THE SQUARE OF ADJACENCY MATRICES

DANIEL JOSEPH KRANDA

ABSTRACT. It can be shown that any symmetric $(0, 1)$-matrix $A$ with $\text{tr} A = 0$ 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 and counting four cycles. Row and column sums are examined as well as the problem of multiple nonisomorphic graphs with the same adjacency matrix squared.

1. INTRODUCTION AND BACKGROUND

This paper aims to determine properties of graphs found by examining the square of the adjacency matrix and vice versa. As a thorough study of the square of the adjacency matrix has not been addressed previously in the literature, we survey several results covering different aspects of the given problem.

Throughout this paper, we will consider only simple, undirected graphs.

Theorem 1.1. 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 with two edges) 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 $v_k$. □

Definition 1.2. A matrix $S$ is square graphic if there is a simple, undirected graph $G$ such that $S = A(G)^2$.

Definition 1.3. 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 $S_1 \sim S_2$.

Theorem 1.4. If $S_1$ is square graphic, then so is $S_2 = P^{-1}S_1P$ for any permutation matrix $P$.

Remark 1.5. If $S_1 \sim S_2$ then $S_1$ is square graphic if and only if $S_2$ is square graphic.

The following results relate the structure of the square of the adjacency matrix of a graph with the structure of that graph. We begin by determining if a graph is bipartite or disconnected by examining the adjacency matrix squared.

Date: May 2, 2014.
Theorem 1.6. 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 $0 < k < n$ and $0$ represents a matrix of all zeros of the appropriate size.

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

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

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. 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

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

where $B_i$ 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 $C = v_{c_0}v_{c_1} \cdots v_{c_{t-1}}v_{c_0}$ 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 $P \cap C = \{v\}$.

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 $P$ is of odd length, consider a neighbor $w$ of $v$, such that $w \in V(C) \subseteq V_1$. Then $uwPu$ 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. \(\square\)

We now give a result on counting four cycles in a graph.
Theorem 1.7. If $S = (s_{ij}) = A(G)^2$ for some graph $G$, then

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

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

Proof. First, we claim that, for $i \neq j$, $\left(\frac{s_{ij}}{2}\right)$ 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 $\left(\frac{s_{ij}}{2}\right)$.

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

Remark 1.8. A necessary condition for a matrix $S$ to be square graphic that can be taken from Theorem 1.7 is that the number $\sum_{i \neq j} \left(\frac{s_{ij}}{2}\right)$ must be divisible by four.

2. Row and Column Sums

We now prove some results relating the row and column sums of the square of the adjacency matrix to properties of the underlying graph.

Definition 2.1. The neighborhood of $v$, $\Gamma(v)$, is the set of all vertices in $G$ adjacent to $v$.

Theorem 2.2. 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 $v_i vu$. 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. \qed
Corollary 2.3. 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 $E_i = \{s_{jj} \text{ such that } v_j \in \Gamma(v_i)\}$ gives the desired result. □

Corollary 2.4. 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 2.5. 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.

3. 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. For example, the graphs in Figures 1 and 2 are non-isomorphic with the same adjacency matrix squared.

The following theorem serves as a starting point for the construction of squares of adjacency matrices corresponding to several non-isomorphic graphs.
Theorem 3.1. We have
\[
\begin{pmatrix}
A(G) & 0 \\
0 & A(G)
\end{pmatrix} \sim \begin{pmatrix}
0 & A(G) \\
A(G) & 0
\end{pmatrix}
\]
if and only if \( G \) is bipartite.

Before the proof of this theorem is given, we recall the following fact from graph theory.

Lemma 3.2. We have \( G \) is bipartite if and only if \( A(G) \sim \begin{pmatrix} 0 & B^T \\ B & 0 \end{pmatrix} \).  

