertices with 3 Neighbors**
1, 2, 4, 8, 7, 15, 13, 14	3, 5, 6, 9, 10, 11, 12, 16	11, 10, 12, 16
1, 2, 4, 12, 11, 15, 13, 14	3, 5, 6, 7, 8, 9, 10, 16	7, 3, 5, 8
1, 2, 6, 8, 7, 15, 11, 12	3, 4, 5, 9, 10, 13, 14, 16	14, 10, 13, 16
1, 2, 6, 14, 13, 15, 11, 12	3, 4, 5, 7, 8, 9, 10, 16	7, 3, 5, 8
1, 2, 10, 12, 11, 15, 7, 8	3, 4, 5, 6, 9, 13, 14, 16	13, 5, 9, 14
1, 2, 10, 14, 13, 15, 7, 8	3, 4, 5, 6, 9, 11, 12, 16	12, 4, 11, 16
1, 3, 4, 8, 6, 14, 13, 15	2, 5, 7, 9, 10, 11, 12, 16	11, 10, 12, 16
1, 3, 4, 12, 10, 14, 13, 15	2, 5, 6, 7, 8, 9, 11, 16	6, 2, 5, 8
1, 3, 7, 8, 6, 14, 10, 12	2, 4, 5, 9, 11, 13, 15, 16	15, 11, 13, 16
1, 3, 7, 15, 13, 14, 10, 12	2, 4, 5, 6, 8, 9, 11, 16	6, 2, 5, 8
1, 3, 11, 12, 10, 14, 6, 8	2, 4, 5, 7, 9, 13, 15, 16	13, 5, 9, 15
1, 3, 11, 15, 13, 14, 6, 8	2, 4, 5, 7, 9, 10, 12, 16	12, 4, 10, 16
1, 5, 6, 8, 4, 12, 11, 15	2, 3, 7, 9, 10, 13, 14, 16	10, 2, 9, 14
1, 5, 6, 14, 10, 12, 11, 15	2, 3, 4, 7, 8, 9, 13, 16	4, 2, 3, 8
1, 5, 7, 8, 4, 12, 10, 14	2, 3, 6, 9, 11, 13, 15, 16	15, 11, 13, 16
1, 5, 7, 15, 11, 12, 10, 14	2, 3, 4, 6, 8, 9, 13, 16	4, 2, 3, 8
1, 5, 13, 14, 10, 12, 4, 8	2, 3, 6, 7, 9, 11, 15, 16	15, 7, 11, 16
1, 5, 13, 15, 11, 12, 4, 8	2, 3, 6, 7, 9, 10, 14, 16	14, 6, 10, 16
1, 9, 10, 12, 4, 8, 7, 15	2, 3, 5, 6, 11, 13, 14, 16	14, 6, 13, 16
1, 9, 10, 14, 6, 8, 7, 15	2, 3, 4, 5, 11, 12, 13, 16	4, 2, 3, 12
1, 9, 11, 12, 4, 8, 6, 14	2, 3, 5, 7, 10, 13, 15, 16	15, 7, 13, 16
1, 9, 11, 15, 7, 8, 6, 14	2, 3, 4, 5, 10, 12, 13, 16	4, 2, 3, 12
1, 9, 13, 14, 6, 8, 4, 12	2, 3, 5, 7, 10, 11, 15, 16	15, 7, 11, 16
1, 9, 13, 15, 7, 8, 4, 12	2, 3, 5, 6, 10, 11, 14, 16	14, 6, 10, 16

Table 5. Paths of Length Eight of Q_4 Starting With Vertex 1.

e. Demonstrating $P(Q_4) = 3$

Above, we established that $P(Q_4) > 2$. Certainly, there are many ways to properly cover Q_4 with three paths and Figure 17 shows an example using two paths of length seven and one path of length three. From this, we can conclude that $P(Q_4) = 3$.

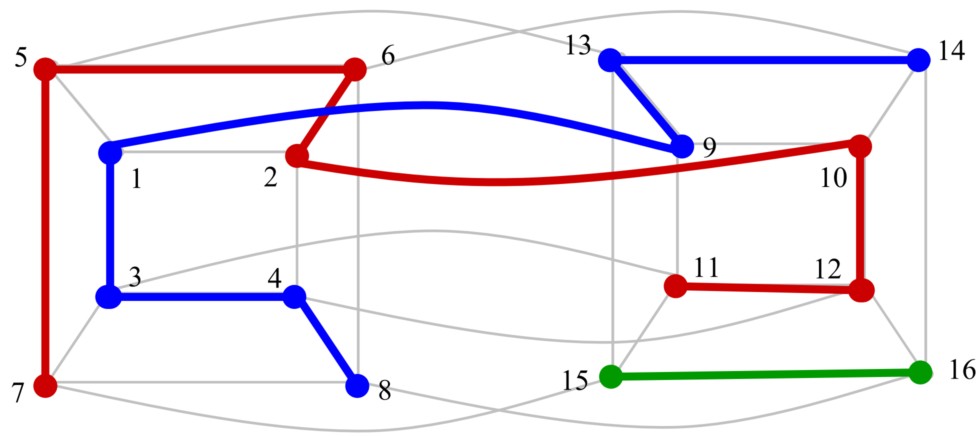


Figure 17. A Path Covering for Q_4 showing that $P(Q_4) \leq 3$.

