Powers of the Adjacency Matrix and the Walk Matrix

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Introduction The aim of this article is to identify and prove various relations between powers of adjacency matrices of graphs and various invariant properties of graphs, in particular distance, diameter and bipartiteness. A relation between the Walk matrix of a graph and a subset of the eigenvectors of the graph will also be illustrated. A number of *Mathematica* procedures are also provided which implement the results described. Note that the procedures are only illustrative; issues of algorithmic efficiency are largely ignored.

Unless specified, all graphs are assumed to be simple and connected, that is, there is at most one edge between each pair of vertices, there are no loops, and there is at least one path between every two vertices. The adjacency matrix A or $A(G)$ of a graph G having vertex set $V = V(G) = \{1, ..., n\}$ is an $n \times n$ symmetric matrix a_{ij} such that $a_{ij} = 1$ if vertices i and j are adjacent and 0 otherwise.

Powers of the Adjacency Matrix

The following well-known result will be used frequently throughout:

Theorem 0.1 *The $(i, j)^{th}$ entry a_{ij}^k of A^k, where $A = A(G)$, the adjacency matrix of G, counts the number of walks of length k having start and end vertices i and j respectively.*

Proof For $k = 1$, $A^k = A$, and there is a walk of length 1 between i and j if and only if $a_{ij} = 1$, thus the result holds. Assume the proposition holds for $k = n$ and consider the matrix $A^{n+1} = A^n A$. By the inductive hypothesis, the $(i, j)^{th}$ entry of A^n counts the number of walks of length n between vertices i and j. Now, the number of walks of length $n + 1$ between i and j equals the number of walks of length n from vertex i to each vertex v that is adjacent to j. But this is the $(i, j)^{th}$ entry of $A^n A = A^{n+1}$ the non-zero entries of the column of A corresponding to v are precisely the first neighbours of v. Thus the result follows by induction on n. ∎

The Diameter of a Graph

Definition 0.1 *The distance between two vertices i and j in a graph G, denoted d_{ij}, is the length of the shortest path between i and j. Clearly, since G is connected such a path must exist.*

Definition 0.2 *The diameter of G is defined to be* $D = \max_{(i,j)\in V}\{d_{ij}\}$.

Remark Although most of the results in this section can be found in [2], most of the proofs appearing here are different.

Lemma 0.2 *Let d_{ij} be the distance between vertices i and j in G. Then for all $k \in \mathbb{N}$, there is a walk of length $d_{ij} + 2k$ between i and j.*

Proof Let $k \in \mathbb{N}$. We shall construct a walk of length $d_{ij} + 2k$ between i and j. Let $i = v_1, v_2, \ldots, v_{p-1}, v_p = j$ be the path of length d_{ij} between i and j. After following this path, follow the cycle v_p, v_{p-1}, v_p k times. The ending vertex is j and the total length of this constructed walk is $d_{ij} + 2k$. ∎

Theorem 0.3 *[2] Let D be the diameter of the graph G. Then the matrix $A^D + A^{D-1}$ has no zero entries.*

Proof Without loss of generality, let D be even. Let $i, j \in V(G)$. If d_{ij} is even, $D - d_{ij}$ is also even, and thus by the previous lemma there is a walk of length $d_{ij} + D - d_{i,j} = D$ between i and j , and thus the (i, j) entry of A^D is greater then 0. If d_{ij} is odd, then $D - d_{ij} - 1$ is even, and thus by the previous lemma, there is a walk between i and j of length $d_{ij} + (D - d_{ij} - 1) = D - 1$. Hence the $(i, j)^{th}$ entry of A^{D-1} is greater than 0. Since the entries of A^D and A^{D-1} are non-negative, in either case, $A^D + A^{D-1}$ has no zero entries. ∎

The converse of this proposition is also true, and provides us with an algorithm for calculating the diameter of the graph.

