On Powers of the Adjacency Matrix Representing Number of Walks in a Graph

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Abstract

An adjacency matrix is a matrix representation of a graph, and when it is studied, it reveals properties of its corresponding graph such as walks and cycles. We will show that the (i, j) entry of a matrix A^k, where A is the adjacency matrix of graph G, represents the number of k length walks from vertices v_i to v_j in G and we will discuss the applications of this theorem in proving the existence of 3-cycles in the graph.

1 Introduction

Graph Theory has been around since the time of Leonhard Euler and has proven to be an interesting mathematical basis for solving some problems which had no solutions before, such as the Königsberg bridge problem, or explaining why certain solutions exists like the four color theorem. New discoveries in graph theory can reveal unexpected applications in real life. In this paper we look at walks in a graph and how they reveal some insights about their them. And the medium through which we will investigate walks are adjacency matrices, which are a basic matrix representation of finite graphs. Using the properties of adjacency matrices we will find out the number of walks of a given length between vertices and existence of cycles.

Adjacency matrices are useful matrix representations of graphs. They have gained popularity over the last century as applications of graph theory were found in fields such as chemistry, operations research, and most importantly, computer science. One example of an application of graph theory in computer science is, using Minimum Spanning Tree Algorithms for finding in data mining, pattern recognition and machine learning [2]. Such a significant application, including others, has led to in-depth study of adjacency matrices.

Adjacency Matrices, as the name implies, are the matrices that represent which vertices in a graph are adjacent. If vertices in a graph are arbitrarily indexed from 1 to n, then the adjacency matrix denotes whether there exists an edge between the two vertices at the element corresponding to the position of their indices.

In section 3 we will prove our main theorem, which states that, the k^{th} power of an adjacency matrix describes the number of k length walks from one vertex to another. As this theorem reveals the possible number of walks of length k between two vertices, we can use properties of graphs and walks to conclude many of our following implications. A simple implication is if we take the sum of the k^{th} power of the adjacency matrix for varying values of k then the resulting matrix shows the total number of walks for any of those varying lengths.

In section 4, we study a significant implication of this theorem which is a proposition that states that by inspecting the number of walks which start and end at the same vertex we can find the presence of cycles within a graph. For graphs without self edges, every element on the diagonal of the adjacency matrix A would be 0. However, once we take the 3^{rd} power of the adjacency matrix, if one of the diagonal positions becomes a non-zero value, then we can conclude that there exists at least one 3-cycle in the graph which contains that corresponding vertex. We can then further investigate this property and arrive at a theorem which tells us the number of 3-cycles in a graph through the trace of the $3rd$ power of the adjacency matrix. In a 3-cycle, if we consider length 3 walks which start and end at the same vertex, there are two walks for each vertex going in opposite directions to each other in the 3-cycle and ending at themselves. With 3 vertices, there would be a total of 6 walks contributed by each cycle of length 3 starting and ending at themselves. We formally prove this theorem and its preceding proposition in this section.

2 Definitions

We will define fundamental concepts required for the theorems and proofs in the sections 3 and 4. We first define graphs which are ordered pairs of a set of vertices and edges [3].

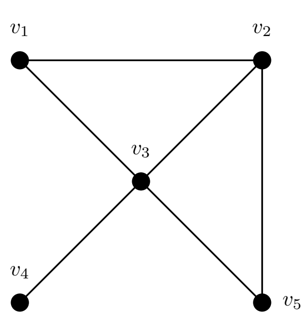
Definition 2.1. *A graph $G = (V, E)$ is an ordered pair of n vertices and m edges, where $V = \{v_1, v_2, ..., v_n\}$ is a set of vertices and $E = \{e_1, e_2, ..., e_m\}$ is the set of edges. Here an edge $e = \{v_x, v_y\} \in E$ such that $v_x, v_y \in V$.*

Graphs are discrete mathematical structures which are represented pictorially as dots that are vertices and lines which connect those dots, that are edges. Graphs have interesting representations more suited for computational purposes such as adjacency matrices. The (i, j) entry of the adjacency matrix is 1 if $\{v_i, v_j\} \in E$, otherwise 0 [5].