6. The Path Cover Number of Q_5

Because $Q_5 = Q_4 \times K_2$, it follows that since $P(Q_4) = 3$, then $P(Q_5) \geq 3$. Since a covering is shown in Figure 18 using only 3 paths, we can then conclude that $P(Q_5) = 3$.

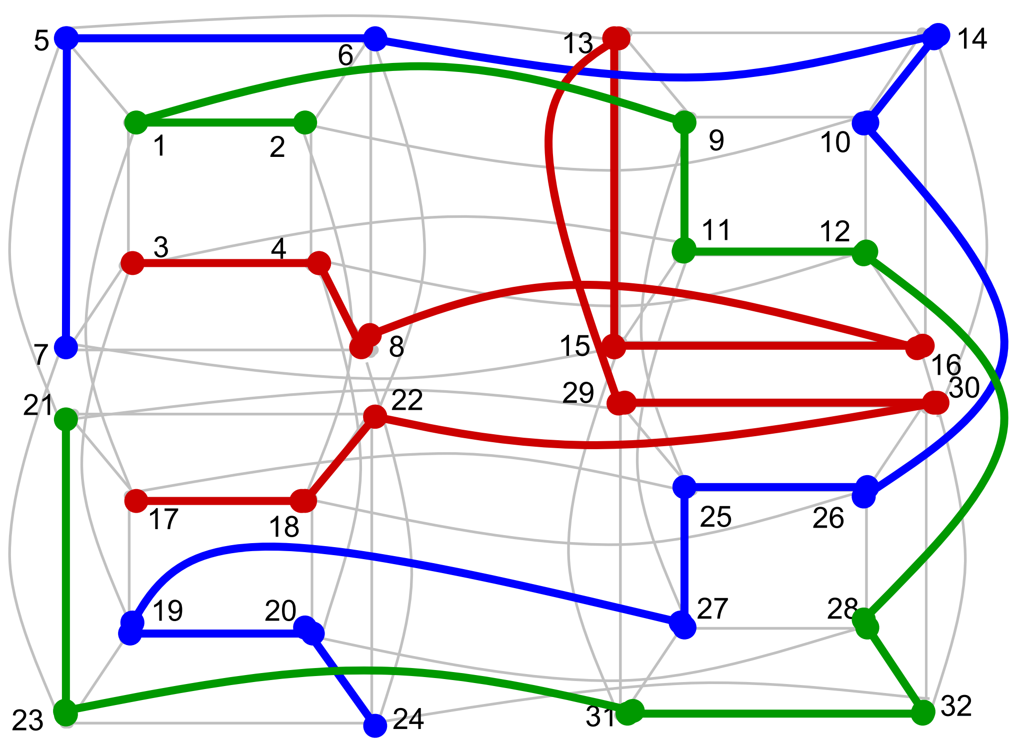


Figure 18. A Path Covering for Q_5 showing that $P(Q_5) \leq 3$.

7. The Path Cover Number of Q_n in General

At this point, it seems that there is no way to determine the path cover number for Q_n in general. Table 6 summarizes our results so far from Q_1 thru Q_5.

Hypercube Q_n	Number of Vertices	Path Cover Number
Q_1	2	1
Q_2	4	2
Q_3	8	2
Q_4	16	3
Q_5	32	3

Table 6. Path Cover Number for Q_1 thru Q_5.

8. The Path Vertex-Deletion Number $\Delta(Q_n)$

Determining the path vertex-deletion number of a graph involves two main steps. First, we need to delete vertices so that we divide the graph into components of vertex disjoint paths. The number of these initially–deleted vertices becomes the lower bound for q. Second, we consider deleting additional vertices that will yield more p paths and thus maximize [p – q]. We begin with $\Delta(Q_1)$.

Proposition 10: $\Delta(Q_1) = 1 - 0 = 1$.

Proof: Since Q_1 is already a vertex disjoint path we can easily see that we do not need to delete any vertices and $\Delta(Q_1) = 1 - 0 = 1$. QED.

Proposition 11: $\Delta(Q_2) = 2 - 2 = 0$.

Proof: Since Q_2 is a cycle of length four, we must delete at least one vertex in order to divide the graph into components that are disjoint paths. Figure 19 shows that when deleting one or two vertices the maximum choices of [p – q] are [1 – 1] or [2 – 2], and so $\Delta(Q_2) = 0$. Note that deleting three vertices would leave one isolated vertex remaining and thus only one path and so $p - q = 1 - 3 = -2$, which is less than zero and so discarded. QED.

