THE SQUARE OF ADJACENCY MATRICES

A Thesis
Submitted to the Graduate Faculty
of the
North Dakota State University
of Agriculture and Applied Science

By

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In Partial Fulfillment of the Requirements
for the Degree of
MASTER OF SCIENCE

Major Department:
Mathematics

October 2011

Fargo, North Dakota

North Dakota State University
Graduate School

Title

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The Supervisory Committee certifies that this ***disquisition*** complies with North Dakota State University's regulations and meets the accepted standards for the degree of

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ABSTRACT

Kranda, Daniel Joseph, M.S., Department of Mathematics, College of Science and Mathematics, North Dakota State University, October 2011. The Square of Adjacency Matrices. Major Professor: Dr. Warren E. Shreve.

It can be shown that any symmetric (0, 1)-matrix A with $\operatorname{tr} A = 0$ can be interpreted as the adjacency matrix of a simple, finite graph. The square of an adjacency matrix $A^2 = (s_{ij})$ has the property that s_{ij} represents the number of walks of length two from vertex i to vertex j. With this information, the motivating question behind this paper was to determine what conditions on a matrix S are needed to have $S = A(G)^2$ for some graph G. Structural results imposed by the matrix S include detecting bipartiteness or connectedness, counting four cycles and determining plausible neighborhoods of vertices. Some characterizations will be given and the problem of when S represents several non-isomorphic graphs is also explored.

ACKNOWLEDGMENTS

I would like to thank Dr. Warren Shreve for his many hours of guidance provided to me during the writing of this thesis.

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CHAPTER 1. INTRODUCTION

This thesis will aim to determine necessary and sufficient conditions for a matrix to represent the square of the adjacency matrix of a graph. Beginning with some background in graph theory and a motivating problem, we will continue with immediate necessary conditions.

Throughout this paper, examples will be provided either as a showcase of the results or to show why certain conditions are not both necessary and sufficient. We will prove several results about the necessary structure of graphs given conditions on the square of the adjacency matrix.

The process of removing vertices of certain degrees and the effect this has on the square of the adjacency matrix is explored.

We will prove characterizations of the squares of the adjacency matrices of several classes of graphs including paths and unions of cycles. Lastly, the problem of determining when a matrix represents several non-isomorphic graphs is explored with a result on constructing such matrices.

A thorough study of the square of the adjacency matrix of a graph has not been addressed previously in the literature, as was determined by an extensive search of MathSciNet and the internet. However, we expect the graph theory community will find this to be a topic of interest.

1.1. Background

Throughout this paper, we will consider only simple, undirected graphs; that is, we will only concern ourselves with graphs that have no loops or multiedges and whose edges have no direction assigned to them. Under these assumptions, we have the following definition.

Definition 1.1. For a graph G on n vertices $\{v_1, v_2, \ldots v_n\}$, the *adjacency matrix of* G, denoted $A(G) = (a_{ij})$, is the $n \times n$ $(0,1)$-matrix with

$$a_{ij} = \begin{cases} 1 \text{ if } v_i v_j \in E(G) \\ 0 \text{ if } v_i v_j \notin E(G). \end{cases}$$

With a simple, undirected graph G, we must have that $\operatorname{tr} A(G) = 0$ and that $A(G)^T = A(G)$. The trace must be zero because we do not allow loops in our graph; that is, $v_i v_i \notin E(G)$ for all i and hence, $a_{ii} = 0$ for all i. The matrix must be symmetric because all edges are undirected; that is, $v_i v_j \in E(G)$ if and only if $v_j v_i \in E(G)$ and hence, $a_{ij} = a_{ji}$.

Definition 1.2. A $(0,1)$-matrix A is *graphic* if there exists a simple undirected graph G such that $A = A(G)$.

Theorem 1.3. *A $(0,1)$-matrix A is graphic if and only if* $\operatorname{tr} A = 0$ *and* $A^T = A$.

Proof. We have already proven the necessity, so suppose A is an $n \times n$, symmetric, $(0,1)$-matrix such that $\operatorname{tr} A = 0$. Let G be a graph on n vertices $\{v_1, v_2, \ldots, v_n\}$ such that $v_i v_j \in E(G)$ if and only if $a_{ij} = a_{ji} = 1$. Then by construction G is a simple undirected graph with $A(G) = A$, and hence, A is graphic. □

Theorem 1.4. *(see Merris, [6], e.g.) Suppose $A = (a_{ij}) = A(G)$ and $B = (b_{ij}) = A(H)$ for some graphs G and H. Then $G \cong H$ if and only if $A = P^{-1}BP$ for some permutation matrix P.*

Proof. Without loss of generality, let $V(G) = V(H) = \{v_1, v_2, \ldots, v_n\}$. If $G \cong H$ then there exists $\phi : V(G) \to V(H)$ such that $v_i v_j \in E(G)$ if and only if $v_{\phi(i)} v_{\phi(j)} \in E(H)$ and so $a_{ij} = b_{\phi(i)\phi(j)}$. Let

$$P = \begin{pmatrix} e_{\phi(1)} & e_{\phi(2)} & \cdots & e_{\phi(n)} \end{pmatrix}$$

where e_i is the ith column of the $n \times n$ identity matrix. Notice that $P^{-1} = P^T$ and so

$$P^{-1}BP = (b_{\phi(i)\phi(j)}) = (a_{ij}) = A.$$

On the other hand, suppose there is a permutation matrix P such that $A = P^{-1}BP$. Since P a permutation matrix, there is $\phi \in S_n$ such that

$$P = \begin{pmatrix} e_{\phi(1)} & e_{\phi(2)} & \cdots & e_{\phi(n)} \end{pmatrix}.$$

Now $v_i v_j \in E(G)$ if and only if $1 = a_{ij} = b_{\phi(i)\phi(j)}$ if and only if $v_{\phi(i)}v_{\phi(j)} \in E(H)$. Therefore, ϕ is an isomorphism between G and H. □

With this background on the adjacency matrix of a graph, we now present an important theorem connecting the square of the adjacency matrix of a graph to properties of the graph. This theorem helps motivate the idea that there is a connection between the squares of adjacency matrices of graphs and properties of the corresponding graphs.

Definition 1.5. In a graph G, a *walk* is an alternating sequence of vertices and edges in G, beginning and ending with vertices so that each vertex is incident to the edges that precede and follow it in the sequence and where the vertices that precede and follow an edge in the sequence are the end vertices of that edge.

In this paper, the length of a walk will be determined by the number of edges in the walk.

Theorem 1.6. *Let $A = (a_{ij}) = A(G)$ for some simple undirected graph G and define $S = (s_{ij}) = A^2$. Then for every i and j, s_{ij} represents the number of two-walks (walks of length two) from vertex v_i to v_j in G.*

Proof. Consider the entry s_{ij} in S. By definition, $s_{ij} = \sum_{k=1}^{n} a_{ik}a_{kj}$ and so one is contributed to the sum only when a_{ik} and a_{kj} are 1. That is, when the edges v_iv_k and v_kv_j are in G, which corresponds to the two-walk from v_i to v_j through v_k. □

It should be noted that this theorem can be extended in the following sense: if A is the adjacency matrix of a graph G and k is some positive integer, then the (i, j)-entry of the matrix A^k represents the number of walks of length k from v_i to v_j. This result can be found in many books on graph theory; see Chartrand and Lesniak, [2], for example.

1.2. Square Graphic Matrices

Definition 1.7. A matrix S is *square graphic* if there is a simple, undirected graph G such that $S = A(G)^2$.

We have seen a characterization of graphic $(0, 1)$-matrices with two simple conditions from Theorem 1.3. With this characterization and the previous definition, the question of determining when a matrix is square graphic is a natural one.

However, there are several immediate necessary conditions for a matrix to be square graphic, that fail to be sufficient conditions. Some of these necessary conditions are listed in the following proposition. First, we introduce some background on the spectra of graphs.

The following theorems are well known from matrix and graph theory and hence the proofs are omitted.

Theorem 1.8. *(Spectral Mapping Theorem)(see Roman, [7], e.g.) If A is an $n \times n$ matrix and p is a polynomial, then the eigenvalues of $p(A)$ are $p(\lambda_1), p(\lambda_2), \ldots, p(\lambda_n)$ where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of A.*

Theorem 1.9. *([7], e.g.) If A is an $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ then*

$$\det A = \prod_{i=1}^{n} \lambda_i \text{ and } \operatorname{tr} A = \sum_{i=1}^{n} \lambda_i.$$

Theorem 1.10. *(see Marcus and Minc, [5], e.g.) If A is a real, symmetric $n \times n$ matrix then all of the eigenvalues of A are real numbers.*

Theorem 1.11. *(Perron-Frobenius Theorem)(see Beineke and Wilson, [1], e.g.) If A is a real, symmetric $n \times n$ matrix whose entries are all non-negative, then $\lambda_1 \geq |\lambda_i|$ for $i = 1, \ldots, n$ and where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of A.*

Definition 1.12. For a vertex v in a graph G, the degree of v, denoted $\deg v$, is the number of vertices adjacent to v in G.

Theorem 1.13. *(First Theorem of Graph Theory)(see Chartrand and Lesniak, [2], e.g.) If G is a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$ then*

$$\sum_{i=1}^{n} \deg v_i = 2m$$

where m is the number of edges in G.

Proposition 1.14. *If $S = A(G)^2 = (s_{ij})$ for some simple, undirected graph G then we have the following:*

(i) $S^T = S$

(ii) $s_{ii} = \deg(v_i)$ *and* $0 \leq s_{ii} \leq n - 1$ *for all* i

(iii) $s_{ij} \leq \min\{s_{ii}, s_{jj}, n-2\}$ *for all* $i \neq j$

(iv) $\operatorname{tr}(S) = 2m$ *where* $m = |E(G)|$ *and so* $0 \leq m \leq n(n-1)$

(v) If λ is an eigenvalue of S then $\lambda \geq 0$

(vi) There exist $e_i \in \{-1, 1\}$ for $i = 2, \ldots, n$ such that $\sqrt{\lambda_1} + \sum_{i=2}^{n} e_i \sqrt{\lambda_i} = 0$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of S.

Proof. Let $A = (a_{ij}) = A(G)$.

(i) We have $S^T = (A^2)^T = A^T A^T = A^2 = S$ since A is symmetric.

(ii) The number of two-walks from vertex v_i to itself is exactly the degree of v_i. Since at most, it can be adjacent to all other vertices in G, we have $\deg v_i = s_{ii} \leq n-1$.

(iii) Suppose $i \neq j$. The number of two-walks from v_i to v_j is the number s_{ij}. A two-walk between v_i and v_j corresponds to a shared neighbor of each vertex, of which, there are at most $\min\{\deg v_i, \deg v_j\} = \min\{s_{ii}, s_{jj}\}$. Since a vertex is never its own neighbor, the greatest number of vertices shared by v_i and v_j is $n-2$. Therefore, $s_{ij} \leq \min\{s_{ii}, s_{jj}, n-2\}$.

(iv) Since $s_{ii} = \deg v_i$ for each i, we have $\operatorname{tr}(S) = \sum \deg(v)$. The result follows from Theorem 1.13.

(v) Since A is a real, symmetric matrix, we know that every eigenvalue of A is a real number. By Theorem 1.8, if λ is an eigenvalue of A then λ^2 must be an eigenvalue of S. Since λ was real, the square must be nonnegative.

(vi) By Theorem 1.8, if λ is an eigenvalue of S then $\sqrt{\lambda}$ or $-\sqrt{\lambda}$ must be an eigenvalue of A. By Theorem 1.9, we have

$$0 = \operatorname{tr} A = \sum_{i=1}^{n} \mu_i = \sum_{j=1}^{n} e_j \sqrt{\lambda_j}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of A. The values of the e_i correspond to the sign needed to recover the eigenvalues of A from the square root of those from S.

Since, by Theorems 1.9 and 1.11, the largest eigenvalue of A must be positive, it must be the case that $e_1 = 1$. Thus,

$$\sqrt{\lambda_1} + \sum_{i=2}^{n} e_i \sqrt{\lambda_i} = 0.$$

□

Theorem 1.15. *If S_1 is square graphic, then so is $S_2 = P^{-1} S_1 P$ for any permutation matrix P.*

Proof. Suppose $S_1 = (s_{ij}) = A(G)^2$ for some graph G on vertices $\{v_1, v_2, \ldots, v_n\}$. If P is a permutation matrix, then there exists $\pi \in S_n$ such that

$$P = \begin{pmatrix} e_{\pi(1)} & e_{\pi(2)} & \cdots & e_{\pi(n)} \end{pmatrix}$$

where e_i is the ith column of the $n \times n$ identity matrix. Now,

$$P^{-1} S_1 P = \begin{pmatrix} e_{\pi(1)}^T \\ e_{\pi(2)}^T \\ \vdots \\ e_{\pi(n)}^T \end{pmatrix} S_1 \begin{pmatrix} e_{\pi(1)} & e_{\pi(2)} & \cdots & e_{\pi(n)} \end{pmatrix} = (s_{\pi(i)\pi(j)}).$$

Consider a renumbering of the vertices of G given by $v_i \mapsto v_{\pi(i)}$. To avoid confusion, denote this graph with G' and let $S_2 = (b_{ij}) = A(G')^2$. We claim now that $S_2 = P^{-1} S_1 P$, but this is immediate, since by definition, $b_{ij} = s_{\pi(i)\pi(j)}$ for all i and j. That is, the number of two-walks from vertex $v_{\pi(i)}$ to $v_{\pi(j)}$ in G' equals the number of two-walks from v_i to v_j in G. Thus, since $P^{-1} S_1 P = S_2 = A(G')^2$, we have that $P^{-1} S_1 P$ is square graphic. □

Since the number of two-walks from a vertex to itself corresponds exactly to the degree of that vertex, the main diagonal of the square of an adjacency matrix will represent the degree sequence of the graph under an appropriate permutation if necessary.