Proof of Theorem 3.1. Suppose \( G \) is bipartite. Then \( A(G) = \begin{pmatrix} 0 & B^T \\ B & 0 \end{pmatrix} \) for some \( m \times n \) matrix \( B \). Consider the permutation matrix
\[
P = \begin{pmatrix}
0 & 0 & I_n & 0 \\
0 & I_m & 0 & 0 \\
I_n & 0 & 0 & 0 \\
0 & 0 & 0 & I_m
\end{pmatrix}.
\]

Then we have
\[
P^{-1} \begin{pmatrix}
0 & 0 & 0 & B^T \\
0 & 0 & B & 0 \\
0 & B^T & 0 & 0 \\
B & 0 & 0 & 0
\end{pmatrix} P = \begin{pmatrix}
0 & B^T & 0 & 0 \\
B & 0 & 0 & 0 \\
0 & 0 & 0 & B^T \\
0 & 0 & B & 0
\end{pmatrix}
\]
and so
\[
\begin{pmatrix}
A(G) & 0 \\
0 & A(G)
\end{pmatrix} \sim \begin{pmatrix}
0 & A(G) \\
A(G) & 0
\end{pmatrix}.
\]
On the other hand, suppose $G$ is nonbipartite. Then
\[
\begin{pmatrix}
  A(G) & 0 \\
  0 & A(G)
\end{pmatrix} = A(G \cup G)
\]
and thus, is the adjacency matrix of a disconnected, nonbipartite graph $H_1$. On the other hand, if $B = A(G)$ then
\[
\begin{pmatrix}
  0 & A(G) \\
  A(G) & 0
\end{pmatrix} = \begin{pmatrix}
  0 & B^T \\
  B & 0
\end{pmatrix}
\]
and thus, is the adjacency matrix of a bipartite graph $H_2$ by Lemma 3.2. Therefore, $H_1 \not\cong H_2$ and hence, $A(H_1) \not\cong A(H_2)$ by Theorem 3.2. □

Remark 3.3. By the previous theorem, given any nonbipartite graph $G$, the graphs whose adjacency matrices are
\[
A(H_1) = \begin{pmatrix}
  A(G) & 0 \\
  0 & A(G)
\end{pmatrix} \quad \text{and} \quad A(H_2) = \begin{pmatrix}
  0 & A(G) \\
  A(G) & 0
\end{pmatrix}
\]
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 3.4. 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,
\[
A = \begin{pmatrix}
  A(G) & 0 & \cdots & 0 \\
  0 & A(G) & \ddots & \vdots \\
  \vdots & \ddots & \ddots & 0 \\
  0 & \cdots & 0 & A(G)
\end{pmatrix}.
\]
If we define $S = A^2$, then $S$ is square graphic since $S = A(\bigcup_{i=1}^{2k} G_i)^2$.

Let $H$ be the bipartite double cover graph of $G$; that is, the graph $H$ such that
\[
A(H) = \begin{pmatrix}
  0 & A(G) \\
  A(G) & 0
\end{pmatrix}
\]
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 $\pi_{2t}$.
For example,

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

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

\[
P_{\pi_2} A = \begin{pmatrix}
A(H) & 0 & \cdots & 0 & 0 & \cdots & 0 \\
0 & A(H) & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & A(H) & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \cdots & 0 & A(G) & \ddots & \ddots \\
0 & \cdots & \cdots & 0 & \cdots & 0 & A(G)
\end{pmatrix}
\]

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

\[
A(G_t) = P_{\pi_2} A = A((\bigcup_{i=1}^{t} H) \cup (\bigcup_{j=1}^{2(k-t)} G)).
\]

Since \( G \) is nonbipartite, we have \( G_i \not\cong G_j \) for \( i \neq j \); however, \( A(G_t)^2 = S \) for all \( t = 1, 2, \ldots, k \) by Theorem 3.1 and Remark 3.3.

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 \( \bigcup_{i=1}^{2k} G \).

Remark 3.5. There are nonbipartite, connected, non-isomorphic graphs whose adjacency matrices squared are similar.

Example 3.6. The graphs \( G \) and \( H \) from Figures 3 and 4, respectively, are non-bipartite, 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. These graphs were found in [?].

With this example, it appears to the author that the problem of duplication is more complicated than initially suspected and will require further study.
Figure 4. Graph $H$