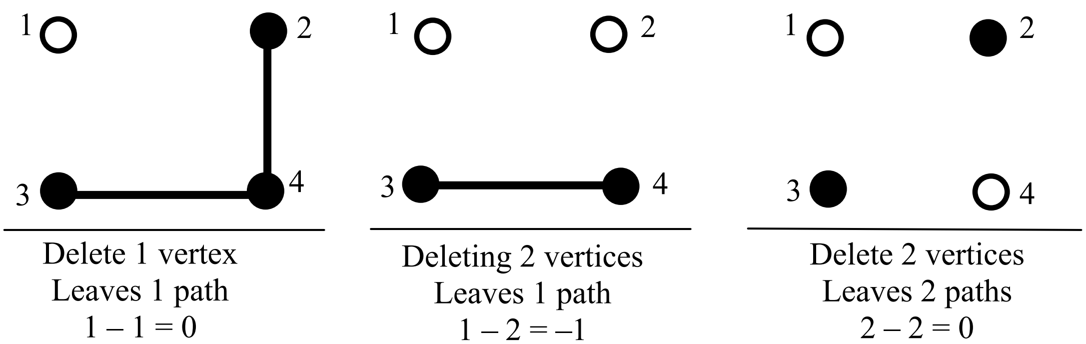
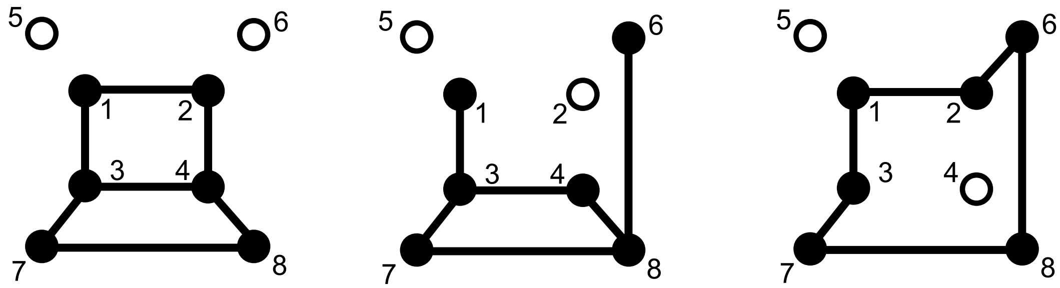


Figure 19. Cases in Determining $\Delta(Q_2)$.

Proposition 12: $\Delta(Q_3) = 4 - 4 = 0$.

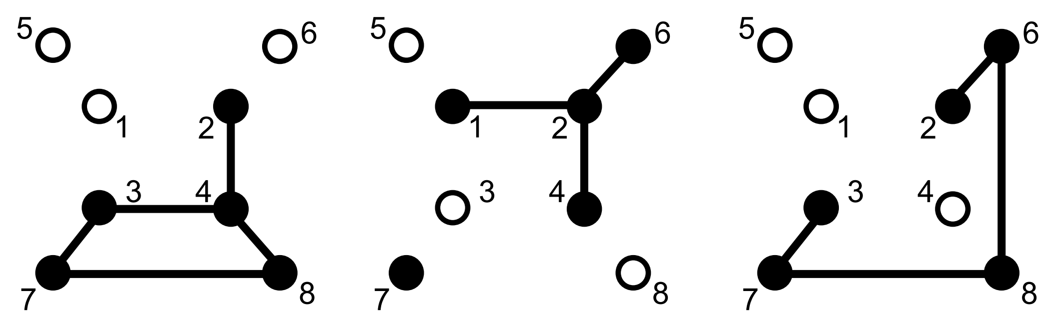
Proof: We begin by deleting vertices of Q_3 in order to divide the graph into components that are disjoint paths. It is easy to see that deleting only one vertex alone will not achieve this since Q_3 has two disjoint cycles, one in each copy of Q_2. Because of the vertex transitivity of the hypercube, we only need to consider the cases where the deleted vertices are different distances apart. In deleting two vertices, there are three unique cases (up to isomorphism) based on the deleted vertices being distance either 1, 2, or 3 away from each other. Three is the largest distance to consider since the diameter of Q_3 is 3. Figure 20 shows that deleting only two vertices, shown as empty circles, still does not achieve dividing the graph into paths.



Deleting 2 vertices, distance = 1 | Deleting 2 vertices, distance = 2 | Deleting 2 vertices, distance = 3

Figure 20. Cases in Determining $\Delta(Q_3)$ using q = 2.

Next, we examine deleting three vertices from Q_3. Again, there are three unique cases to consider. If we denote the deleted vertices A, B, and C, and denote the distance between each of these points as: (A to B, B to C, A to C), then the three unique cases are: (1, 1, 2), (2, 2, 2), and (1, 2, 3). Figure 21 shows that only in the final case, with distances between deleted vertices (1, 2, 3), do we finally divide the graph into components of vertex disjoint paths and attain p – q = –2.