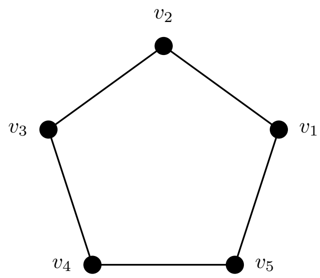
Definition 2.2. *Let $G = (V, E)$ be a graph and let $V = \{v_1, v_2, ..., v_n\}$, then the (i, j) entry of the adjacency matrix A of graph G is defined as:*

$$A_{i,j} = \begin{cases} 1 & if\{v_i, v_j\} \in E \\ 0 & otherwise \end{cases}$$

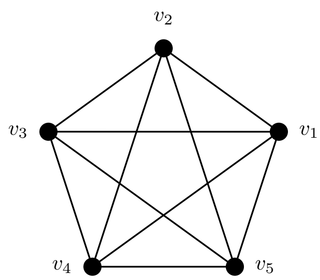
Adjacency matrices differ according to their corresponding graphs. An undirected adjacency matrix is symmetric whereas a directed one is not. For a weighted graph, the corresponding elements of the edges in the adjacency matrix are replaced with their weights. Having defined adjacency matrices we can imagine what the adjacency matrices of certain types of graphs would look like. For example, the adjacency matrix of a complete graph will have 1 at every element except on the diagonal which would be 0, and the adjacency matrix of a cycle will have its row sum and column sum equalling exactly 2. Examples of graphs and related adjacency matrices are shown below in Figure 2.1.



$$A_1 = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$



$$A_2 = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$



$$A_3 = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

Figure 2.1 As shown above, the graphs are placed with their respective adjacency matrices to their right. From top to bottom: a graph with its matrix A_1, the 5-cycle with its matrix A_2, and the complete graph K_5 with its matrix A_5.

We will now define walks which will be a key concept in proving our main theorem. A Walk is the sequence of vertices and edges we traverse while travelling from on starting vertex to an ending vertex [3].

Definition 2.3. *Let $G = (V, E)$ be a graph and $e_i = \{v_{i-1}, v_i\} \in E$ for $i = 1$ to n where $n \in \mathbb{N}$, then a sequence $(v_0, e_1, v_1, e_2, v_2, ..., e_n, v_n)$ is called a walk in G.*

Walks can contain repeated elements and their length is the number of edge elements contained in the sequence. Therefore if we infinitely repeat the same elements we can get infinite length walks from finite graphs. Walks also help in defining more concepts such as paths. Paths are walks without repeated elements [3]

Definition 2.4. *A path P in $G = (V, E)$ is a walk such that every element in the walk is unique and if there exists a path P between any two vertices $v_i, v_j \in V$ then we say G is connected.*

Paths do not have repeated elements unlike walks, hence every element in a path is unique. Paths are also used to define cycles which will be another important concept used in section 4. Cycles are paths which start and end at the same vertex [3].

Definition 2.5. *A cycle C in graph G is a path such that it starts and ends at the same vertex and a graph which only consists of a cycle of length n is called an n-cycle or C_n.*

The n-cycle graphs are also referred to as n-gons as they can be depicted and n sided polygons. For example, 3-cycle can also be called the triangle. Some examples of cycles are shown below in Figure 2.2. We will find the existence of 3-cycles by checking diagonal of the third power of the adjacency matrix in section 4.

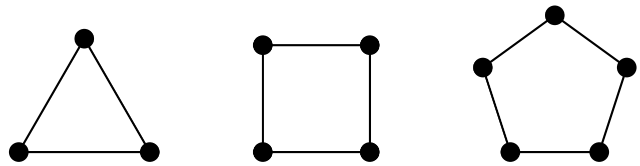


Figure 2.2 These are examples of cycles. From left to right: 3-cycle, 4-cycle, and 5-cycle

We will now define the trace of a matrix and introduce its use in proving the existence of 3-cycles in A^3. The trace of a matrix is the sum of its diagonal elements [4].

Definition 2.6. *Let A be a matrix. Then its trace is defined as,*

$$Tr(A) = \sum_{k=1}^{n} A_{(k,k)}$$

The trace of a matrix is the sum of its diagonal elements and as these diagonal elements are the number of length 3 walks in A^3, such that A is an adjacency matrix. The sum of the diagonal elements tells the total number of length 3 walks in the original graph.

3 Powers of Adjacency Matrix and Walks

As hinted to in the introduction, the k^{th} power of the adjacency matrix indicates the number of walks of length k at its i^{th} row and j^{th} column [5]. We first state this theorem and then rigorously prove it.

Theorem 3.1. *Let A be an adjacency matrix of graph G. Then the (i, j) entry of A^k represents the number of possible walks of length k from vertices v_i to v_j in G.*

Proof. We will use proof by induction on the power k to prove this theorem,
Consider the proposition $P(k)$: The (i, j) entry in A^k represents the number of possible walks from v_i to v_j of length k in the original graph.