This means that we inherit, as necessary conditions, all the conditions for a degree sequence to be graphic. For example, we have the theorems of Havel-Hakimi and Erdős-Gallai which can be found in many books on graph theory; see Chartrand and Lesniak, [2], for example.

Definition 1.16. We will say S_1 and S_2 are *similar* if there is a permutation matrix P such that $S_2 = P^{-1}S_1P$. In this case, we write $S_1 \sim S_2$.

Remark 1.17. It can be shown that being *similar* is an equivalence relation.

Notice by Theorem 1.15, if $S_1 \sim S_2$ then S_1 is square graphic if and only if S_2 is square graphic.

Remark 1.18. There are matrices that satisfy the conditions from Proposition 1.14 that fail to be square graphic.

Example 1.19. *Consider the square matrix*

$$S = \begin{pmatrix} 3 & 2 & 1 & 1 & 1 & 1 \\ 2 & 3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 2 & 1 & 1 \\ 1 & 1 & 2 & 3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 & 2 \\ 1 & 1 & 1 & 1 & 2 & 3 \end{pmatrix}.$$

Certainly, S is a real, symmetric matrix. The trace of S is 18, which is even. The eigenvalues of S, listed with multiplicity, are $\{9, 3, 3, 1, 1, 1, 0, 0, 0\}$. *Finally, we have*

$$3 + \sqrt{3} - \sqrt{3} - 1 - 1 - 1 + 0 + 0 + 0 = 0$$

and hence, condition (vi) is satisfied. However, the only 3-regular graphs on 6 vertices are $K_{3,3}$ and $K_3 \times K_2$ (see Harary, [4], e.g.) whose adjacency matrices squared are

$$A(K_{3,3})^2 \sim \begin{pmatrix} 3 & 3 & 3 & 0 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 \end{pmatrix}$$

and

$$A(K_3 \times K_2)^2 \sim \begin{pmatrix} 3 & 2 & 0 & 1 & 1 & 2 \\ 2 & 3 & 1 & 0 & 2 & 1 \\ 0 & 1 & 3 & 2 & 2 & 1 \\ 1 & 0 & 2 & 3 & 1 & 2 \\ 1 & 2 & 2 & 1 & 3 & 0 \\ 2 & 1 & 1 & 2 & 0 & 3 \end{pmatrix}.$$

Since each has entries of zero, it is clear that S is not similar to either matrix, and hence, is not square graphic.

Remark 1.20. Note that Theorem 1.15 and Definition 1.16 do not say anything about isomorphisms of graphs. The proof differs from Theorem 1.4 as we are not dealing with adjacency matrices and so we cannot say anything directly about when vertices are adjacent.

The theorem is still important, as it allows us to take a given matrix and permute it into a different form if it is convenient. If we can show the permuted matrix is graphic, then we know the original matrix must be graphic. However, there are graphs such that $A(G)^2 \sim A(H)^2$ and $G \ncong H$.

Example 1.21. *Consider the two graphs from Figures* 1 *and* 2, *each on six vertices with six edges.*

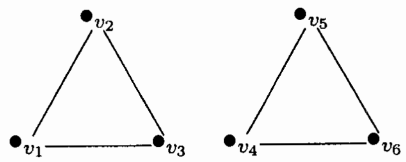

Figure 1. $C_3 \cup C_3$

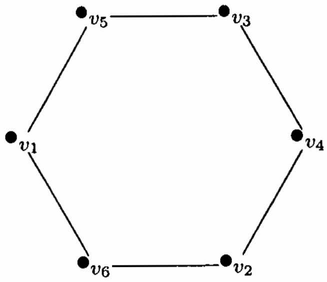

Figure 2. C_6

Note that we have

$$A(C_6)^2 = A(C_3 \cup C_3)^2 = \begin{pmatrix} 2 & 1 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 & 2 \end{pmatrix},$$

but $C_6 \ncong C_3 \cup C_3$

In many of the results to follow, we will be considering matrices with blocks consisting of all zeros. In order to avoid cumbersome notation, a bold zero will represent a matrix consisting of all zeros of the appropriate size according to the context.

Proposition 1.22. *If $S_1 = A(G)^2$ and $S_2 = A(H)^2$ for some graphs G and H then*

$$A(G \cup H)^2 \sim \begin{pmatrix} S_1 & \mathbf{0} \\ \mathbf{0} & S_2 \end{pmatrix}.$$

Proof. Consider the graph $G \cup H$ and a labeling such that the first n vertices belong to the component of $G \cup H$ consisting of G and the next m vertices belong to the component of $G \cup H$ consisting of H. Then certainly there are no new two-walks between G and H when viewed as components of the graph $G \cup H$. And the two-walks of G and H as components of $G \cup H$ are exactly those of G and H, respectively.

That is,

$$A(G \cup H)^2 \sim \begin{pmatrix} S_1 & \mathbf{0} \\ \mathbf{0} & S_2 \end{pmatrix}.$$

□

Definition 1.23. We define $J_{m \times n}$ to be the $m \times n$ matrix whose entries are all one. We will shorten $J_{n \times n}$ to J_n.

Definition 1.24. The join of two graphs G and H on distinct vertex sets $V(G)$ and $V(H)$ is the graph $G + H$ with $V(G + H) = V(G) \cup V(H)$ and $E(G + H) = E(G) \cup E(H) \cup \{e = uv \mid u \in V(G), v \in V(H)\}$.

Proposition 1.25. *Let $S_1 = (s'_{ij}) = A(G)^2$ and $S_2 = (s''_{ij}) = A(H)^2$ for some graphs G and H on n and m vertices, respectively. Then*

$$A(G + H)^2 \sim \begin{pmatrix} S_1 + mJ_n & S \\ S^T & S_2 + nJ_m \end{pmatrix}$$

where $S = (s_{ij})$ is the $n \times m$ matrix with $s_{ij} = s'_{ii} + s''_{jj}$ for all i and j.

Proof. Consider the graph $G + H$ and a labeling such that the first n vertices correspond the vertices originating from G and the next m vertices correspond to the vertices originating from H.

By definition of the join operation, we add every edge starting at a vertex in G and ending at a vertex in H. Thus,

$$A(G+H) \sim \begin{pmatrix} A(G) & J_{n\times m} \\ J_{m\times n} & A(H) \end{pmatrix}.$$

And hence,

$$A(G+H)^2 \sim \begin{pmatrix} A(G)^2 + mJ_n & A(G)J_{n\times m} + J_{n\times m}A(H) \\ J_{m\times n}A(G) + A(H)J_{m\times n} & A(H)^2 + nJ_m \end{pmatrix}.$$

Now we only need to show that the (i,j)-entry of $A(G)J_{n\times m} + J_{n\times m}A(H) = (s_{ij})$ is exactly $s'_{ii} + s''_{jj}$. Consider the entry s_{ij}, it corresponds to the sum of the (i,j)-entries from $A(G)J_{n\times m}$ and $J_{n\times m}A(H)$. But the (i,j)-entry of $A(G)J_{n\times m}$ is exactly the sum of the elements in the ith row of $A(G)$. As this counts the vertices adjacent to vertex v_i in G, this term is exactly s'_{ii}. Similarly, the (i,j)-entry of $J_{n\times m}A(H)$ is the sum of the elements in the jth column of $A(H)$. This corresponds to s''_{jj}, and hence, $s_{ij} = s'_{ii} + s''_{jj}$.

Therefore, $A(G)J_{n\times m} + J_{n\times m}A(H) = S$ as desired and so,

$$A(G+H)^2 \sim \begin{pmatrix} S_1 + mJ_n & S \\ S^T & S_2 + nJ_n \end{pmatrix}.$$

□

Remark 1.26. The previous result can also be proven by counting two-walks in the graph $G + H$. As it is slightly less elegant, that proof was omitted in favor of the one given.

Proposition 1.27. *Let* $A(G)^2 = (s'_{ij})$ *and* H *be a subgraph of* G. *If* $A(G \setminus \{e \notin E(H)\})^2 = (s''_{ij})$ *then* $s''_{ij} \leq s'_{ij}$ *for all* i *and* j.

Proof. First notice that the graph $\overline{H} = G \setminus \{e \notin E(H)\}$ corresponds to the subgraph $H \cup \{v \in V(G) \setminus V(H)\}$ in G. The reason for this construction and not looking at the subgraph H directly is so we are able to compare matrices of the same size.

Notice, since edges are only removed from G to obtain $\overline{H}$, the number of two-walks among any vertices in $\overline{H}$ is not increased. Thus, we have the desired result. □

Example 1.28. *The converse of Proposition* 1.27 *is false. That is, if* $A(G)^2 = (s'_{ij})$ *and* $A(H)^2 = (s''_{ij})$ *for some graphs* G *and* H *and* $s''_{ij} \leq s'_{ij}$ *for all* i *and* j *then* H *is not necessarily a subgraph of* G.

Consider, for example, the graphs in Figures 3 *and* 4 *and their corresponding adjacency matrices squared.*

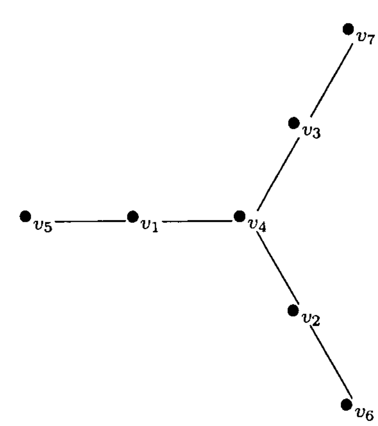

Figure 3. G; a subdivision of $K_{1,3}$

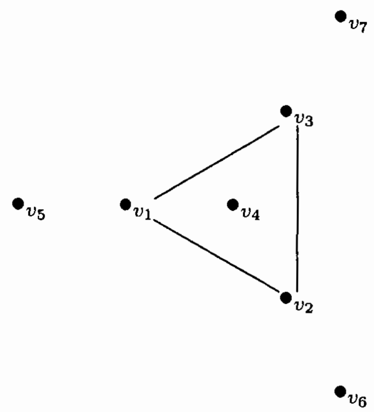

Figure 4. $H = C_3 \cup \{v_4, \ldots, v_7\}$

We have

$$A(G)^2 = (s'_{ij}) = \begin{pmatrix} 2 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

and

$$A(H)^2 = (s''_{ij}) = \begin{pmatrix} 2 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Thus, $s''_{ij} \leq s'_{ij}$ *for all* i *and* j*, but* H *is not a subgraph of* G*.*

1.3. Preliminary Structure Results

The following results relate the structure of the square of the adjacency matrix of a graph with the structure of that graph.

Theorem 1.29. *Suppose S is an $n \times n$ matrix such that $S = A(G)^2$. Then G is bipartite or disconnected if and only if* $S \sim \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}$ *where B_1 is a $k \times k$ matrix with $0 < k < n$.*

Proof. First suppose that G is disconnected with a connected component H on k vertices with $0 < k < n$. Then there are no two-walks from any vertex of H to any vertex of $G \setminus H$. Therefore, renumbering the vertices of G if necessary, we have

$$A(G)^2 \sim \begin{pmatrix} A(H)^2 & 0 \\ 0 & A(G \setminus H)^2 \end{pmatrix}.$$

Setting $B_1 = A(H)^2$ and $B_2 = A(G \setminus H)^2$, it is clear $A(G)^2$ has the desired form.

Now, suppose G is bipartite with partite sets X and Y and that $A(G)^2 = (s_{ij})$. Without loss of generality, we have $X = \{v_1, v_2, \ldots, v_k\}$ (otherwise, relabel the graph accordingly). Since G is bipartite, every two-walk must begin and end in the same partite set. If there is a two-walk $v_i v_j v_k$ with $v_i \in X$ and $v_k \in Y$, then since $v_j \in X$ or $v_j \in Y$ we must have an edge among the vertices of a partite set, which is a contradiction. Hence, $s_{ij} = s_{ji} = 0$ for all $i = 1, 2, \ldots, k$ and $j = k+1, \ldots, n$. Therefore,

$$A(G)^2 = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}$$

where B_1 is $k \times k$ with $0 < k < n$.

To prove the sufficiency of the statement, assume by the contrapositive that G

is connected and nonbipartite. By contradiction, assume

$$A(G)^2 = (s_{ij}) = \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}$$

where B_1 is $k \times k$ with $0 < k < n$. Let $V_1 = \{v_1, v_2, \ldots, v_k\}$ and $V_2 = \{v_{k+1}, \ldots, v_n\}$. Under these assumptions, we must have $s_{ij} = s_{ji} = 0$ for all $i = 1, \ldots, k$ and $j = k+1, \ldots, n$.

Since G is nonbipartite, there is an odd cycle C in G of length t. Without loss of generality, there is a $v \in V(C) \cap V_1$. We now claim that $V(C) \subseteq V_1$.

Write $C = v_{c_0} v_{c_1} \ldots v_{c_{t-1}} v_{c_0}$ where the indices are c_i with $i \mod t$. Then without loss of generality, $v = v_{c_0} \in V_1$. Notice that we must have $v_{c_{i+2}} \in V_1$ whenever $v_{c_i} \in V_1$. Otherwise, if $v_{c_i} \in V_1$ and $v_{c_{i+2}} \in V_2$ then $s_{c_i c_{i+2}} \neq 0$ which is a contradiction, because $c_i \in \{1, \ldots, k\}$ and $c_{i+2} \in \{k+1, \ldots, n\}$. Therefore, $v_{c_{2p}} \in V_1$ for $p = 0, 1, 2, \ldots, t-1$. But since C is of odd length, this forces $V(C) \subseteq V_1$, proving the claim.