Deleting 3 vertices, distances = 1, 1, 2 | Deleting 3 vertices, distance = 2, 2, 2 | Deleting 3 vertices, distance = 1, 2, 3, p – q = 1 – 3 = –2

Figure 21. Cases in Determining $\Delta(Q_3)$ using q = 3.

We now consider deleting additional vertices in an effort to find a higher value for $p - q$, continuing with $q = 4$. If we delete four vertices, that leaves four vertices remaining, and the largest number of paths we can achieve would be four disjoint paths of length one. If we consider that the hypercube is bipartite and delete the four vertices of one bipartite set, we will leave the four vertices from the other bipartite set. Since no two vertices in a bipartite set are adjacent, we know these remaining vertices will form the four disjoint paths that we are trying to achieve. So, given that the size of each bipartite set is 2^{n-1}, we can see that deleting one set yields $p - q = 2^{n-1} - 2^{n-1} = 4 - 4 = 0$. See Figure 22.

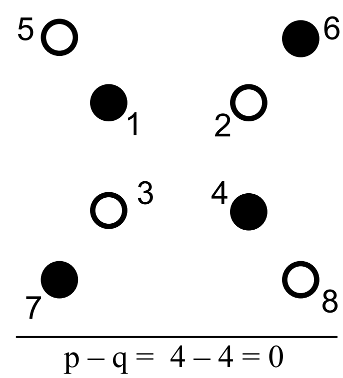


Figure 22. Determining $\Delta(Q_3)$ using $q = 4$.

To conclude this proof, we must address two additional cases not yet covered in determining $\Delta(Q_3)$ and show that both yield $p - q < 0$. First, we consider deleting four vertices but not from the same bipartite set. Then, of the four remaining vertices, at least two will be adjacent, and therefore the largest number of paths we can achieve is three, leaving $p - q \leq 3 - 4 = -1$, which is less than zero and so discarded. Finally, we consider deleting five or more vertices. Since this would yield three or less vertices remaining, the best we can achieve for $p - q \leq 3 - 5 = -2$, which again is less than zero and so discarded.

We can see now the maximum choice for $p - q = 2^{n-1} - 2^{n-1} = 4 - 4 = 0$ and therefore can conclude that $\Delta(Q_3) = 0$. Note that any other choices for p and q in determining $\Delta(Q_3)$ other than $p = q = 2^{n-1}$ will yield $p - q < 0$. QED.

Theorem 13: $\Delta(Q_n) = 2^{n-1} - 2^{n-1} = 0$ for $n \geq 2$

Proof: We have already shown that Theorem 13 is true for $n = 2, 3$. Additionally, we can certainly see that by deleting one bipartite set of vertices from Q_n, we will achieve $p - q = 2^{n-1} - 2^{n-1} = 0$, $n \geq 2$. The goal now will be demonstrating that all other choices for p and q yield $p - q < 0$. We note here that Q_n, $n \geq 3$, contains 2^{n-3} copies of Q_3 and the key to this proof will be focusing on how those copies are divided into vertex disjoint paths.

Case 1: Deleting three vertices for every copy of Q_3 in Q_n.

Based on the third construction shown in Figure 21, we can see that we must delete a minimum of three vertices within all copies of Q_3 that exist in Q_n, $n > 3$ in order to divide Q_n into vertex disjoint paths. We certainly may have to delete more vertices; three is simply a lower bound. Figure 21 shows that deleting these three vertices within each copy of Q_3 will create a single path P_5, within each copy. The best we can do to maximize p under this scenario is for these paths to remain vertex disjoint and so p would equal the number of copies of Q_3. Therefore if we denote the number of copies of Q_3 in Q_n ($n \geq 3$) as x, then the maximum we can achieve is

$$p - q = x - 3x = -2x \text{ and so } \mathbf{p - q < 0.}$$

Case 2: Deleting three vertices in some copies of Q_3 while deleting four vertices in the remaining copies of Q_3 in Q_n.

Since there are 2^{n-3} copies of Q_3 in Q_n, we let y be number of copies in which we delete three vertices, leaving $2^{n-3} - y$ copies remaining. For each copy where we delete 3 vertices, we will again create one path P_5, and for each copy where we delete four vertices, the best we can do is to create fours paths P_1. As in case 1, we maximize p when these paths remain disjoint between different copies of Q_3. Therefore, in this case,

$$p \leq 1 \cdot y + 4 \cdot (2^{n-3} - y) \text{ and}$$

$$q = 3 \cdot y + 4 \cdot (2^{n-3} - y), \text{ so}$$

$$p - q \leq [y + 4 \cdot (2^{n-3} - y)] - [3y + 4 \cdot (2^{n-3} - y)]$$

$$\leq y - 3y = -2y \text{ and it follows that } \mathbf{p - q < 0}.$$

Case 3: Deleting four vertices in each copy of Q_3, where at least one deleted vertex is not in the same bipartite set as the other deleted vertices.