For the base case we will prove $P(1)$ is true. In the original adjacency matrix, if (i, j) entry is 1 then the v_i is adjacent to v_j. Therefore, there exists an edge between v_i and v_j. We can define a walk $W = (v_i, \{v_i, v_j\}, v_j)$, here W has a length 1 so we can consider the adjacency matrix A as representing walks of length 1 between vertices. Hence $P(1)$ is true.

We shall consider the inductive case. Let $P(k)$ be true, we will prove $P(k + 1)$. $P(k)$ states that the (i, j) entry of A^k is the number of walks from v_i to v_j of length k. Let us consider the matrix equation $A^k A = A^{k+1}$, which is shown below in in figure 3.1.

$$\begin{bmatrix} \mathrm{A}^k_{(1,1)} & \cdots & \mathrm{A}^k_{(1,t)} & \cdots & \mathrm{A}^k_{(1,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}^k_{(i,1)} & \cdots & \mathrm{A}^k_{(i,t)} & \cdots & \mathrm{A}^k_{(i,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}^k_{(n,1)} & \cdots & \mathrm{A}^k_{(n,t)} & \cdots & \mathrm{A}^k_{(n,n)} \end{bmatrix} \begin{bmatrix} \mathrm{A}_{(1,1)} & \cdots & \mathrm{A}_{(1,j)} & \cdots & \mathrm{A}_{(1,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}_{(t,1)} & \cdots & \mathrm{A}_{(t,j)} & \cdots & \mathrm{A}_{(t,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}_{(n,1)} & \cdots & \mathrm{A}_{(n,j)} & \cdots & \mathrm{A}_{(n,n)} \end{bmatrix} = \begin{bmatrix} \mathrm{A}^{k+1}_{(1,1)} & \cdots & \mathrm{A}^{k+1}_{(1,j)} & \cdots & \mathrm{A}^{k+1}_{(1,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}^{k+1}_{(i,1)} & \cdots & \mathrm{A}^{k+1}_{(i,j)} & \cdots & \mathrm{A}^{k+1}_{(i,n)} \\ \vdots & & \vdots & & \vdots \\ \mathrm{A}^{k+1}_{(n,1)} & \cdots & \mathrm{A}^{k+1}_{(n,j)} & \cdots & \mathrm{A}^{k+1}_{(n,n)} \end{bmatrix}$$

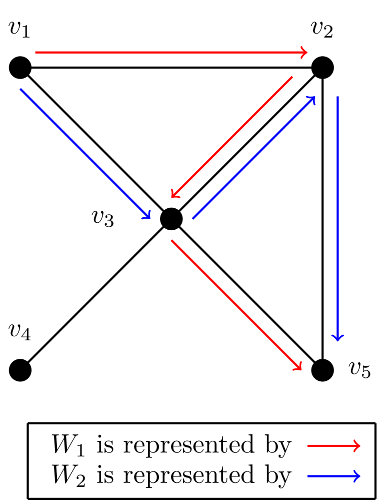
Figure 3.1 Expanded form of the matrix equation

According to our inductive assumption, we know that the (i, t) entry of A^k, let us call it $A^k_{(i,t)}$, represents the number of possible walks of length k from v_i to v_t, where $t \in \{1, ..., n\}$. And we know by the definition of adjacency matrices that the (t, j) entry of A, let us call it $A_{(t,j)}$, represents if v_t and v_j are adjacent or not by being 1 or 0. Hence if we were to multiply A^k and A, in that order, the (i, j) entry of the resulting matrix A^{k+1} would be the product of the i^{th} row vector of A^k and the j^{th} column vector of A. Thus we get,

$$A^{k+1}_{(i,j)} = \sum_{t=1}^{n} A^k_{(i,t)} A_{(t,j)}$$

Here, $A^k_{(i,t)}$ represents the number of walks of length k from v_i to v_t. Hence, if v_t is adjacent to v_j then we can conclude that there must also exist $A^k_{(i,t)}$ walks of length $k + 1$ from v_i to v_j where the second last vertex in the walk, the one before v_j, is v_t. If v_t is not adjacent to v_j then there are 0 walks from v_i to v_j such that the second last vertex is v_t. Therefore the term $A^k_{(i,t)} A_{(t,j)}$ represents the number of walks from v_i to v_j with second last vertex v_t.If we find the sum of all these terms for all possible second to last vertices $t = \{1, ..., n\}$, then the sum represents the total number of walks of length $k + 1$ from v_i to v_j. $\square$

Let us consider the example of a graph used in the introduction and the 3^{rd} power of its adjacency matrix as shown below in Figure 3.2.



$$A^3 = \begin{bmatrix} 2 & 5 & 6 & 1 & 2 \\ 5 & 4 & 6 & 2 & 5 \\ 6 & 6 & 4 & 4 & 6 \\ 1 & 2 & 4 & 0 & 1 \\ 2 & 5 & 6 & 1 & 2 \end{bmatrix}$$

Figure 3.3 The matrix A is the adjacency matrix of the graph shown above.