Now, if there is a vertex $u \in V(G \setminus C)$ then since G is assumed to be connected, there exists a path P from u to a vertex v on C so that $P \cap C = \{v\}$ (see Figure 5).

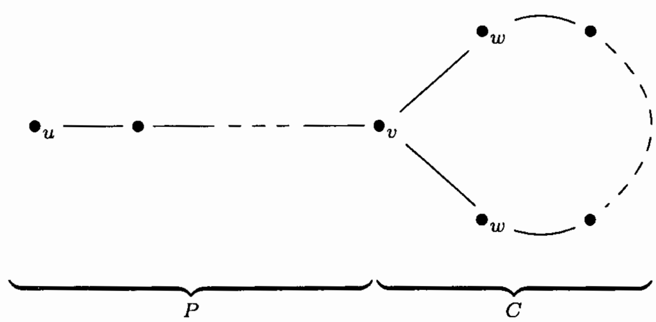

Figure 5. P and C

If P is of even length, then since every second vertex from v on P must also be in V_1, we have that $u \in V_1$. If a vertex of even distance from v is not in V_1, we would contradict the assumption that there are no two-walks starting in V_1 and ending in V_2.

If P is of odd length, consider a neighbor w of v, such that $w \in V(C) \subseteq V_1$. Then $wvPu$ is a path of even length, and the argument from above forces $u \in V_1$.

Therefore, every vertex of G must be in V_1, making $|V_1| = n$ and $|V_2| = 0$ which is a contradiction. Therefore, we have proven the claim by contrapositive. That is, if G is nonbipartite and connected, then $A(G)^2$ is not similar to a block diagonal matrix. □

Definition 1.30. The *neighborhood of a vertex* v in a graph G is the set $\Gamma(v) = \{u \in V(G) \text{ such that } uv \in E(G)\}$.

Corollary 1.31. *Suppose* $S = A(G)^2$ *is an* $n \times n$ *matrix such that* $S \sim \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}$ *where* B_1 *is a* $k \times k$ *matrix with* $0 < k < n$. *Then we have the following:*

(i) If B_1 *or* B_2 *is similar to a block diagonal matrix with two or more blocks, then* G *is disconnected.*

(ii) If $\operatorname{tr} B_1$ *or* $\operatorname{tr} B_2$ *is odd, then* G *is bipartite or has a bipartite component.*

(iii) If $\operatorname{tr} B_1 \neq \operatorname{tr} B_2$*, then* G *is disconnected.*

Proof. (i) By the previous theorem, we know G is disconnected or bipartite. Suppose, without loss of generality, that

$$B_1 \sim \begin{pmatrix} B_{11} & \mathbf{0} \\ \mathbf{0} & B_{12} \end{pmatrix}$$

where B_{11} is size $l \times l$ with $0 < l < k$.

Assume by contradiction, that G is connected. This implies G is a connected, bipartite graph such that

$$A(G)^2 \sim \begin{pmatrix} B_{11} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_{12} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B_2 \end{pmatrix} = (s_{ij}).$$

Let the partite sets of G be X and Y.

First, we claim that for any proper, nonempty subset $E \subset X$ there exists a two-walk from some u in E to some v in $X \setminus E$. To prove the claim, suppose by contradiction there is a subset $E \subset X$ such that there is no two-walk between every u in E and every v in $X \setminus E$. This gives us that

$$\{\Gamma(u) \mid u \in E\} \cap \{\Gamma(v) \mid v \in X \setminus E\} = \emptyset$$

which implies G must be disconnected, which is a contradiction.

Define the sets following sets of vertices: $V_1 = \{v_1, \ldots, v_l\}$, $V_2 = \{v_{l+1}, \ldots, v_k\}$ and $V_3 = \{v_{k+1}, \ldots, v_n\}$. By the previous claim, we now have that vertices from distinct vertex sets V_i and V_j must be in distinct partite sets. However, since there are only two partite sets and three sets of vertices without two-walks between them, there must be a u and v in the same partite set from distinct sets of vertices V_i and V_j. This contradicts G being connected; therefore, G must have been disconnected to start.

(ii) By the previous theorem, G must be disconnected or bipartite. Suppose, without loss of generality, that $\operatorname{tr} B_1$ is odd and that G is not bipartite and has no bipartite component. Then G must be disconnected and each connected component must be nonbipartite. Then if H is a connected component of G, by the previous theorem, H is not similar to a block diagonal matrix.

Let $H_1, \ldots, H_k$ be the distinct connected components of G and relabel G so that the vertices of H_1 are $\{v_1, v_2, \ldots, v_{k_1}\}$, the vertices of H_2 are $\{v_{k_1+1}, \ldots, v_{k_1+k_2}\}$ and so on. Then we have

$$S \sim A(G)^2 \sim \begin{pmatrix} A(H_1)^2 & 0 & \cdots & 0 \\ 0 & A(H_2)^2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & A(H_k)^2 \end{pmatrix}.$$

Therefore, there is a set $E \subset \{1, 2, \ldots, k\}$ such that B_1 is similar to a block diagonal matrix whose blocks are $A(H_i)^2$ with $i \in E$. Thus,

$$\operatorname{tr} B_1 = \sum_{i \in E} \operatorname{tr} A(H_i)^2$$

but each $A(H_i)^2$ is graphic; hence, $\operatorname{tr} A(H_i)^2$ is even for each i. Therefore, $\operatorname{tr} B_1$ must be even, which is a contradiction. Thus, G must be bipartite or have a bipartite component.

(iii) By the previous theorem, we know G must be disconnected or bipartite. Suppose $\operatorname{tr} B_1 \neq \operatorname{tr} B_2$ and by contradiction, that G is connected. Relabel G so that the partite sets of vertices are $X = \{v_1, v_2, \ldots, v_k\}$ and $Y = \{v_{k+1}, v_{k+2}, \ldots, v_n\}$. Then since the only two-walks in G are from one partite set to itself, we must have that, without loss of generality, entries of B_1 correspond to the number of two-walks among vertices in X and entries of B_2 to those among vertices in Y. A similar argument from (i) shows that the partite sets cannot be split among the vertices corresponding to the blocks B_1 and B_2.

Now every edge in G must go between the partite sets X and Y. Thus, if we wish to count the edges in G, it would be enough to add the degrees of the vertices in one partite set. Since the number of edges in a graph is fixed, we can add the degrees of the vertices from one partite set and we must get the same result as when we add the degrees of the vertices from the other partite set.

Since the degrees of the vertices of G lie on the main diagonal of S, by our labeling of G we have $\operatorname{tr} B_1 = \operatorname{tr} B_2$, which is a contradiction. Therefore, G must have been disconnected to start. □

Example 1.21 shows that it will be impossible, in general, to detect connectivity from the square of the adjacency matrix of a graph. However, an optimistic point of view could be that there are multiple graphs associated to a given matrix, thus making the task of determining if a matrix is square graphic possibly easier.

Theorem 1.32. *If $S = (s_{ij}) = A(G)^2$ for some graph G, then*

$$\frac{1}{4}\sum_{i \neq j} \binom{s_{ij}}{2}$$

is the number of distinct cycles of length four in G.

Proof. First, we claim that, for $i \neq j$, $\binom{s_{ij}}{2}$ counts the number of distinct cycles of length four on which vertices v_i and v_j sit opposite. To prove the claim, let $v_i, v_j \in V(G)$ and notice every two-walk from v_i to v_j corresponds to a shared neighbor of the two. Now, a cycle of length four on which v_i and v_j sit opposite occurs when there is a two-walk from v_i to v_j and a different two-walk from v_j to v_i. In other words, v_i and v_j sit opposite on a cycle of length four when we can choose two distinct vertices u and v that are neighbors of both v_i and v_j. Since the number of shared neighbors of v_i and v_j is exactly s_{ij}, the number of cycles of length four on which v_i and v_j sit opposite is $\binom{s_{ij}}{2}$.

Consider a cycle of length four in G: $uvwxu$. In the sum $\sum_{i \neq j} \binom{s_{ij}}{2}$, this cycle is counted once by each of $\binom{s_{uw}}{2}$, $\binom{s_{wu}}{2}$, $\binom{s_{vx}}{2}$, and $\binom{s_{xv}}{2}$. Thus, to count each four cycle in G exactly once, we divide this sum by four. □

Remark 1.33. A necessary condition for a matrix S to be graphic that can be taken from Theorem 1.32 is that the number $\sum_{i \neq j} \binom{s_{ij}}{2}$ must be divisible by four.

Example 1.34. *Considering again the matrix from Example* 1.19 *that satisfied all the conditions from Proposition* 1.14*, we can now use the previous theorem to detect the fact that it is not square graphic. We have*

$$S = \begin{pmatrix} 3 & 2 & 1 & 1 & 1 & 1 \\ 2 & 3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 2 & 1 & 1 \\ 1 & 1 & 2 & 3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 & 2 \\ 1 & 1 & 1 & 1 & 2 & 3 \end{pmatrix}$$

and thus, $\sum_{i \neq j} \binom{s_{ij}}{2} = 6$*, which is not divisible by four, meaning S is not graphic.*

CHAPTER 2. REMOVING VERTICES

The following are several results dealing with the removal of vertices of certain degrees and the effect on the square of the adjacency matrix.

2.1. Full and Null Degree

The following definition will be needed in future results. It can be used as a way to reduce the size of the square of an adjacency matrix and corresponds to the removal of vertices from the graph.

Definition 2.1. If A is an $n \times n$ matrix, let A_{ij} be the $(n-1) \times (n-1)$ matrix formed by deleting the ith row and jth column from A.

We start our exploration of the removal of vertices with the removal of vertices with 'full' and 'null' degrees. That is, vertices adjacent to all other vertices in the graph and vertices adjacent to no other vertices in the graph.

Lemma 2.2. *Suppose $S = (s_{ij})$ is an $n \times n$ matrix such that $s_{pp} = n - 1$ for some p. If S is square graphic, then so is $S_{pp} - J_{(n-1)}$. Also, if $S' = (s'_{ij})$ is an $n \times n$ square graphic matrix, then*

$$S = \begin{pmatrix} & & & & s'_{11} \\ & S' + J_n & & & s'_{22} \\ & & & & \vdots \\ & & & & s'_{nn} \\ s'_{11} & s'_{22} & \cdots & s'_{nn} & n \end{pmatrix}$$

is an $(n+1) \times (n+1)$ square graphic matrix.

Proof. Assume $S = A(G)^2$ for some graph G and that, without loss of generality, $s_{nn} = n - 1$. If $s_{pp} = n - 1$, then the permutation simultaneously swapping row and column p with row and column n results in $s_{nn} = n - 1$. Then $\deg(v_n) = n - 1$ and vertex v_n is adjacent to each vertex v_i for $i = 1, 2, \ldots, n - 1$. Now for all i and j between 1 and $n - 1$, not necessarily distinct, we have the two-walk $v_i v_n v_j$ which contributes a one to s_{ij}. Every other two-walk from v_i to v_j must go through a vertex different from v_n. Thus, the removal of vertex v_n from G decreases s_{ij} by exactly one for all i and j between 1 and $n - 1$. Since all other two-walks are preserved, we have $A(G \setminus \{v_n\})^2 = S_{nn} - J_{(n-1)}$. Hence, $S_{nn} - J_{(n-1)}$ is square graphic, as, in general, is $S_{pp} - J_{(n-1)}$.

Now, suppose $S' = (s'_{ij})$ is an $n \times n$ graphic matrix such that $S' = A(G)^2$ for some graph G on the vertices $\{v_1, v_2, \ldots, v_n\}$. Consider the graph $G + \{v_{n+1}\}$. Since $A(\{v_{n+1}\})^2 = (0)$, by Proposition 1.25 we have

$$A(G + \{v\})^2 = \begin{pmatrix} & & & s'_{11} \\ & S' + J_n & & s'_{22} \\ & & & \vdots \\ s'_{11} & s'_{22} & \cdots & n \end{pmatrix}$$

and hence, is square graphic. □

Lemma 2.3. *Let $S = (s_{ij})$ be an $n \times n$ matrix such that $s_{pp} = n - 1$ for some p. If S is square graphic then $s_{pq} = s_{qp} = s_{qq} - 1$ for all $q \neq p$.*

Proof. Suppose $S = A(G)^2$ for some graph G. Then in G, $\deg(v_p) = n - 1$ implies that $v_p v_q \in E(G)$ for all $q \neq p$. For each neighbor v of v_q with $v \neq v_p$ (of which there are $\deg(v_q) - 1$) we get the two-walk $v_p v v_q$. Since every two-walk from v_p to any vertex v_q must have this form, there are $\deg(v_q) - 1$ two-walks from v_p to v_q. Thus, $s_{pq} = \deg(v_q) - 1 = s_{qq} - 1$ for all $q \neq p$. Also, by symmetry, it follows that $s_{qp} = s_{qq} - 1$, proving the claim. □

Theorem 2.4. *Let $S = (s_{ij})$ be an $n \times n$ matrix such that $s_{pp} = n - 1$ for some p and $s_{pq} = s_{qp} = s_{qq} - 1$ for all $q \neq p$ then S is square graphic if and only if $S_{pp} - J_{n-1}$ is square graphic.*

Proof. Apply Lemma 2.2 and Lemma 2.3. □

Theorem 2.5. *Suppose $S = (s_{ij})$ is an $n \times n$ matrix such that $s_{pp} = 0$ for some p and that $s_{pq} = s_{qp} = 0$ for all $q \neq p$. Then S is square graphic if and only if S_{pp} is square graphic.*

Proof. Suppose $S = A(G)^2$. Then in G, v_p corresponds to a degree zero vertex; that is, an isolated vertex. Therefore, there are no two-walks to, from, or through vertex v_p. The removal of this vertex results in the graph $G \setminus \{v_p\}$ with $A(G \setminus \{v_p\})^2 = S_{pp}$. Therefore, S_{pp} is square graphic.