Since this means that at least two vertices in one copy of Q_3 will be adjacent and thus form a path of at least length two, p can be at most $2^{n-1} - 1$ and thus

$$p - q \leq (2^{n-1} - 1) - (2^{n-1}) = -1, \text{ so } \mathbf{p - q < 0}.$$

Case 4: Deleting five or more vertices in at least one copy of Q_3.

For any copy of Q_3 that we delete at least five vertices, the maximum number of paths remaining will be three if they are all disjoint paths of length one. Here, we denote the number of copies of Q_3 in which we delete 3, 4, or 5 vertices to be x, y, and $(2^{n-3} - x - y)$, respectively. Therefore, under these conditions,

$$p \leq 1 \cdot x + 4 \cdot y + 3 \cdot (2^{n-3} - x - y) \text{ and}$$

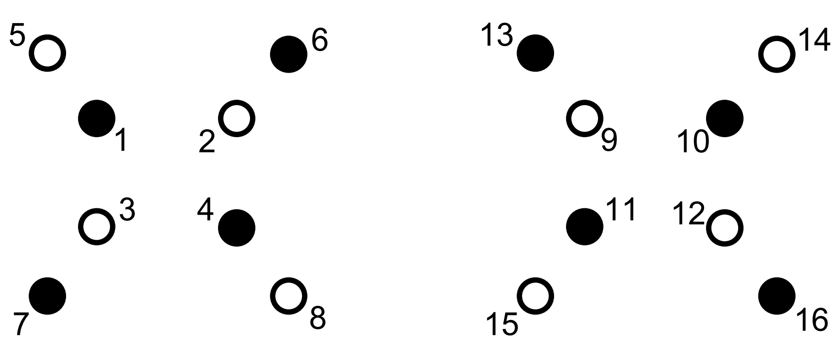
$$q = 3 \cdot x + 4 \cdot y + 5 \cdot (2^{n-3} - x - y), \text{ so}$$

$$p - q \leq [x + 4y + 3 \cdot (2^{n-3} - x - y)] - [3x + 4y + 5 \cdot (2^{n-3} - x - y)]$$

$$\leq -2x - 2 \cdot (2^{n-3} - x - y) = -2 \cdot (2^{n-3} - 2x - y) \text{ and we have } \mathbf{p - q < 0}.$$

Since we have shown that all other choices for p and q other than $p = q = 2^{n-1}$ yield $p - q < 0$, we can conclude that $\Delta(Q_n) = 2^{n-1} - 2^{n-1} = 0$, $n \geq 2$. QED.

Figure 23 shows $\Delta(Q_4)$ by applying Theorem 13.



$$p - q = 2^{n-1} - 2^{n-1} = 8 - 8 = 0$$

Figure 23. Determining $\Delta(Q_4)$.

9. Summary of Results for the Inverse Eigenvalue Problem of Q_n

Table 7 lists the results we have found, or conjectured, for the hypercube for $M(Q_n)$, $mr(Q_n)$, $P(Q_n)$, and $\Delta(Q_n)$.

Hypercube Q_n	**$M(Q_n) = mr(Q_n)$**	**$P(Q_n)$**	**$\Delta(Q_n)$**
Q_1	1	1	1
Q_2	2	2	0
Q_3	4	2	0
Q_4	8	3	0
Q_5	16	3	0

Table 7. Summary Table for the Inverse Eigenvalue Problem of the Hypercube.

Since Q_1 is a tree, our results agree with Theorem 6 agrees that tells us

$$M(Q_1) = mr(Q_1) = P(Q_1) = \Delta(Q_1).$$

For Q_2 we have

$$M(Q_2) = mr(Q_2) = P(Q_2) > \Delta(Q_2).$$

Now, using Theorems 7, 9 and 13, we can easily conclude the following:

Theorem 14: $M(Q_n) = mr(Q_n) > P(Q_n) > \Delta(Q_n)$, for $n \geq 3$.

IV. THE ENERGY OF THE HYPERCUBE

A. INTRODUCTION

The energy E(G) of a graph G is defined to be the sum of the absolute values of the eigenvalues of the adjacency matrix of G [13]. For certain special graphs, this is easy to determine in general. For instance, the complete graph K_n has n eigenvalues {n–1 , –1, –1, –1, . . ., –1}, so its energy is $E(K_n) = (1)(n - 1) + (n - 1)(1) = 2n - 2$. In other cases, we can only provide bounds for the energy of certain types of graphs. For instance, Koolen and Moulton showed that for any graph with order n and size m, $E(G) \le \sqrt{2mn}$, and, if we only consider the order, $E(G) \le \frac{n}{2}(1+\sqrt{n})$ [14]. Additionally, they showed that if G is bipartite, then $E(G) \le \frac{n}{\sqrt{8}}(\sqrt{2}+\sqrt{n})$ [15]. In the next section, we derive several equivalent formulas for the energy of the hypercube Q_n.