In this example we consider the matrix A^3 which is the 3^{rd} power of the original adjacency matrix. Therefore it represents the number of possible length 3 walks in the original graph G. We see that the $(1, 5)$ entry of the matrix is 2. This means that there exist 2 possible walks of length 3 which start from v_1 and end at v_5. We can write out these walks as the sequences W_1 and W_2, where $W_1 = (v_1, \{v_1, v_2\}, v_2, \{v_2, v_3\}, v_3, \{v_3, v_5\}, v_5)$ and $W_2 = (v_1, \{v_1, v_3\}, v_3, \{v_3, v_2\}, v_2, \{v_2, v_5\}, v_5)$. W_1 is shown in red whereas W_2 is shown in blue.

Let us consider a corollary that states that the sum of different powers of an adjacency matrix represents the number of walks of lengths of those powers [1].

Corollary 3.1. *Let $B = \sum_{k \in I} A^k$, where $I \subseteq \mathbb{N}$ and A is an adjacency matrix. Then the (i, j) entry of B represents the number of possible walks from v_i to v_j for all lengths $k \in I$.*

We see that this corollary can easily be proven using Theorem 3.1. This result helps in computing the possible number of walks in graphs if the length of those walks can vary.

4 Existence of 3-Cycles

An interesting application of Theorem 3.1 is proving the existence of 3-cycles. As we discussed in the previous section, the (i, j) entry of the matrix A^k, where A is the adjacency matrix of G, is equal to the number of walks of length k from v_i to v_j. Hence, the entry (i, i) of A^k would be equal to the number of walks of length k which start and end at v_i. If $A^k_{(i,i)} > 0$ and k is even, then there exist walks of even length which start and end at v_i. But as walks can have repeated elements, we can have the first half of the walk be unique but the second half repeat the first half sequence backwards. However, for odd length walks we cannot retrace our walk like we did for the even cases. Therefore every element in a walks of length 3 which starts and ends at the same vertex is unique [4]. Which leads to the following proposition.

Proposition 4.1. *If there exists a walk W from v_i to itself of length 3, then every element of the sequence W is unique except the starting and ending vertex v_i.*

Proof. We will prove this proposition using proof by contradiction. We will assume that there exists a walk of length 3 from v_i to itself but some elements are repeated. Let $W = (v_i, e_1, v_1, e_2, v_2, e_3, v_i)$ be the walk. Also we know that there are 3 vertices and 3 edges in this walk. As this is a simple graph we know there cannot exist an edge from a vertex to itself. Therefore as all $\binom{3}{2}$ edges are represented. Let us assume any two of the vertices v_x, v_y in this sequence are equal, then we can find an edge e, such that $e = \{v_x, v_y\}$, but simple graphs do not have an edge between themselves, therefore this is a contradiction and all vertices are unique. Let us consider the cases for the edges now:

- Assume $e_1 = e_2$. This would imply $v_i = v_2$ as edges contain only two elements. But as vertices cannot equal each other this is a contradiction.
- Assume $e_1 = e_3$. This would imply $v_1 = v_2$, this is again a contradiction as vertices cannot equal each other.
- Assume $e_2 = e_3$. This would imply $v_i = v_1$, without loss of generality.
- Assume $e_1 = e_2 = e_3$. This implies $e_1 = e_2$ which implies $v_i = v_2$ without loss of generality.

Therefore we considered all cases for the elements in walk W were repeated and all resulted in contradictions. Therefore we overall got a contradiction assuming that any element in the walk is repeated. Hence all elements in the walk of length 3 must be unique except v_i. □

As we have proven that a walk of length 3 has all unique elements except for the staring and ending element, we can then see that these properties correspond to a 3-cycle. Therefore we can say if $A^3_{(i,i)} > 0$, then v_i lies on a 3-cycle.

The diagonal of A^3 tells us about the existence of walks and proposition 4.1 tells us about the existence of 3-cycles if the walks do exist. We can then search for a pattern between the diagonal of A^3 and the number of 3-cycles. The number of walks from a vertex to itself in a 3-cycle are 2, both going in an opposite direction to each other. Therefore, as there are 3 vertices in a 3-cycle, every 3-cycle contributes 6 total walks to the diagonal of A^3 [4]. Which leads us to the next theorem.