For the converse, consider the $(n-1) \times (n-1)$ matrix $S_{pp} = A(G)^2$. Then the addition of an isolated vertex v_n results in no additional two-walks among any vertices of G. Then we have

$$A(G \cup \{v_n\})^2 = \begin{pmatrix} & & & 0 \\ & S_{pp} & & 0 \\ & & & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \sim S.$$

Therefore, S must also be square graphic. □

By Theorem 2.4 and 2.5, when deciding if an $n \times n$ matrix S is square graphic, if the off-diagonal elements satisfy the proper hypotheses, we can reduce the problem to looking at the matrix formed from S by removing any rows and columns whose diagonal element is zero or $n - 1$.

Example 2.6. *This example will illustrate the use of the previous two results to determine if a matrix is square graphic. Consider the matrix*

$$S = \begin{pmatrix} 4 & 3 & 2 & 0 & 2 & 2 & 2 & 3 \\ 3 & 4 & 2 & 0 & 2 & 2 & 2 & 3 \\ 2 & 2 & 4 & 0 & 2 & 2 & 2 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & 0 & 4 & 2 & 2 & 3 \\ 2 & 2 & 2 & 0 & 2 & 4 & 3 & 3 \\ 2 & 2 & 2 & 0 & 2 & 3 & 4 & 3 \\ 3 & 3 & 3 & 0 & 3 & 3 & 3 & 6 \end{pmatrix}.$$

By Theorem 2.5, *S is square graphic if and only if*

$$S_{44} = \begin{pmatrix} 4 & 3 & 2 & 2 & 2 & 2 & 3 \\ 3 & 4 & 2 & 2 & 2 & 2 & 3 \\ 2 & 2 & 4 & 2 & 2 & 2 & 3 \\ 2 & 2 & 2 & 4 & 2 & 2 & 3 \\ 2 & 2 & 2 & 2 & 4 & 3 & 3 \\ 2 & 2 & 2 & 2 & 3 & 4 & 3 \\ 3 & 3 & 3 & 3 & 3 & 3 & 6 \end{pmatrix}$$

is square graphic.

Notice, there is a diagonal entry corresponding to a vertex of full degree and that the off-diagonal entries satisfy the proper hypotheses.

By Theorem 2.4, S_{44} *is square graphic if and only if the following matrix is square graphic, which by Examples* 1.19 *and* 1.34, *is not.*

$$(S_{44})_{77} - J_6 = \begin{pmatrix} 3 & 2 & 1 & 1 & 1 & 1 \\ 2 & 3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 2 & 1 & 1 \\ 1 & 1 & 2 & 3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 & 2 \\ 1 & 1 & 1 & 1 & 2 & 3 \end{pmatrix}$$

Therefore, S is not square graphic.

2.2. Row and Column Sums

While at first it may appear off-topic, the following results give an interpretation of the row and column sums of the square of an adjacency matrix. This interpretation will be useful later in this section in providing more results on the removal of vertices.

Theorem 2.7. *If $S = (s_{ij}) = A(G)^2$ for some graph G then*

$$\sum_{j=1}^{n} s_{ij} = \sum_{j=1}^{n} s_{ji} = \sum_{v \in \Gamma(v_i)} \deg(v)$$

and thus, if $s_{ii} \neq 0$

$$\frac{1}{s_{ii}} \sum_{j=1}^{n} s_{ij}$$

gives the average degrees of the neighbors of v_i.

Proof. Consider $v_i \in G$ and some $v \in \Gamma(v_i)$. Then there are exactly $\deg v$ two-walks of the form $v_i v u$. Since every two-walk starting at v_i must go through some neighbor of v_i, by taking the sum of the degrees of the neighbors of v_i, we will have counted all possible two-walks from v_i. On the other hand, $\sum_j s_{ij}$ gives the total number of two-walks starting at v_i. Thus,

$$\sum_{j=1}^{n} s_{ij} = \sum_{v\in\Gamma(v_i)} \deg(v).$$

The number of summands on the right hand side is exactly $|\Gamma(v_i)| = \deg(v_i) = s_{ii}$. Dividing across gives the desired result. □

Corollary 2.8. *If $S = (s_{ij}) = A(G)^2$ for some graph G then for each i there is $E_i \subseteq \{s_{11}, s_{22}, \ldots, s_{nn}\} \setminus \{s_{ii}\}$ (viewed as a multiset if necessary) such that $|E_i| = s_{ii}$ and*

$$\sum_{s\in E_i} s = \sum_{j=1}^{n} s_{ij}.$$

Proof. We have

$$\sum_{j=1}^{n} s_{ij} = \sum_{v\in\Gamma(v_i)} \deg(v)$$

and since $|\Gamma(v_i)| = \deg(v_i) = s_{ii}$, the number of summands on the right hand side of this equation is s_{ii}. For each $v_j \in \Gamma(v_i)$, we have $\deg(v_j) = s_{jj}$. Taking $E_i = \{s_{jj}$ such that $v_j \in \Gamma(v_i)\}$ gives the desired result. □

Corollary 2.9. *If $S = (s_{ij}) = A(G)^2$ where G is a k-regular graph, then*

$$\sum_{j=1}^{n} s_{ij} = \sum_{j=1}^{n} s_{ji} = k^2.$$

Proof. We have

$$\sum_{j=1}^{n} s_{ij} = \sum_{v\in\Gamma(v_i)} \deg(v) = \sum_{v\in\Gamma(v_i)} k = k^2$$

since $|\Gamma(v_i)| = \deg(v_i) = k$ for all i. □

It should be noted that, the previous results can be used to determine if a matrix S is square graphic as shown in the next example.

Example 2.10. *Consider the matrix*

$$S = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}.$$

Then by the previous results, if S were square graphic, then the average degree of the neighbors of v_2 would be

$$\frac{1}{s_{22}} \sum_{i=1}^{4} s_{2i} = \left(\frac{1}{2}\right)(5) = \frac{5}{2}.$$

This implies that v_2 must have a neighbor of degree at least 3, which is impossible given the diagonal of S. Therefore, S cannot be square graphic.

2.3. More Removal Results

Theorem 2.11. *Suppose $S = (s_{ij})$ is square graphic. If $s_{pp} = 1$ for some p then there exists $q \neq p$ such that $s_{pq} = s_{qp} = 0$; $s_{qq} = \sum_{i=1}^{n} s_{pi}$; and*

$$\begin{pmatrix} s_{11} & \cdots & s_{1q} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots & & \vdots \\ s_{q1} & \cdots & s_{qq} - 1 & \cdots & s_{qn} \\ \vdots & & \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nq} & \cdots & s_{nn} \end{pmatrix}_{pp}$$

is also square graphic.

Proof. Assume $S = (s_{ij}) = A(G)^2$ for some graph G and that $s_{pp} = 1$. Then we have $\deg(v_p) = 1$; that is, there is exactly one q such that v_p is adjacent to v_q. If $s_{pq} \neq 0$ then there is a two-walk $v_p v v_q$ for some vertex $v \neq v_q$. But $\deg(v_p) = 1$, therefore, this is a contradiction. Thus, $s_{pq} = s_{qp} = 0$

Now, by Theorem 2.7,

$$\sum_{i=1}^{n} s_{pi} = \sum_{v\in\Gamma(v_p)} \deg(v) = \deg(v_q) = s_{qq}$$

since $\Gamma(v_p) = \{v_q\}$.

Finally, since the only two-walk through vertex v_p is $v_q v_p v_q$, when vertex v_p is removed from G, $\deg(v_q)$ is reduced by one and all other two-walks among vertices in $G \setminus \{v_p\}$ are preserved. Therefore,

$$A(G\setminus\{v_p\})^2 = \begin{pmatrix} s_{11} & \cdots & s_{1q} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots & & \vdots \\ s_{q1} & \cdots & s_{qq}-1 & \cdots & s_{qn} \\ \vdots & & \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nq} & \cdots & s_{nn} \end{pmatrix}_{pp}$$

and hence, is square graphic. □

Theorem 2.12. *Suppose $S = (s_{ij})$ is an $n \times n$ square graphic matrix with $n \geq 2$. If $s_{pp} = n - 2$ for some p then there exists $q \neq p$ such that $s_{qq} = \operatorname{tr} S - s_{pp} - \sum_{i=1}^{n} s_{pi}$; $s_{pq} = s_{qp} = s_{qq}$; $s_{ij} > 0$ for all $i, j \in \{1, \ldots, n\} \setminus \{p, q\}$; and if $S' = (s'_{ij})$ where*

$$s'_{ij} = \begin{cases} s_{ij} - 1 \text{ if } i,j \in \{1,\ldots,n\}\setminus\{q\} \\ s_{ij} \text{ else} \end{cases}$$

then S'_{pp} is also square graphic.

Proof. Assume $S = (s_{ij}) = A(G)^2$ for some graph G and that $s_{pp} = n - 2$. Then in G, vertex v_p is adjacent to all but one vertex, call it v_q. By Theorem 2.7, the sum of the entries of the pth row of S is the same as the sum of the degrees of the neighbors of v_p. Thus, we have

$$\sum_{i=1}^{n} s_{pi} = \big(\sum_{j=1}^{n} s_{jj}\big) - s_{qq} - s_{pp}$$

since v_p is adjacent to all vertices in G except v_q and itself. Rewritten, we have

$$\sum_{i=1}^{n} s_{pi} = \operatorname{tr} S - s_{qq} - s_{pp}$$

which gives us the following equation for the degree of v_q:

$$\deg(v_q) = s_{qq} = \operatorname{tr} S - s_{pp} - \sum_{i=1}^{n} s_{pi}.$$

Next, notice for every pair of distinct vertices $v_i, v_j \in V(G) \setminus \{v_p, v_q\}$, v_p is a common neighbor. That is, there is the two-walk $v_i v_p v_j$ in G, and hence, $s_{ij} > 0$ for all $i, j \in \{1, \ldots, n\} \setminus \{p, q\}$.

Now, every two-walk from v_p to v_q must go through a shared neighbor. Since v_p is adjacent to all the neighbors of v_q, each will contribute exactly one two-walk. Therefore, $s_{pq} = s_{qp} = \deg(v_q) = s_{qq}$.

Finally, the removal of vertex v_p from G will decrease the degree of every vertex by one except that of v_q, since v_p is adjacent to all vertices but v_q. Also, since for each vertex v_i and v_j adjacent to v_p we have the two-walk $v_i v_p v_j$, the removal of vertex v_p will result in the decrease of s_{ij} and s_{ji} by one. This occurs for every pair of vertices except any containing v_q. That is, s_{ij} is decreased by one for all $i, j \in \{1, \ldots, n\} \setminus \{q\}$ after the removal of vertex v_p.

Therefore, $A(G \setminus \{v_p\})^2 = S'_{pp}$ as described, and hence is square graphic. □

Theorem 2.13. *Suppose $S = (s_{ij})$ is an $n \times n$ square graphic matrix with $n \geq 3$. If $s_{pp} = 2$ for some p then there exist distinct $q, r \in \{1, \ldots, n\} \setminus \{p\}$ (say $q < r$ without loss of generality) such that $s_{qq} + s_{rr} = \sum_{i=1}^{n} s_{pi}$; $s_{pq} = s_{pr} \in \{0, 1\}$; $s_{qr} = s_{rq} > 0$;*

and

$$\begin{pmatrix} s_{11} & \cdots & s_{1q} & \cdots & s_{1r} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ s_{q1} & \cdots & s_{qq}-1 & \cdots & s_{qr}-1 & \cdots & s_{pn} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ s_{r1} & \cdots & s_{rq}-1 & \cdots & s_{rr}-1 & \cdots & s_{rn} \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nq} & \cdots & s_{nr} & \cdots & s_{nn} \end{pmatrix}_{pp}$$

is also square graphic.

Proof. Assume $S = (s_{ij}) = A(G)^2$ for some graph G and that $s_{pp} = 2$. Then we have that $\deg(v_p) = 2$; that is, there are two vertices v_q and v_r adjacent to v_p.

By Theorem 2.7,

$$\sum_{i=1}^{n} s_{pi} = \sum_{v \in \Gamma(v_p)} \deg(v) = \deg(v_q) + \deg(v_r) = s_{qq} + s_{rr}$$

since $\Gamma(v_p) = \{v_q, v_r\}$.

Now, either $v_q v_r \in E(G)$ or $v_q v_r \notin E(G)$. If $v_q v_r \in E(G)$ then we have the two-walks $v_p v_q v_r$ and $v_p v_r v_q$ in G. Hence, if $v_q v_r \in E(G)$ then $s_{pr} = s_{pq} = 1$.

If $v_q v_r \notin E(G)$ then there is not two-walk from v_p to either v_q or v_r. Hence, if $v_q v_r \notin E(G)$ then $s_{pr} = s_{pq} = 0$.

Next, we know $s_{qr} = s_{rq} > 0$ since there is at least the two-walk $v_q v_p v_r$ between v_q and v_r.

The removal of vertex v_p from G decreases the degrees of v_q and v_r by one. That is, s_{qq} and s_{rr} are reduced by one after the removal of v_p. Since v_p is only adjacent to these two vertices, all other degrees are unaffected.

Also, the only two-walk through v_p is $v_q v_p v_r$ (by symmetry, $v_r v_p v_q$). Thus, s_{qr}

and s_{rq} are both decreased by one, and all other off-diagonal entries are unaffected after the removal of vertex v_p.