B. APPLIED TO THE HYPERCUBE

1. Deriving the equation for E(Q_n)

Using Table 1 in Chapter II.C.1, we can determine the absolute values of eigenvalues (with multiplicity) for the hypercube to be as summarized here in Table 8.

	Absolute Values of Eigenvalues	Multiplicity
Q_n	$\lambda = n, n-2, n-4, \ldots, n-4, n-2, n$	$\binom{n}{0}, \binom{n}{1}, \binom{n}{2}, \ldots \binom{n}{n-1}, \binom{n}{n}$

Table 8. Absolute Values of the Eigenvalues of the Adjacency Matrix of Q_n with Multiplicity.

Thus, we can see that the energy of the hypercube is given by

$$E(Q_n) = (n)\binom{n}{0} + (n-2)\binom{n}{1} + (n-4)\binom{n}{2} + ... + (n-4)\binom{n}{n-2} + (n-2)\binom{n}{n-1} + (n)\binom{n}{n}.$$

We now consider the symmetry in the above equation and focus on the two cases, one when n is odd and the other when n is even. To illustrate, consider Q_5 and Q_6:

$$E(Q_5) = (5)\binom{5}{0} + (3)\binom{5}{1} + (1)\binom{5}{2} \qquad + \qquad (1)\binom{5}{3} + (3)\binom{5}{4} + (5)\binom{5}{5} \; = \; 60.$$

$$E(Q_6) = (6)\binom{6}{0} + (4)\binom{6}{1} + (2)\binom{6}{2} + (0)\binom{6}{3} + (2)\binom{6}{4} + (4)\binom{6}{5} + (6)\binom{6}{6} \; = \; 120.$$

First, it is easy to see that the first eigenvalue (in absolute value) equals the last, the second equals the second last and so forth. When n is odd, we have pairs of eigenvalues in absolute value to be

$$\{n, n, n-2, n-2, \ldots 5, 5, 3, 3, 1, 1\}.$$

When n is even, we have pairs of eigenvalues in absolute value to be

$$\{n, n, n-2, n-2, \ldots 4, 4, 2, 2, 0\}.$$

Since the zero eigenvalue can be discarded when determining the energy, we can see that the smallest eigenvalues (in absolute value) is $\lambda = 1$ when n is odd and $\lambda = 2$ when n is even. It will be useful later to express this minimum as $\lambda_{min} = \left(n - 2\cdot\left\lfloor \frac{n-1}{2} \right\rfloor\right)$.

Since $\binom{n}{k} = \binom{n}{n-k}$, we can see that the eigenvalues with these pairs of coefficients above have the same multiplicity. In the case where n is even, the $\binom{n}{n/2}$ term occurs only once, but the corresponding eigenvalue is zero (and is thus discarded in calculating the energy). Based on these considerations, we can see that in general

$$E(Q_n) = 2\left[(n)\binom{n}{0} + (n-2)\binom{n}{1} + (n-4)\binom{n}{2} + \ldots + \left(n - 2\left\lfloor \frac{n-1}{2} \right\rfloor\right)\binom{n}{\left\lfloor \frac{n-1}{2} \right\rfloor}\right].$$

We have proven the following theorem:

Theorem 15: $E(Q_n) = \sum_{i=0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} 2(n-2i)\binom{n}{i}$.

In Table 9, we calculate the energy for Q_n ($1 \le n \le 4$) in both ways: on the left, using this formula, and on the right using the definition of energy by listing and adding the absolute values of the eigenvalues (excluding zeros).

Using Theorem 15	**Using the Definition**
$E(Q_1) = \sum_{i=0}^{0} 2(1-2i)\binom{1}{i} = 2(1-2\cdot 0)\binom{1}{0} = 2$	$1 + 1 = 2$
$E(Q_2) = \sum_{i=0}^{0} 2(2-2i)\binom{2}{i} = 2(2-2\cdot 0)\binom{2}{0} = 4$	$2 + 2 = 4$
$E(Q_3) = \sum_{i=0}^{1} 2(3-2i)\binom{3}{i}$ $= 2\left[(3-2\cdot 0)\binom{3}{0} + (3-2\cdot 1)\binom{3}{1}\right] = 12$	$3 + 1 + 1 + 1 + 1 +$ $1 + 1 + 3 = 12$
$E(Q_4) = \sum_{i=0}^{1} 2(4-2i)\binom{4}{i}$ $= 2\left[(4-2\cdot 0)\binom{4}{0} + (4-2\cdot 1)\binom{4}{1}\right] = 24$	$4 + 2 + 2 + 2 + 2 + 2 +$ $2 + 2 + 2 + 4 = 24$

Table 9. Calculating $E(Q_n)$ in Two Ways for $1 \le n \le 4$.