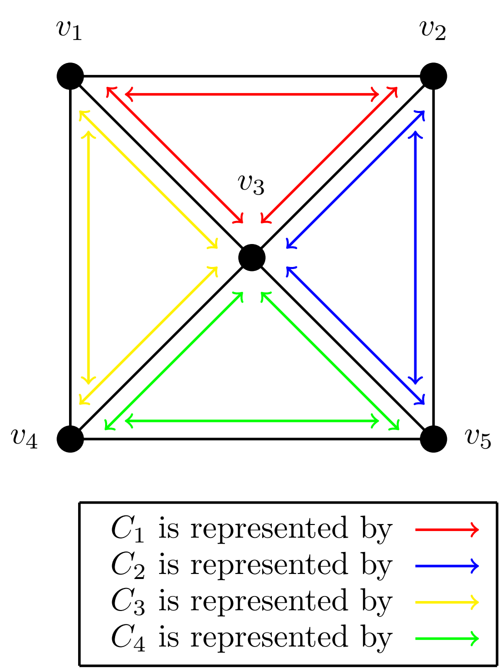
Theorem 4.1. *The number of* 3*-cycles in a graph* G *with adjacency matrix* A *is* n*, such that*

$$n = \frac{Tr(A^3)}{6}$$

where Tr *is the trace function of a matrix.*

Proof. Let $G = (V, E)$ We know that all 3-length walks which start and end at a vertex v_i are part of cycles. And we know that the (i, i) entry of A^3 is the number of length 3 walks from v_i to itself. Therefore $Tr(A^3)$ is the sum of all length 3 walks for all vertices in the graph G which start and end at the same vertex. Let us consider a cycle $C = (v_i, v_j, v_k)$, then let us create a walk $W = (v_i, \{v_i, v_j\}, v_j, \{v_j, v_k\}, v_k, \{v_k, vi\}, v_i)$, where $\{v_i, v_j, v_k\} \subset V$ and the sets between the vertices are their corresponding edges. Then we can permute the first 3 vertices of the cycle C and write them as W to obtain all walks related to that cycle. Therefore for one cycle C there exist $3! = 6$ total walks. Hence as only 3-cycle contribute length 3 walks starting and ending at the same vertex and every 3-contributes exactly 6 walks, then the total number of length 3 walks starting and ending at the same vertex, that is, $Tr(A^3)$ is divisible by 6 □

We can visualize and apply this theorem below in Figure 4.1



$$A^3 = \begin{bmatrix} 4 & 8 & 8 & 8 & 4 \\ 8 & 4 & 8 & 4 & 8 \\ 8 & 8 & 8 & 8 & 8 \\ 8 & 4 & 8 & 4 & 8 \\ 4 & 8 & 8 & 8 & 4 \end{bmatrix}$$

Figure 4.1 We can visualize the 4 different 3-cycles of this example graph C_1,C_2,C_3 and C_4 while comparing them to A^3 and its trace.

In this graph we can see that there are 4 3-cycles. Represented by C_1, C_2, C_3 and C_4. And we see that,

$$\begin{aligned}\frac{Tr(A^3)}{6} &= \frac{(4+4+8+4+4)}{6} \\ &= \frac{24}{6} \\ &= 4\end{aligned}$$

As there are 4 cycles in this graph, this theorem gives us the correct number of cycles once we apply it to the trace of A^3.

References

[1] Stephen Andrilli and David Hecker. Chapter 8 - additional applications. In Stephen Andrilli and David Hecker, editors, *Elementary Linear Algebra (Fourth Edition)*, pages 491 – 585. Academic Press, Boston, fourth edition edition, 2010.

[2] Murat Kirişci and Deniz Öncel. The new algorithm involving minimum spanning tree for computer networks in a growing company. *İSTANBUL TİCARET ÜNİVERSİTESİ FEN BİLİMLERİ DERGİSİ*, 16(32):1–14, 2017.

[3] E. Keith Lloyd, Jiri Matousek, and Jaroslav Nesetril. Invitation to discrete mathematics. *The Mathematical Gazette*, 83(498):561, 1999.

[4] Jagdish Kumar Pahade and Manoj Jha. Trace of positive integer power of adjacency matrix. *Global Journal of Pure and Applied Mathematics*, 13(6):2079–2087, 2017.

[5] Dragan Stevanović. Chapter 1 - introduction. In Dragan Stevanović, editor, *Spectral Radius of Graphs*, pages 1 – 13. Academic Press, Boston, 2015.