Therefore,

$$A(G \setminus \{v_p\})^2 = \begin{pmatrix} s_{11} & \cdots & s_{1q} & \cdots & s_{1r} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ s_{q1} & \cdots & s_{qq}-1 & \cdots & s_{qr}-1 & \cdots & s_{pn} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ s_{r1} & \cdots & s_{rq}-1 & \cdots & s_{rr}-1 & \cdots & s_{rn} \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nq} & \cdots & s_{nr} & \cdots & s_{nn} \end{pmatrix}_{pp}$$

and hence, is square graphic. □

Theorem 2.14. *Suppose $S = (s_{ij})$ is an $n \times n$ square graphic matrix with $n \geq 3$. If $s_{pp} = n - 3$ for some p then there exist $q, r \in \{1, \ldots, n\} \setminus \{p\}$ such that $s_{qq} + s_{rr} = \operatorname{tr} S - s_{pp} - \sum_{i=1}^{n} s_{pi}$; $s_{ij} > 0$ for all $i, j \in \{1, \ldots, n\} \setminus \{p, q, r\}$; and if $S' = (s'_{ij})$ where*

$$s'_{ij} = \begin{cases} s_{ij} - 1 \text{ if } i, j \in \{1, \ldots, n\} \setminus \{q, r\} \\ s_{ij} \text{ else} \end{cases}$$

then S'_{pp} is also square graphic.

Proof. Assume $S = (s_{ij}) = A(G)^2$ for some graph G and that $s_{pp} = n - 3$. Then in G, vertex v_p is adjacent to all but two vertices, call them v_q and v_r.

By Theorem 2.7 and a similar argument as in Theorem 2.12, we have

$$s_{qq} + s_{rr} = \operatorname{tr} S - s_{pp} - \sum_{i=1}^{n} s_{pi}.$$

Next, notice for every pair of distinct vertices $v_i, v_j \in V(G) \setminus \{v_p, v_q, v_r\}$, v_p is a common neighbor. That is, there is the two-walk $v_i v_p v_j$ in G, and hence, $s_{ij} > 0$ for all $i, j \in \{1, \ldots, n\} \setminus \{p, q, r\}$.

Finally, the removal of vertex v_p from G will decrease the degree of every vertex by one except vertices v_q and v_r. That is, s_{ii} is reduced by one for all $i \in \{1, \ldots, n\} \setminus \{p, q, r\}$ after the removal of vertex v_p. Since we have the two-walk $v_i v_p v_j$ for all v_i and v_j adjacent to v_p, the removal of v_p from G reduces s_{ij} and s_{ji} by one. That is, s_{ij} is decreased by one for all $i, j \in \{1, \ldots, n\} \setminus \{p, q, r\}$ after the removal of vertex v_p.

Therefore, $A(G \setminus \{v_p\})^2 = S'_{pp}$ as described and hence, is square graphic. □

Remark 2.15. It is possible to use the results from the previous sections to help determine plausible neighborhoods given a matrix. These techniques can help build a candidate graph for a given matrix. This process is highlighted in the following example.

Example 2.16. *Consider the matrix*

$$S = (s_{ij}) = \begin{pmatrix} 4 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 3 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 3 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 2 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 2 \end{pmatrix}.$$

Notice that $s_{11} = 7 - 3 = 4$. *Thus, if* $S = A(G)^2$ *for some graph* G *then* v_1 *is* *not adjacent to two vertices v_q and v_r. By Theorem 2.14, we know*

$$s_{qq} + s_{rr} = \operatorname{tr} S - s_{11} - \sum_{i=1}^{7} s_{1i} = 16 - 10 - 4 = 2.$$

The only choice for q and r is 2 and 3. That is, if G exists, vertex v_1 is adjacent to all vertices except v_2 and v_3.

Continuing by looking at vertices v_2 and v_3 and using ideas from Theorem 2.11, we see that each must be adjacent to a vertex of degree 3. Since $s_{25} \neq 0$, we know v_2 is adjacent to v_4. Similarly, since $s_{34} \neq 0$, we know v_3 is adjacent to v_5.

Next, by Theorem 2.7,

$$\sum_{i=1}^{7} s_{4i} = \sum_{i=1}^{7} s_{5i} = 8$$

tells us the sum of the degrees of the neighbors of each vertex. Since each v_4 and v_5 is already adjacent to a vertex of degree 4 and of degree 1, we know each must be adjacent to a vertex of degree 3. That is, v_4 must be adjacent to v_5.

By a similar argument, we see that v_6 and v_7 must be adjacent to each other. This gives us one plausible graph B (see Figure 6) with the forced adjacencies occurring.

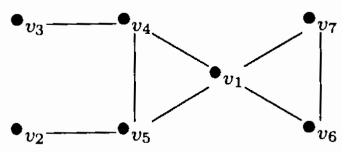

Figure 6. B; a candidate for $S = A(B)^2$

To determine that S is indeed square graphic, we check to see that $S = A(B)^2$ as desired.

CHAPTER 3. CHARACTERIZATIONS

There are several classes of graphs of which the square of the adjacency matrix determines the graph. The graphs included next are the empty graph on n vertices, the complete graph on n vertices, the complete bipartite graph with partite sets of size m and n, the n-point star, 1-regular graphs, 2-regular graphs and paths.

3.1. Empty, Complete and Complete Bipartite Graphs

Theorem 3.1. *We have $S \sim A(\overline{K_n})^2$ if and only if S is the $n \times n$ matrix consisting of all zeros.*

Proof. First, suppose $S = (s_{ij}) \sim A(\overline{K_n})^2$. Since $\overline{K_n}$ has no edges, there are no two-walks between any vertices v_i and v_j, distinct or otherwise. That is, for all i and j, we have $s_{ij} = 0$. Hence, S is the $n \times n$ matrix consisting of all zeros.

On the other hand, suppose $S = (s_{ij})$ such that $s_{ij} = 0$ for all i and j. In a labeled $\overline{K_n}$, there are no two-walks between any vertices v_i and v_j, distinct or otherwise. That is, $A(\overline{K_n})^2$ is the $n \times n$ matrix consisting of all zeros. Hence, $S = A(\overline{K_n})^2$.

It should be noted that this is indeed a characterization of this matrix. Let S be the $n \times n$ matrix consisting of all zeros. If $S = A(G)^2$ for some G, then, by the main diagonal of S, we know the degree sequence of G must be $\underbrace{0, 0, \ldots, 0}_{n}$. Therefore, if $S = A(G)^2$, then $G = \overline{K_n}$. Since we have shown S is square graphic, we now know that S uniquely determines $A(\overline{K_n})^2$. □

Theorem 3.2. *For $n \geq 2$, we have $S \sim A(K_n)^2$ if and only if $S = (n-2)J_n + I_n$.*

Proof. First, suppose $S = (s_{ij}) \sim A(K_n)^2$ and consider v_i in K_n. Since v_i is adjacent to all other vertices, we must have $s_{ii} = n - 1$. Now, if v_j is some other vertex, then

v_i and v_j have all other vertices as common neighbors. That is, v_k is adjacent to both v_i and v_j, for all $k \in \{1, 2, \ldots, n\} \setminus \{i, j\}$. Through each of these shared neighbors, v_k, is the two-walk $v_i v_k v_j$ from v_i to v_j. Since there are $n-2$ choices for v_k, we must have $s_{ij} = n - 2$ for all $i \neq j$. Therefore, $S = (n-2)J_n + I_n$.

On the other hand, suppose $S = (s_{ij}) = (n-2)J_n + I_n$. In a labeled K_n, every vertex v_i is adjacent to all other vertices in K_n, of which there are $n-1$. That is, all entries on the main diagonal of $A(K_n)^2$ must be $n-1$. Through a similar argument as above, there are $n-2$ two-walks between any two distinct vertices v_i and v_j. Hence, every off-diagonal entry of $A(K_n)^2$ must be $n-2$. Therefore, $S = A(K_n)^2$.

Note that this is indeed a characterization of this matrix. Let $S = (n-2)J_n + I_n$. If $S = A(G)^2$ for some G, then the main diagonal of S would force $G = K_n$. Since we have shown S is square graphic, we now know that S uniquely determines $A(K_n)^2$. □

Definition 3.3. A symmetric matrix S is called *reducible* if it can be placed into block diagonal form by a series of simultaneous row/column permutations. That is, S is reducible if it is similar to a block diagonal matrix. A matrix is called *irreducible* otherwise.

Theorem 3.4. *Let $S = (s_{ij})$ be an $(m+n) \times (m+n)$ matrix with $m, n \geq 1$. We have $S \sim A(K_{m,n})^2$ if and only if there is $E \subseteq \{1, 2, \ldots, m+n\}$ such that $|E| = m$ and*

$$s_{ij} = \begin{cases} n \text{ when } i, j \in E \\ m \text{ when } i, j \in \{1, 2, \ldots, m+n\} \setminus E \\ 0 \text{ otherwise.} \end{cases}$$

Proof. Suppose $S \sim A(K_{m,n})^2 = (s_{ij})$ and let $X, Y \subseteq V(K_{m,n})$ be the partite sets of the graph such that $|X| = m$ and $|Y| = n$. Let $E = \{i \mid v_i \in X\}$ and notice that $|E| = |X| = m$. Now, if v_i is in X, then v_i is adjacent to exactly those vertices not in

X, of which there are n. Therefore, $\deg(v_i) = n$ for all v_i in X and hence, $s_{ii} = n$ for all i in E.

Next, if v_i and v_j are distinct vertices from E, then each is adjacent to every vertex in Y. Thus, there are n two-walks between v_i and v_j, one for each of the n neighbors v_i and v_j share. Hence, $s_{ij} = s_{ji} = n$ for all i and j in E.

Now, if v_i is in X and v_j is in Y, then there are no two-walks from v_i to v_j or vice versa. Hence, $s_{ij} = s_{ji} = 0$ for all i in E and all j in $\{1, 2, \ldots, m+n\} \setminus E$.

Finally, by a similar argument as before, if v_i and v_j are distinct vertices in Y, then $\deg(v_i) = m$ and there are m two-walks between v_i and v_j. Hence, $s_{ii} = s_{ij} = s_{ji} = m$ for all i and j in $\{1, 2, \ldots, m+n\} \setminus E$.

Putting all of this together and using the above definition for the set E, we see that the entries of S have the desired form.

To prove the converse, consider a matrix S and a set E such that the entries of S satisfy the given conditions. Consider a labeling of $K_{m,n}$ with partite sets X and Y by defining $X = \{v_i \mid i \in E\}$ and $Y = \{v_j \mid j \notin E\}$. Then, under this labeling, a similar argument as above shows that we have $A(K_{m,n})^2 = S$.

Consider a matrix S and a set E such that the entries of S satisfy the given conditions and suppose that $S = A(G)^2$ for some graph G. Through an appropriate series of permutations, we have $S \sim \begin{pmatrix} nJ_m & \mathbf{0} \\ \mathbf{0} & mJ_n \end{pmatrix}$.

By Theorem 1.29, we know that G would have to be bipartite or disconnected. But since each block is irreducible, if G were disconnected then each block would represent a nonbipartite, connected component. However, by Proposition 1.14, the off-diagonal entries of each block would have to be at most one less than each diagonal entry if they were to be graphic. Since this is not the case, each block by itself is not graphic and hence, G must be bipartite and connected.

By a similar argument as in Corollary 1.31.(i), the partite sets of G must be

$X = \{v_1, \ldots, v_m\}$ and $Y = \{v_{m+1}, \ldots, v_{m+n}\}$. Since no two vertices from the same partite set are adjacent and $\deg(u) = n$ for $u \in X$ and $\deg(v) = m$ for $v \in Y$, it must be that every vertex from X is adjacent to every vertex in Y. Therefore, G must be $K_{m,n}$. □

Remark 3.5. The n-point star is a special case of the complete bipartite graph with partite sets of size m and n, where we take $m = 1$. Thus, the n-point star is uniquely determined and has the following form:

$$A(K_{1,n})^2 \sim \begin{pmatrix} n & 0 \\ 0 & J_n \end{pmatrix}.$$

3.2. One- and Two-Regular Graphs

Theorem 3.6. *We have $S \sim A(\bigcup_{i=1}^{k} K_2)^2$ if and only if $S = I_{2k}$.*

Proof. First, suppose $S \sim A(\bigcup_{i=1}^{k} K_2)^2$. Then all of the $2k$ vertices have degree one and there are no two-walks between any two distinct vertices. Therefore, $S = I_{2k}$.

Now, suppose $S = I_{2k}$. If $S = A(G)^2$ for some graph G, then since the main diagonal of S determines the degrees of the vertices of G, G would have to be 1-regular. As the size of S determines the order of G, G would have $2k$ vertices. Finally, as there are no nonzero, off-diagonal entries, this implies that G would have no two-walks between any two distinct vertices. Therefore, $G = \bigcup_{i=1}^{k} K_2$. □

Before giving the characterization of 2-regular graphs, some lemmas are needed.

Lemma 3.7. *If $S = (s_{ij})$ is an $n \times n$ irreducible matrix with $n \geq 3$, such that:*

(i) S is symmetric,

(ii) $s_{ii} = 2$ for all $i = 1, \ldots, n$,

(iii) $\sum_{j=1}^{n} = 4$ *for all* $i = 1, \ldots, n,$

(iv) $s_{ij} \in \{0, 1\}$ *for all* $i \neq j$

then $S \sim T_n$ *where* $T_n = (t_{ij})$ *is the* $n \times n$ *matrix defined as follows:*

(i) $t_{ii} = 2$ *for* $i = 1, \ldots, n$

(ii) $t_{(i+)i} = t_{i(i+1)} = 1$ *for* $i = 1, \ldots, n-1$

(iii) $t_{1n} = t_{n1} = 1$

(iv) $t_{ij} = 0$ *otherwise.*

That is,

$$S \sim T_n = \begin{pmatrix} 2 & 1 & 0 & \cdots & & \cdots & 0 & 0 & 1 \\ 1 & 2 & 1 & \ddots & & & & 0 & 0 \\ 0 & 1 & 2 & \ddots & & & & & 0 \\ \vdots & \ddots & \ddots & \ddots & & & & & \vdots \\ & & & & \ddots & & & & \\ \vdots & & & & & \ddots & \ddots & \ddots & \vdots \\ 0 & & & & & \ddots & 2 & 1 & 0 \\ 0 & 0 & & & & \ddots & 1 & 2 & 1 \\ 1 & 0 & 0 & \cdots & & \cdots & 0 & 1 & 2 \end{pmatrix}.$$

Proof. Suppose S is an $n \times n$ irreducible matrix that satisfies the four conditions from the hypothesis. Assume by contradiction that $S \not\sim T_n$; that is, $P^{-1}SP \neq T_n$ for all permutation matrices P. Then, working from the top left corner of S, down and to the right, swapping rows and columns as needed to permute S into T_n, there must be some $k < n$ such that $s_{ij} = t_{ij}$ and $s_{ji} = t_{ji}$ for $i = 1, \ldots, k-1$ and $j = 1, \ldots, n$, but there is no permutation swapping rows/columns to complete the next step to permute

S into T_n. Otherwise, we could continue this process for the n rows and columns and permute S into T_n which would contradict our assumption.