In Table 10, we summarize $E(Q_n)$ for $1 \leq n \leq 12$.

Q_n	Energy
Q_1	2
Q_2	4
Q_3	12
Q_4	24
Q_5	60
Q_6	120

Q_n	Energy
Q_7	280
Q_8	560
Q_9	1,260
Q_{10}	2,520
Q_{11}	5,544
Q_{12}	11,088

Table 10. $E(Q_n)$ for $1 \leq n \leq 12$.

2. Proving $E(Q_n) = 2 \cdot E(Q_{n-1})$ for n Even

Observation of the above table seems to show that, for n even, $E(Q_n) = 2 \cdot E(Q_{n-1})$. By applying Theorem 15 and letting n = 2k, this observation suggests that

$$\sum_{i=0}^{\left\lfloor \frac{2k-1}{2} \right\rfloor} 2(2k-2i)\binom{2k}{i} = 2\left[\sum_{i=0}^{\left\lfloor \frac{2k-1-1}{2} \right\rfloor} 2(2k-1-2i)\binom{2k-1}{i}\right].$$

By simplifying the upper limit of the summation using $\left\lfloor \frac{2k-1}{2} \right\rfloor = \left\lfloor \frac{2k-1-1}{2} \right\rfloor = k-1$ we state the following theorem.

Theorem 16: $\sum_{i=0}^{k-1}(2k-2i)\binom{2k}{i} = 2\left[\sum_{i=0}^{k-1}(2k-2i-1)\binom{2k-1}{i}\right]$.

Proof: First, we expand the summation of the right side, obtaining the sum

$$2\left[(2k-1)\binom{2k-1}{0} + (2k-3)\binom{2k-1}{1} + (2k-5)\binom{2k-1}{2} + \ldots + 3\binom{2k-1}{k-2} + 1\binom{2k}{k-1}\right].$$

Now, we show that the left side is equal to the right side. We proceed by expanding the left side to obtain

$$2k\binom{2k}{0} + (2k-2)\binom{2k}{1} + (2k-4)\binom{2k}{2} + \dots + 6\binom{2k}{k-3} + 4\binom{2k}{k-2} + 2\binom{2k}{k-1}.$$

Since there is only one way to choose zero objects from a set of any size, we can replace the first term in the expansion of $\binom{2k}{0}$ with $\binom{2k-1}{0}$. We then apply Pascal's identity $\left(\binom{k}{i} = \binom{k-1}{i} + \binom{k-1}{i-1}\right)$ to all of the other terms on the left side, and so we have

$$2k\binom{2k-1}{0} + (2k-2)\left[\binom{2k-1}{0} + \binom{2k-1}{1}\right] + (2k-4)\left[\binom{2k-1}{1} + \binom{2k-1}{2}\right] + \dots$$
$$+ 4\left[\binom{2k-1}{k-3} + \binom{2k-1}{k-2}\right] + 2\left[\binom{2k-1}{k-2} + \binom{2k-1}{k-1}\right].$$

We distribute the terms {2k, 2k – 2, 2k – 4, . . . , 4, 2} within each bracketed group of combinations and now have

$$2k\binom{2k-1}{0} + (2k-2)\binom{2k-1}{0} + (2k-2)\binom{2k-1}{1} + (2k-4)\binom{2k-1}{1} + (2k-4)\binom{2k-1}{2} + \dots$$
$$+ 4\binom{2k-1}{k-3} + 4\binom{2k-1}{k-2} + 2\binom{2k-1}{k-2} + 2\binom{2k-1}{k-1}.$$

We now use the associative law of addition to regroup the combinations as follows:

$$\left[2k\binom{2k-1}{0} + (2k-2)\binom{2k-1}{0}\right] + \left[(2k-2)\binom{2k-1}{1} + (2k-4)\binom{2k-1}{1}\right] + \left[(2k-4)\binom{2k-1}{2} + \dots\right.$$
$$\left. + 4\binom{2k-1}{k-3}\right] + \left[4\binom{2k-1}{k-2} + 2\binom{2k-1}{k-2}\right] + \left[2\binom{2k-1}{k-1}\right].$$

Next, we simplify the equation inside each bracket to get

$$\left[(4k-2)\binom{2k-1}{0}\right] + \left[(4k-6)\binom{2k-1}{1}\right] + \left[(4k-10)\binom{2k-1}{2}\right] + \dots$$
$$+\left[10\binom{2k-1}{k-3}\right] + \left[6\binom{2k-1}{k-2}\right] + \left[2\binom{2k-1}{k-1}\right].$$

Finally, if we factor out a two from each term, we have the following:

$$2\left[(2k-1)\binom{2k-1}{0} + (2k-3)\binom{2k-1}{1} + (2k-5)\binom{2k-1}{2} + \dots\right.$$
$$\left. + 5\binom{2k-1}{k-3} + 3\binom{2k-1}{k-2} + 1\binom{2k-1}{k-1}\right].$$

This is precisely equal to the right side of Theorem 16, which is what we were trying to show. QED.