It should be noted that such a process can be started, as the first row/column of S must have $s_{11} = 2$ and exactly two other entries equal to 1, say in positions s_{1i} and s_{1j}. A permutation changing this first row/column of S to the first row/column of T_n corresponds to the permutation $\pi = (i2)(jn)$. Thus, the first row and column of $P_\pi^{-1} S P_\pi$ are those of T_n

Note that another permutation changing the first row/column of S to that of T_n is $\pi = (in)(j2)$. The same argument will work for either case, so, without loss of generality, choose the permutation for which the most rows/columns of S can be permuted to those of T_n.

Since each row/column sum is four, $s_{ii} = 2$ and $s_{ij} \in \{0, 1\}$ for each $i \neq j$, we must have two ones off of the main diagonal in each row and column. By assumption, we have permuted the first $k - 1$ rows/columns of S into those of T_n. Therefore, we must have $s_{k(k-1)} = s_{(k-1)k} = 1$ and the other nonzero, off-diagonal entry from row/column k must be in position s_{kl} (s_{lk}, respectively) where $k+1 \leq l \leq n$. However, if $s_{k(k+1)} = s_{(k+1)k} = 1$ then row/column k matches that of T_n which is a contradiction. Thus, $l > k + 1$.

If $k + 1 < l < n$ then $s_{kl} = 1$ and $s_{il} = 0$ for $i = 1, \ldots, k - 1$ by assumption (similarly, $s_{lk} = 1$ and $s_{li} = 0$ for $i = 1, \ldots, k-1$). Therefore, a permuting row/column l with row/column $k + 1$ does not affect the rows/columns already moved into the proper positions. Thus, such a permutation can be carried out to permute the first k rows/columns of S into those of T_n, which is a contradiction (consider, $\pi = (l\ (k+1))$ for example).

Hence, $l = n$ and the two nonzero, off-diagonal entries of row k are $s_{k(k-1)}$ and s_{kn}. Similarly, the two nonzero, off-diagonal entries of column k are $s_{(k-1)k}$ and s_{nk}.

Therefore, we have

$$
S \sim \left(\begin{array}{cccccc|cccc}
2 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 \\
1 & 2 & 1 & & & \vdots & & & & 0 \\
0 & 1 & 2 & \ddots & & \vdots & & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & 0 & & & & \vdots \\
0 & & & \ddots & 2 & 1 & & & & 0 \\
0 & \cdots & \cdots & 0 & 1 & 2 & 0 & \cdots & 0 & 1 \\
\hline
0 & & & & & 0 & 2 & & & 0 \\
\vdots & & & & & \vdots & & \ddots & & \vdots \\
0 & & & & & 0 & & & 2 & 0 \\
1 & 0 & \cdots & \cdots & 0 & 1 & 0 & \cdots & 0 & 2
\end{array}\right)
$$

where the upper left corner highlighted with vertical and horizontal bars is size $k \times k$.

Hence, after permuting row/column n with row/column $k+1$ we have:

$$
S \sim \left(\begin{array}{ccccccc|cccc}
2 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\
1 & 2 & 1 & & & \vdots & 0 & & & & 0 \\
0 & 1 & 2 & \ddots & & \vdots & \vdots & & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & 0 & \vdots & \vdots & & & \vdots \\
\vdots & & & \ddots & 2 & 1 & 0 & & & & 0 \\
0 & \cdots & \cdots & 0 & 1 & 2 & 1 & 0 & \cdots & & 0 \\
1 & 0 & \cdots & \cdots & 0 & 1 & 2 & 0 & \cdots & & 0 \\
\hline
0 & & & \cdots & & 0 & 0 & 2 & & & \vdots \\
\vdots & & & & & \vdots & \vdots & & \ddots & & \vdots \\
0 & & & & & & & & & 2 & 0 \\
0 & 0 & \cdots & \cdots & 0 & 0 & 0 & \cdots & \cdots & 0 & 2
\end{array}\right).
$$

Notice now that S has been decomposed into block diagonal form with at least two blocks: one in the upper left corner of size $(k+1) \times (k+1)$ and possibly more further down and to the right in the matrix. These blocks are highlighted using the vertical and horizontal bars in the matrix. However, S was assumed to be irreducible, so this is a contradiction. Since this case is forced by the assumption that $S \not\sim T_n$, that assumption must have been false to begin with. That is, under the given hypotheses, S is similar to T_n. □

Lemma 3.8. *Let T_n be defined as in Lemma 3.7. If n is odd and at least 3 then $T_n \sim A(C_n)^2$.*

Proof. Consider an unlabeled C_n. Choose a vertex and label it vertex 1. Label every other vertex with $2, \ldots, n$ moving around the cycle. Since n is odd, this process labels the graph without labeling any vertex twice or missing a label on any vertex.

We claim now that a two-walk exists between two vertices if and only if they form the neighborhood of a vertex. To see this, suppose there is a two-walk between vertices i and j. Then there is a vertex k such that ikj is in C_n. That is, $\{i,j\} \subseteq \Gamma(k)$. But since $|\Gamma(k)| = 2$, we have $\Gamma(k) = \{i,j\}$. On the other hand, if $\Gamma(k) = \{i,j\}$, then there is the two-walk ikj in C_n, thus proving the claim.

Now, by the way we have labeled C_n, the only possible neighborhoods are of the form $\{i, i+1\}$ for $i = 1, 2, \ldots, n-1$ and $\{n, 1\}$. Thus, in $A(C_n)^2 = (s_{ij})$, we have $s_{i(i+1)} = s_{(i+1)i} = s_{n1} = s_{1n} = 1$ for $i = 1, 2, \ldots, n-1$. Since there are no other possible two-walks between distinct vertices, every other off-diagonal entry must be zero. Also, since the degree of every vertex is 2, we must have $s_{ii} = 2$ for $i = 1, 2, \ldots, n$.

Therefore, under this labeling, $A(C_n)^2 = T_n$ and in general, $A(C_n)^2 \sim T_n$. □

Lemma 3.9. *Let T_n be defined as in Lemma 3.7. If $n = 2q$ where q is an integer* *greater than 2, then* $A(C_n)^2 \sim \begin{pmatrix} T_q & \mathbf{0} \\ \mathbf{0} & T_q \end{pmatrix}$.

Proof. Consider an unlabeled C_n. Choose a vertex and label it vertex 1. Label every other vertex with $2, 3, \ldots, q$ moving around the cycle. Since n is even, C_n is bipartite with partite sets both of size q. We have that every two-walk beginning in one partite set ends in the same partite set; hence, the labeling of the first q vertices as described labels one partite set completely.

Next, choose an unlabeled vertex from the other partite set and label it vertex $q+1$. Label every other vertex with $q+2, \ldots, 2q$ moving around the cycle. Again, since the remaining unlabeled vertices are all in the same partite set, such a labeling will work.

By a similar argument from the proof of Lemma 3.8, a two-walk exists between vertices i and j with $i \neq j$ if and only if $\Gamma(k) = \{i, j\}$ for some vertex k. Let $A(C_n)^2 = (s_{ij})$. Since the only possible neighborhoods are of the form $\{i, i+1\}$ for $i = 1, \ldots, q-1, q+1, \ldots, 2q-1$; and the sets $\{q, 1\}$ and $\{2q, q+1\}$, we must have

$$s_{i(i+1)} = s_{(i+1)i} = s_{q1} = s_{1q} = s_{2q(q+1)} = s_{(q+1)2q} = 1$$

and all other off-diagonal entries must be zero. Also, since the degree of every vertex is 2, we must have $s_{ii} = 2$ for $i = 1, 2, \ldots, n$. Therefore, under this labeling,

$$A(C_n)^2 = \begin{pmatrix} T_q & \mathbf{0} \\ \mathbf{0} & T_q \end{pmatrix}$$

and, in general, the two matrices are similar. □

Remark 3.10. If we define $T_2 = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$, then the previous lemma extends to

$n = 2q$ where q is an integer at least 2. When $q = 2$ then we have exactly the square of the adjacency matrix of a C_4.

$$A(C_4)^2 \sim \begin{pmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{pmatrix}.$$

Remark 3.11. Notice that when $n = 2q$ with q odd, then Lemma 3.9 tells us that $A(C_n)^2 \sim \begin{pmatrix} T_q & \mathbf{0} \\ \mathbf{0} & T_q \end{pmatrix}$ and Lemma 3.8 gives that $T_q \sim A(C_q)^2$. Therefore,

$$A(C_n)^2 \sim \begin{pmatrix} T_q & \mathbf{0} \\ \mathbf{0} & T_q \end{pmatrix} \sim \begin{pmatrix} A(C_q)^2 & \mathbf{0} \\ \mathbf{0} & A(C_q)^2 \end{pmatrix} \sim A(C_q \cup C_q)^2.$$

That is, the squares of the adjacency matrices of C_{2q} and $C_q \cup C_q$ are indistinguishable. This generalizes Example 1.21.

Remark 3.12. Note that when n is even, T_n is not square graphic. To see this, suppose it were, then by the main diagonal of T_n, it would have to be the square of the adjacency matrix of a union of cycles. Also, since it is irreducible, by Theorem 1.29, if $T_n \sim A(G)^2$ then G must be connected and nonbipartite. These two conditions force $T_n \sim A(C_n)^2$; however, C_n is bipartite because n is even. Therefore, T_n is not square graphic.

We are now prepared to characterize the squares of the adjacency matrices of 2-regular graphs.

Theorem 3.13. *We have $S \sim A(\bigcup_{i=1}^{l} C_{k_i})^2$ if and only if $S = (s_{ij})$ is an $n \times n$ symmetric matrix such that* *(i)* $s_{ii} = 2$ *for all* i

(ii) $\sum_{j=1}^{n} s_{ij} = 4$ *for each* i

(iii) if

$$S \sim \begin{pmatrix} S_1 & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ \mathbf{0} & S_2 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & S_m \end{pmatrix}$$

with each S_i *irreducible, then each block of even size appears an even number of times.*

Proof. First, suppose $S \sim A(\bigcup_{i=1}^{l} C_{k_i})^2$. Consider a relabeling of the graph so that the vertices so that $V(C_{k_1}) = \{1, \ldots, k_1\}$, $V(C_{k_2}) = \{k_1 + 1, \ldots, k_1 + k_2\}$ and so on.

Then we have

$$S \sim A(\bigcup_{i=1}^{l} C_{k_i})^2 \sim \begin{pmatrix} A(C_{k_1})^2 & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ \mathbf{0} & A(C_{k_2})^2 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & A(C_{k_l})^2 \end{pmatrix}.$$

By Lemmas 3.8 and 3.9, each of $A(C_{k_i})^2 \sim T_{k_i}$ when k_i is odd and at least 3 and $A(C_{k_i})^2 \sim \begin{pmatrix} T_{q_i} & \mathbf{0} \\ \mathbf{0} & T_{q_i} \end{pmatrix}$ when $k_i = 2q_i$ for some integer q_i at least 2.

Notice, the definition of each T_{n_i} guarantees each diagonal element is 2 and every row and column sum is 4.

Thus, after a renumbering, we have

$$S \sim \begin{pmatrix} T_{m_1} & 0 & \cdots & \cdots & 0 \\ 0 & T_{m_2} & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & T_{m_p} \end{pmatrix}.$$

Note that by Remark 3.12, whenever m_i is even, there must be some j such that $m_i = m_j$. That is, each block of even size shows up as a pair; that is, every block of even size shows up an even number of times. If not, then S would not be graphic, which is a contradiction. Also, each T_{m_i} is irreducible by construction, and so S has the desired form.

On the other hand, suppose

$$S \sim \begin{pmatrix} S_1 & 0 & \cdots & \cdots & 0 \\ 0 & S_2 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & S_m \end{pmatrix}$$

where each S_i is irreducible and every block of even size shows up an even number of times. Notice that we must have the size of each S_i be at least 2×2. Otherwise, we would not satisfy the conditions that all diagonal elements are two and row sums and column sums are four.

Now, each S_i satisfies the conditions of Lemma 3.7, and hence, $S_i \sim T_{n_i}$ for some n_i.

If $S_i \sim T_{n_i}$ with n_i odd, then by Lemma 3.8, $T_{n_i} \sim A(C_{n_i})^2$.