3. An Alternate Equation for the Energy of the Hypercube

Since $E(Q_n) = 2 \cdot E(Q_{n-1})$ for n even, there might be two separate, identifiable sub-sequences of $E(Q_n)$ for n being even and for n being odd. We study this next.

a. Sequence of $E(Q_n)$ for n Even

Let n be even. The first six terms of $E(Q_n)$ starting with n = 2, are 4, 24, 120, 560, 2520, and 11088. In searching the On-Line Encyclopedia of Integer Sequences [16], we find an exact match with sequence number A002011 which has the formula: $\frac{4\cdot(2n+1)!}{(n!)^2}$, except that this sequence starts at n = 0 and the sequence of $E(Q_n)$ starts with n = 2. Therefore, if we replace n with $\frac{n}{2}-1$ in the formula for the A002011 sequence, we can conjecture that

$$E(Q_n) = \sum_{i=0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} 2(n-2i)\binom{n}{i} = \frac{4(n-1)!}{\left(\left(\frac{n}{2}-1\right)!\right)^2}.$$

b. Sequence of $E(Q_n)$ for n Odd

Let n be odd. The first six terms of $E(Q_n)$ starting with n = 1, are 2, 12, 60, 280, 1260 and 5544. Again, in searching the On-Line Encyclopedia of Integer Sequences [16], we find an exact match with sequence number A005430 which has the formula: $n\binom{2n}{n}$ also starting with n = 1. Therefore, if we replace n with $\frac{n+1}{2}$, we can conjecture that

$$E(Q_n) = \sum_{i=0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} 2(n-2i)\binom{n}{i} = \left(\frac{n+1}{2}\right)\binom{n+1}{\frac{n+1}{2}}.$$

c. Furthering the Conjectures for $E(Q_n)$ for n Even and Odd

Earlier, we proved that $E(Q_n) = 2 \cdot E(Q_{n-1})$, $n \geq 2$, using our established formula for $E(Q_n)$. We show now that our conjectured alternate formulas for E(Qn) for n even also satisfy $E(Q_n) = 2 \cdot E(Q_{n-1})$. Although this does not prove conclusively these are alternate formulas for E(Qn), it does help substantiate the conjectures. Let n be even, we then have

$$E(Q_n) \; = \; 2 \cdot E(Q_{n-1})$$

$$\frac{4(n-1)!}{\left(\left(\frac{n}{2}-1\right)!\right)^2} = 2\left[\left(\frac{n-1+1}{2}\right)\binom{n-1+1}{\frac{n-1+1}{2}}\right]$$

$$= n\binom{n}{\frac{n}{2}}.$$

We proceed by showing how the left-hand-side is equal to the right-hand-side.

$$\frac{4(n-1)!}{\left(\left(\frac{n}{2}-1\right)!\right)^2} = \frac{4(n-1)!}{\left(\frac{n}{2}-1\right)!\left(\frac{n}{2}-1\right)!}\cdot\frac{\left(\left(\frac{n}{2}\right)!\right)^2}{\left(\left(\frac{n}{2}\right)!\right)^2} = \frac{\left(\frac{n}{2}\right)^2 4(n-1)!}{\left(\left(\frac{n}{2}\right)!\right)^2} = \frac{n^2(n-1)!}{\left(\frac{n}{2}\right)!\left(\frac{n}{2}\right)!} = n\binom{n}{\frac{n}{2}}.$$

d. A Conjectured Alternate Formula for $E(Q_n)$

Based on the results of the previous two sections, we now conjecture a more concise formula for Q_n than that originally provided in Theorem 15.

$$E(Q_n) = \begin{cases} \dfrac{n+1}{2}\dbinom{n+1}{\frac{n+1}{2}} & \text{for n odd;} \\ n\dbinom{n}{\frac{n}{2}} & \text{for n even.} \end{cases}$$

V. TOPICS FOR FURTHER RESEARCH

A. APPLICATION

Although the hypercube has numerous applications to coding theory as well as the study of Boolean functions, there are currently no specific applications known to us for the spectral graph theory analysis of the hypercube provided in this paper. Since the energy of a graph is used in chemistry to approximate certain aspects of molecules, the focal point on finding applications of the energy of the hypercube should start in this area.

B. OPEN QUESTIONS

There are several unanswered questions noted throughout this paper, both with respect to the inverse eigenvalue problem as well as the energy of the hypercube.

1. Is there a general formula for $P(Q_n)$?

2. Is there any relationship between the maximum multiplicity of the possible eigenvalues $M(Q_n)$ and $E(Q_n)$?

3. Can we generalize the results we derived for the energy of the hypercube to find the energy of other graph Cartesian products?

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