If $S_i \sim T_{n_i}$ with n_i even, then by assumption there is a matching $S_j \sim T_{n_j}$ where

$n_j = n_i$. Then by Lemma 3.9, we have

$$\begin{pmatrix} S_i & \mathbf{0} \\ \mathbf{0} & S_j \end{pmatrix} \sim \begin{pmatrix} T_{n_i} & \mathbf{0} \\ \mathbf{0} & T_{n_i} \end{pmatrix} \sim A(C_{2n_i})^2.$$

Therefore, there exists a union of cycles so that the square of the adjacency matrix gives S. That is, $S \sim A(\bigcup_{i=1}^{l} C_{k_i})^2$ for some integers k_i at least 3. □

Remark 3.14. For the converse in the previous theorem, it should be noted that the graph associated to S is not necessarily unique. As seen in Remark 3.11, every pair of irreducible blocks of size $q \times q$ with q odd can be viewed as the square of the adjacency matrix of $C_q \cup C_q$ or as the square of the adjacency matrix of C_{2q}. In either case, however, S is the square of the adjacency matrix of a union of cycles.

The use of *characterization* differs in the previous result from other results in this section in that, there are multiple, non-isomorphic graphs that might have the same matrix as the square of their adjacency matrix. However, all of these graphs must be the union of cycles. With more restrictive conditions in Theorem 3.13, we could force uniqueness of the associated graph.

3.3. Paths

This section is broken up into two parts. The first part of this section deals with paths on an even number of vertices and the second deals with those on an odd number of vertices. Before giving the characterization of paths on an even number of vertices, some notation will be introduced and some lemmas will be needed.

Because of the discrepancies among texts in the notation used in describing paths of a certain length, the author would like to make a special note here that P_n will be used to denote paths on n vertices.

Lemma 3.15. *Let $S = (s_{ij})$ be an $n \times n$ irreducible matrix with $n \geq 3$ such that:*

(i) S *is symmetric*

(ii) $s_{ij} \in \{0,1\}$ *for all* $i \neq j$

(iii) *there exists some* r *such that* $s_{rr} = 1$ *and* $s_{ii} = 2$ *for all* $i \neq r$

(iv) *there exists some* $t \neq r$ *such that* $\sum_{i=1}^{n} s_{it} = 3, \sum_{i=1}^{n} s_{ir} = 2$, *and for all* $j \in \{1, \ldots, n\} \setminus \{r, t\}$ *we have* $\sum_{i=1}^{n} s_{ij} = 4$.

Then $S \sim W_n$ *where* $W_n = (w_{ij})$ *is the* $n \times n$ *matrix defined as follows:*

(i) $w_{11} = 1$ *and* $w_{ii} = 2$ *for* $i = 2, \ldots, n$

(ii) $w_{i(i+1)} = w_{(i+1)i} = 1$ *for* $i = 1, \ldots, n-1$

(iii) $w_{ij} = 0$ *otherwise.*

That is,

$$S \sim W_n = \begin{pmatrix} 1 & 1 & 0 & \cdots & & \cdots & 0 & 0 & 0 \\ 1 & 2 & 1 & \ddots & & & & 0 & 0 \\ 0 & 1 & 2 & \ddots & & & & & 0 \\ \vdots & \ddots & \ddots & \ddots & & & & & \vdots \\ & & & & \ddots & & & & \\ \vdots & & & & & \ddots & \ddots & \ddots & \vdots \\ 0 & & & & & \ddots & 2 & 1 & 0 \\ 0 & 0 & & & & \ddots & 1 & 2 & 1 \\ 0 & 0 & 0 & \cdots & & \cdots & 0 & 1 & 2 \end{pmatrix}.$$

Proof. Suppose S is an $n \times n$ irreducible matrix that satisfies the four conditions from the hypothesis. Assume by contradiction that $S \not\sim W_n$; that is, $P^{-1}SP \neq W_n$ for all permutation matrices P. Then, working from the top left corner of S, down and to the right, swapping rows and columns as needed to permute S into W_n, there must be some $k < n$ such that $s_{ij} = w_{ij}$ and $s_{ji} = w_{ji}$ for $i = 1, \dots, k-1$ and $j = 1, \dots, n$, but there is no permutation swapping rows/columns to complete the next step to permute S to W_n. Otherwise, we could continue this process for the n rows and columns and permute S into W_n which would be a contradiction.

It should be noted that such a process can be started. First recall that $s_{rr} = 1$ for some r, and apply the permutation changing row/column 1 with row/column r. Thus, S is similar to a matrix $S' = (s'_{ij})$ where $s'_{11} = 1$. By assumption, there is some entry $s'_{1j} = s'_{j1} = 1$ and $s'_{1k} = s'_{k1} = 0$ for $k \in \{2, \dots, n\} \setminus \{j\}$. Now, there is a permutation changing the jth row/column of S' to the second row/column of S'. That is, there is some permutation matrix P so that the first row of $P^{-1}SP$ is

$$\begin{pmatrix} 1 & 1 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Now, we must have $s_{kk} = 2$ and the kth row/column sum is either 3 or 4 by assumption. If the kth row/column sum is 3, then since the first $k-1$ rows and columns are assumed to be those of W_n, the nonzero off-diagonal entries of row and column k are $s_{(k-1)k} = s_{k(k-1)} = 1$. Therefore, we have

$$S \sim \left(\begin{array}{ccccc|ccc} 1 & 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 1 & 2 & \ddots & \ddots & \vdots & & & \\ 0 & \ddots & \ddots & \ddots & 0 & \vdots & & \vdots \\ \vdots & \ddots & \ddots & 2 & 1 & & & \\ 0 & \cdots & 0 & 1 & 2 & 0 & \cdots & 0 \\ \hline 0 & & \cdots & & 0 & 2 & & \\ \vdots & & & & \vdots & & \ddots & \\ 0 & & \cdots & & 0 & & & 2 \end{array}\right).$$

That is, S can be decomposed into block diagonal form with at least two blocks: one in the upper left corner of size $k \times k$ and possibly more further down and to the right in the matrix. These blocks are highlighted using the vertical and horizontal bars in the matrix. This implies that S is reducible, which is a contradiction.

Therefore, the kth row/column sum must be 4 and so the nonzero off-diagonal entries of row and column k are $s_{(k-1)k} = s_{k(k-1)} = 1$ and $s_{kl} = s_{lk} = 1$ for some $k+1 \leq l \leq n$. But notice, if $l = k+1$ then row/column k matches that of W_n which is a contradiction. Thus, $l > k+1$.

If $k+1 < l \leq n$ then since $s_{il} = s_{li} = 0$ for $i = 1, \ldots, k-1$ by assumption, there is a permutation moving row/column l to row/column $k+1$ which does not affect the rows/columns already moved into the proper positions. Thus, such a permutation can be carried out to permute the first k rows/columns of S into those of W_n, which is a contradiction.

Since in every case we reach a contradiction, our assumption that $S \not\sim W_n$ must have been false to begin with. That is, under the given hypotheses, S is similar to W_n. □

Lemma 3.16. *Let $n = 2k$ for some integer $k \geq 2$ and W_k be as defined in Lemma 3.15. Then* $A(P_n)^2 \sim \begin{pmatrix} W_k & \mathbf{0} \\ \mathbf{0} & W_k \end{pmatrix}$.

Proof. Consider an unlabeled P_n. Choose an end vertex and label it vertex 1. Moving towards the other end vertex, label every other vertex with $2, \ldots, k$, ending on the vertex next to the other end vertex. Since P_n is bipartite with partite sets both of size k, we have labeled one partite set completely.

Next, choose the unlabeled end vertex and label it vertex $k+1$. As before, moving towards the other end vertex, label every other vertex with $k+2, \ldots, 2k$. This completely labels the second partite set of P_n.

If $A(P_n)^2 = (s_{ij})$ then we have $s_{11} = s_{(k+1)(k+1)} = 1$ and $s_{ii} = 2$ for $i \in \{1,\ldots,n\} \setminus \{1, k+1\}$. Note that two-walks only exist between vertices in the same partite set, thus by construction, $s_{ij} = s_{ji} = 0$ for all $i = 1,\ldots,k$ and $j = k+1,\ldots,2k$.

As for two-walks among vertices in the same partite set, this labeling of P_n gives us that $s_{i(i+1)} = s_{(i+1)i} = 1$ for $i = 1,\ldots,k-1$ and $i = k+1,\ldots,2k-1$. These are in fact, the only nonzero off-diagonal elements. Therefore, under this labeling $A(P_n)^2 = \begin{pmatrix} W_k & \mathbf{0} \\ \mathbf{0} & W_k \end{pmatrix}$ and in general, the two matrices are similar. □

Theorem 3.17. *Let $n = 2k$ for some integer $k \geq 2$ and $S = (s_{ij})$ be an $n \times n$ symmetric matrix such that:*

(i) $s_{ij} \in \{0,1\}$ for all $i \neq j$

(ii) there exist distinct r_1 and r_2 such that $s_{r_1r_1} = s_{r_2r_2} = 1$ and $s_{ii} = 2$ for $i \in \{1,\ldots,n\} \setminus \{r_1, r_2\}$

(iii) there are $t_1, t_2 \in \{1,\ldots,n\} \setminus \{r_1, r_2\}$ such that the t_1 and t_2 row and column sums are 3; the r_1 and r_2 row and column sums are 2 and every other row and column sum is 4.

(iv) there is $E \subseteq \{1,\ldots,n\}$ such that $|E| = k$ with $r_1 \in E$ and $r_2 \notin E$ and either $t_1 \in E$ and $t_2 \notin E$ or $t_1 \notin E$ and $t_2 \in E$. For every $i \in E$ and $j \notin E$, $s_{ij} = 0$. Also, for every $C \subseteq E$ there is some $i \in C$ and $j \in E \setminus C$ such that $s_{ij} \neq 0$ and for every $C \subseteq E^c$ there is some $i \in C$ and $j \in E^c \setminus C$ such that $s_{ij} \neq 0$.

Then $S \sim A(P_n)^2$.

Proof. Suppose S is an $n \times n$ symmetric matrix that satisfies the four conditions from the hypothesis. Then by simultaneously permuting the rows and columns of S whose indices are in the set E to the first k rows and columns, we see that S is similar to a block diagonal matrix with two blocks on the main diagonal, both of size $k \times k$. Thus, without loss of generality, we assume $E = \{1, \ldots, k\}$ and so $S = \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}$.

Next, notice again by condition (iv), that B_1 and B_2 are irreducible. To see this, suppose by contradiction that B_1 was not irreducible. Then B_1 can be decomposed into block diagonal form. That is, there is $C \subseteq \{1, \ldots, k\}$ such that for all $i \in C$ and $j \in \{1, \ldots, k\} \setminus C$ we have $s_{ij} = 0$. However, this is a contradiction, so B_1 must be irreducible. A similar argument shows B_2 is also irreducible.

Now, B_1 and B_2 each satisfy the conditions from Lemma 3.15 and hence, $B_1 \sim W_k$ and $B_2 \sim W_k$. Therefore, $S \sim \begin{pmatrix} W_k & \mathbf{0} \\ \mathbf{0} & W_k \end{pmatrix} \sim A(P_n)^2$ by Lemma 3.16. □

In order to characterize paths of odd length, we go through similar steps as with paths of even length. However, the process is slightly more cumbersome as we are unable to use the symmetries we did in the even length case.

Lemma 3.18. *Let $S = (s_{ij})$ be an $n \times n$ irreducible matrix with $n \geq 2$ such that:*

(i) S is symmetric

(ii) $s_{ij} \in \{0, 1\}$ for all $i \neq j$

(iii) there exist distinct r_1 and r_2 such that $s_{r_1 r_1} = s_{r_2 r_2} = 1$ and $s_{ii} = 2$ for all $i \in \{1, \ldots, n\} \setminus \{r_1, r_2\}$

(iv) we have $\sum_{i=1}^{n} s_{ir_1} = \sum_{i=1}^{n} s_{ir_2} = 2$, and for all $j \in \{1, \ldots, n\} \setminus \{r_1, r_2\}$ we have $\sum_{i=1}^{n} s_{ij} = 4$.

Then $S \sim W'_n$ where $W'_n = (w'_{ij})$ is the $n \times n$ matrix defined as follows:

(i) $w'_{11} = w'_{nn} = 1$ and $w'_{ii} = 2$ for $i = 2, \ldots, n-1$

(ii) $w'_{i(i+1)} = w'_{(i+1)i} = 1$ *for* $i = 1, \ldots, n-1$

(iii) $w'_{ij} = 0$ *otherwise.*

Lemma 3.19. *Let* $S = (s_{ij})$ *be an* $n \times n$ *irreducible matrix with* $n \geq 2$ *such that:*

(i) S *is symmetric*

(ii) $s_{ij} \in \{0, 1\}$ *for all* $i \neq j$

(iii) $s_{ii} = 2$ *for all* i

(iv) *there exist distinct* r_1 *and* r_2 *such that* $\sum_{i=1}^{n} s_{ir_1} = \sum_{i=1}^{n} s_{ir_2} = 3$, *and for all* $j \in \{1, \ldots, n\} \setminus \{r_1, r_2\}$ *we have* $\sum_{i=1}^{n} s_{ij} = 4$.

Then $S \sim W''_n$ *where* $W''_n = (w''_{ij})$ *is the* $n \times n$ *matrix defined as follows:*

(i) $w''_{ii} = 2$ *for all* i

(ii) $w''_{i(i+1)} = w''_{(i+1)i} = 1$ *for* $i = 1, \ldots, n-1$

(iii) $w''_{ij} = 0$ *otherwise.*

Remark 3.20. The proofs for Lemmas 3.18 and 3.19 are omitted to avoid redundancy. A similar argument as performed in the proofs of Lemmas 3.7 and 3.15 forces the above matrices to be similar to the described matrices.

Lemma 3.21. *Let* $n = 2k + 1$ *for some integer* $k \geq 2$. *Let* W'_{k+1} *and* W''_k *be as described in Lemma* 3.18 *and* 3.19, *respectively. Then* $A(P_n)^2 \sim \begin{pmatrix} W'_{k+1} & \mathbf{0} \\ \mathbf{0} & W''_k \end{pmatrix}$.

Proof. Consider an unlabeled P_n. Choose an end vertex and label it vertex 1. Moving towards the other end vertex, label every other vertex with $2, \ldots, k, k+1$, ending on the other end vertex. This labels one partite set completely.

Next, choose the unlabeled vertex adjacent to vertex 1 and label it vertex $k+2$. Moving towards vertex $k+1$, label every other vertex with $k+3, \dots, 2k+1$, ending on the vertex adjacent to vertex $k+1$. This labels the other partite set completely.

If $A(P_n)^2 = (s_{ij})$ then we have $s_{11} = s_{(k+1)(k+1)} = 1$ and $s_{ii} = 2$ for $i \in \{1, \dots, n\} \setminus \{1, k+1\}$. As there are no two-walks between vertices from distinct partite sets, we have $s_{ij} = 0$ for all $i = 1, \dots, k+1$ and $j = k+2, \dots, 2k+1$.

For two-walks among vertices in the same partite set, under this labeling we have $s_{i(i+1)} = s_{(i+1)i} = 1$ for $i = 1, \dots, k$ and $i = k+2, \dots, 2k$. As these are the only nonzero off-diagonal elements, under this labeling of P_n, we have $A(P_n)^2 = \begin{pmatrix} W'_{k+1} & \mathbf{0} \\ \mathbf{0} & W''_k \end{pmatrix}$. In general, the two matrices are similar. □

Theorem 3.22. *Let $n = 2k+1$ for some integer $k \geq 2$ and $S = (s_{ij})$ be an $n \times n$ symmetric matrix such that:*

(i) $s_{ij} \in \{0, 1\}$ *for all* $i \neq j$

(ii) there exist distinct r_1 and r_2 such that $s_{r_1 r_1} = s_{r_2 r_2} = 1$ and $s_{ii} = 2$ for $i \in \{1, \dots, n\} \setminus \{r_1, r_2\}$

(iii) there are $t_1, t_2 \in \{1, \dots, n\} \setminus \{r_1, r_2\}$ such that the t_1 and t_2 row and column sums are 3; the r_1 and r_2 row and column sums are 2 and every other row and column sum is 4.

(iv) there is $E \subseteq \{1, \dots, n\}$ such that $|E| = k+1$ with $r_1, r_2 \in E$ and $t_1, t_2 \notin E$. For every $i \in E$ and $j \notin E$, $s_{ij} = 0$. Also, for every $C \subsetneq E$ there is some $i \in C$ and $j \in E \setminus C$ such that $s_{ij} \neq 0$ and for every $C \subsetneq E^c$ there is some $i \in C$ and $j \in E^c \setminus C$ such that $s_{ij} \neq 0$.

Then $S \sim A(P_n)^2$.

Proof. Suppose S is an $n \times n$ symmetric matrix that satisfies the four conditions from the hypothesis. Then by simultaneously permuting the rows and columns of S whose indices are in the set E to the first $k+1$ rows and columns, we see that S is similar to a block diagonal matrix with two blocks on the main diagonal. Thus, without loss of generality, we assume $E = \{1, \ldots, k+1\}$ and so $S = \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}$.

By a similar argument from the proof of Theorem 3.17, both B_1 and B_2 are irreducible.

Now, B_1 satisfies the conditions from Lemma 3.18 and B_2 satisfies the conditions from Lemma 3.19 and hence, $B_1 \sim W'_{k+1}$ and $B_2 \sim W''_k$. Therefore,

$$S \sim \begin{pmatrix} W'_{k+1} & \mathbf{0} \\ \mathbf{0} & W''_k \end{pmatrix} \sim A(P_n)^2$$

by Lemma 3.21. □

CHAPTER 4. DUPLICATION

Determining when a given matrix was square graphic lead to the interesting problem of determining when a matrix represented the square of the adjacency matrix of several non-isomorphic graphs. It has already been shown in Example 1.21 that this can occur and was further generalized in Lemma 3.9 and the following Remark 3.11. In a sense, such matrices are a sort of dual for matrices which uniquely determine a graph, as was explored in the previous chapter.

The following theorem serves as a starting point for the construction of squares of adjacency matrices corresponding to several non-isomorphic graphs.

Theorem 4.1. *We have*

$$\begin{pmatrix} A(G) & \mathbf{0} \\ \mathbf{0} & A(G) \end{pmatrix} \sim \begin{pmatrix} \mathbf{0} & A(G) \\ A(G) & \mathbf{0} \end{pmatrix}$$

if and only if G is bipartite.

Before the proof of this theorem is given, we first need the following fact from graph theory, stated without proof here.

Lemma 4.2. *We have G is bipartite if and only if* $A(G) \sim \begin{pmatrix} \mathbf{0} & B^T \\ B & \mathbf{0} \end{pmatrix}$.

Proof of Theorem 4.1. Suppose G is bipartite. Then $A(G) = \begin{pmatrix} \mathbf{0} & B^T \\ B & \mathbf{0} \end{pmatrix}$ for some $m \times n$ matrix B. Consider the permutation matrix

$$P = \begin{pmatrix} \mathbf{0} & \mathbf{0} & I_n & \mathbf{0} \\ \mathbf{0} & I_m & \mathbf{0} & \mathbf{0} \\ I_n & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & I_m \end{pmatrix}.$$

Then we have

$$P^{-1}\begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & B^T \\ \mathbf{0} & \mathbf{0} & B & \mathbf{0} \\ \mathbf{0} & B^T & \mathbf{0} & \mathbf{0} \\ B & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} P = \begin{pmatrix} \mathbf{0} & B^T & \mathbf{0} & \mathbf{0} \\ B & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & B^T \\ \mathbf{0} & \mathbf{0} & B & \mathbf{0} \end{pmatrix}$$

and so

$$\begin{pmatrix} A(G) & \mathbf{0} \\ \mathbf{0} & A(G) \end{pmatrix} \sim \begin{pmatrix} \mathbf{0} & A(G) \\ A(G) & \mathbf{0} \end{pmatrix}.$$

On the other hand, suppose G is nonbipartite. Then

$$\begin{pmatrix} A(G) & \mathbf{0} \\ \mathbf{0} & A(G) \end{pmatrix} = A(G \cup G)$$

and thus, is the adjacency matrix of a disconnected, nonbipartite graph H_1. On the other hand, if $B = A(G)$ then

$$\begin{pmatrix} \mathbf{0} & A(G) \\ A(G) & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & B^T \\ B & \mathbf{0} \end{pmatrix}$$

and thus, is the adjacency matrix of a bipartite graph H_2 by Lemma 4.2. Therefore, $H_1 \not\cong H_2$ and hence, $A(H_1) \not\sim A(H_2)$ by Theorem 1.4. □

Remark 4.3. By the previous theorem, given any nonbipartite graph G, the graphs whose adjacency matrices are

$$A(H_1) = \begin{pmatrix} A(G) & \mathbf{0} \\ \mathbf{0} & A(G) \end{pmatrix} \text{ and } A(H_2) = \begin{pmatrix} \mathbf{0} & A(G) \\ A(G) & \mathbf{0} \end{pmatrix}$$

are non-isomorphic graphs with $A(H_1)^2 = A(H_2)^2$.

It should be noted that $H_1 \cong G \cup G$ and H_2 is known as the bipartite double cover graph of G or the Kronecker cover of G.

This result can be used to build matrices S with arbitrarily many non-isomorphic graphs whose adjacency matrix squared is S. This process is described in the following theorem.

Theorem 4.4. *For every positive integer k and integer $n \geq 3$, there exists a matrix S of size $(2kn) \times (2kn)$ such that $A(G_i)^2 = S$ for $k+1$ non-isomorphic graphs $G_1, G_2, \ldots, G_{k+1}$.*

Proof. Let G be a nonbipartite graph on n vertices. Note, $n \geq 3$ since we must have an odd cycle in G the smallest of which is length 3. Let A be the block diagonal matrix with $2k$ copies of $A(G)$ on the main block-diagonal. That is,

$$A = \begin{pmatrix} A(G) & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & A(G) & & \vdots \\ \vdots & & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & A(G) \end{pmatrix}.$$

If we define $S = A^2$, then S is square graphic since $S = A(\bigcup_{i=1}^{2k} G)^2$.

Let H be the bipartite double cover graph of G; that is, the graph H such that

$$A(H) = \begin{pmatrix} \mathbf{0} & A(G) \\ A(G) & \mathbf{0} \end{pmatrix}$$

and define the permutation $\pi_{2t} = (12)(34)\cdots(2(t-1)\ 2t)$ for each $t = 1, 2, \ldots, k$. For each permutation, let $P_{\pi_{2t}}$ be the block permutation matrix of size $(2kn) \times (2kn)$ swapping n rows of I_{2kn} at a time according to the permutation π_{2t}.

For example,

$$P_{\pi_2} = \begin{pmatrix} \mathbf{0} & I_n & \mathbf{0} & \cdots & \mathbf{0} \\ I_n & \mathbf{0} & \mathbf{0} & & \vdots \\ \mathbf{0} & \mathbf{0} & I_n & & \vdots \\ \vdots & & & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & I_n \end{pmatrix}.$$

Then, for every $t = 1, 2, \ldots, k$ we have

$$P_{\pi_{2t}}A = \begin{pmatrix} A(H) & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & A(H) & \ddots & \vdots & \vdots & & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} & \vdots & & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & A(H) & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & A(G) & \ddots & \vdots \\ \vdots & & & \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & \cdots & \mathbf{0} & A(G) \end{pmatrix}$$

where there are t copies of $A(H)$ and $2(k-t)$ copies of $A(G)$ on the main block diagonal. Next, define the graphs G_t by

$$A(G_t) = P_{\pi_{2t}}A = A((\bigcup_{i=1}^{t} H) \cup (\bigcup_{j=1}^{2(k-t)} G)).$$

Since G is nonbipartite, we have $G_i \ncong G_j$ for $i \neq j$; however, $A(G_t)^2 = S$ for all $t = 1, 2, \ldots, k$ by Theorem 4.1 and Remark 4.3.

Therefore, S is $(2kn) \times (2kn)$ and the square of the adjacency matrix for the $k+1$ non-isomorphic graphs: $G_1, \ldots, G_{k-1}, G_k$ and $\bigcup_{i=1}^{2k} G$. □

Example 4.5. *When $n = 3$ we have the unique nonbipartite graph K_3. Thus, if $k = 3$, then a matrix S of size 18×18 that is the square of the adjacency matrix of* *four non-isomorphic graphs is*

$$S = \begin{pmatrix} A(K_3)^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & A(K_3)^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & A(K_3)^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & A(K_3)^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & A(K_3)^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & A(K_3)^2 \end{pmatrix}.$$

The four non-isomorphic graphs with S as the square of the adjacency matrix are: $\bigcup_{i=1}^{6} K_3, C_6 \cup \left(\bigcup_{i=1}^{4} K_3\right), \left(\bigcup_{i=1}^{2} C_6\right) \cup \left(\bigcup_{i=1}^{2} K_3\right)$ *and* $\bigcup_{i=1}^{3} C_6$.

The previous result had stood for several months as the only way to construct non-isomorphic groups of similar graphs. Because of this, the author proposed the following conjecture:

Conjecture 4.6. *If G and H are both nonbipartite, connected, non-isomorphic graphs then it must be the case that $A(G)^2 \not\sim A(H)^2$.*

This was until the following counterexample was found.

Example 4.7. *The graphs G and H from Figures 7 and 8, respectively, are nonbipartite, connected, non-isomorphic graphs whose adjacency matrices squared are similar.*

Note that in each graph, the vertices labeled v_1 are identified; and so, G and H are both 4-regular.

Also note that these graphs are cospectral; that is, the spectra of each adjacency matrix is the same. These graphs were found in [3].

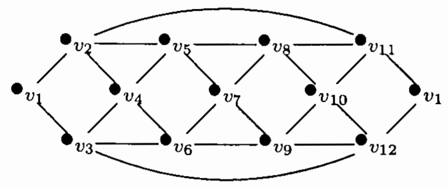

Figure 7. Graph G

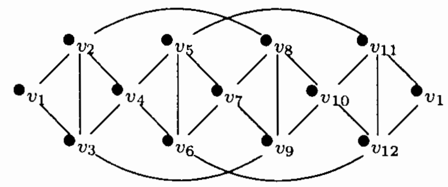

Figure 8. Graph H

With this example, it appears to the author that the problem of duplication is more complicated than initially suspected and will require further study.

CHAPTER 5. CONCLUSION AND FURTHER RESEARCH

While a true characterization of the squares of adjacency matrices remains unknown, we have given several nontrivial necessary conditions. We have also given several characterizations of classes of graphs.

Through the study of the removal of vertices and the effect on the square of the adjacency matrix, new techniques in determining when a matrix is square graphic were found and demonstrated. These approaches have proven to be effective in finding a plausible set of graphs for a given matrix.

The final section of this paper was aimed at the question of determining when a matrix is the square of the adjacency matrix of several non-isomorphic graphs. It was shown, that for a given positive integer n, there is a matrix S and $n+1$ non-isomorphic graphs, so that S is the square of the adjacency matrix of these graphs.

The motivating question behind this paper has been to determine when a matrix is square graphic. This question remains unanswered in the general case. Further research into these matrices and their properties can be done in order to better answer this question.

Determining other properties imposed on the graph by the matrix, and vice versa, is one direction to be further explored.

As a way to further our understanding of square graphic matrices, additional study may include finding characterizations of other classes of graphs. For example, what other conditions on a matrix S with a diagonal consisting of all k's must we have so that S is the square of the adjacency matrix of a k-regular graph, where k is an integer at least 3?

Certainly, further research can be done in the area of determining exactly when a matrix represents several non-isomorphic graphs. This problem appears to the author be more complex than initially supposed as is indicated by the pair of non-isomorphic, nonbipartite, connected graphs whose adjacency matrices squared are similar.

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