Theorem 0.4 *[2] Let d be the smallest natural number such that, $A^d + A^{d-1}$ has no zero entries. Then $d = D$, the diameter of G.*

Proof By Theorem 0.3, d can be found such that $A^d + A^{d-1}$ has no zero entries. Hence $d \leq D$. Suppose $d < D$. Let (i, j) be a pair of vertices at a distance D apart in G. then the ijth entries of A^d and of A^{d-1} are both zero, a contradiction. Thus $d \geq D$. Also for any two vertices i, j, a_{ij}^D or a_{ij}^{D-1} is non-zero, so that $d \leq D$. Thus $d = D$ as required.

Corollary 0.5 *Let d be the smallest natural number such that $(A + I)^d$ has no zero entries. Then $d = D$ the diameter of G.*

Proof $(I + A)^d = I + dA + \ldots + A^d$, where the entries of each A^i are non-negative, and coefficients are positive. Thus the $(i, j)^{th}$ entry of $(A + I)^d$ is non-zero if and only if, $a_{ij}^k > 0$ for some $1 \leq k \leq d$. Suppose $A^d + A^{d-1}$ has a zero entry (i, j). Then there must be some $A^k, 1 \leq k \leq d - 2$ such that the $(i, j)^{th}$ entry of A^k is non-zero, i.e. There is a walk of length k from i to j. Now either $(d - k)$ is even or $(d - k - 1)$ is even. Thus by lemma 2.1, there is a walk of length $k + (d - k) = d$ or $k + (d - k - 1) = d - 1$ between i and j. This implies that the $(i, j)^{th}$ entry of $A^{d-1} + A^d$ is non-zero which is a contradiction. Thus d is the smallest natural number such that $A^d + A^{d-1}$ has no zero entries. The result follows by the previous proposition. ∎

This corollary provides us with a very simple algorithm to determine the diameter of a graph G from its adjacency matrix:

```
HasZeros[m_] := MemberQ[Flatten[m], 0]

Diam[G_] := Module[{d = 1, m2 = m = A + IdentityMatrix[Length[A]]},
        While [HasZeros[m], m = m.m2;   d++];  d]
```

Theorem 0.6 *The diameter D of a (connected) graph G is less than the number of distinct eigenvalues of the adjacency matrix.*

Proof Let the number of distinct eigenvalues of the adjacency matrix A be r. Since A is real and symmetrical, it is diagonalizable. Then the minimal polynomial $m_T(x)$ of A has degree r and $m_T(A) = \mathbf{0}$.

We will show that there exist elements in $\{I, A, \ldots A^D\}$ which are not linear combinations of their predecessors, and thus show that $\{I, A, \ldots A^D\}$ is linearly independent, which implies that there is no polynomial of degree D or less satisfied by A. Consider $d = d_{ij} \leq D$, for some $i, j \in V(G)$. It follows, by definition of d_{ij}, that $a^d_{ij} \neq 0$ and $a^t_{ij} = 0$ for $t < d$. Thus it is impossible that A^d is a linear combination of its predecessors. It follows that $r \geq D + 1$ as required. ∎

Tests for Bipartiteness

By observing powers of the adjacency matrix A, it is possible to determine whether G is bipartite through a simple test.

Definition 0.3 *The index of a graph G is defined to be the smallest γ such that A^γ has no zero entries.*

Note that not every graph has an index as will be seen soon. We will require the following lemma:

Lemma 0.7 *Let D be the diameter of the graph G having adjacency matrix A. If there are two columns r_i, r_j in A^D which are orthogonal, then G is necessarily bipartite.*

Proof Let r_i, r_j be two orthogonal columns in A^D. Partition V into the sets V_1 and V_2, where V_1 is the set of vertices having non-zero entries in r_i and V_2 is the set of vertices having zero entries in r_i. Then any two vertices in the same class are not adjacent. Suppose for contradiction that vertices $k, l \in V_1$ are adjacent. Then $a^D_{ki}, a^D_{li} > 0$, and thus $a^D_{kj} = a^D_{lj} = 0$. Thus the distances d_{kj} and d_{lj} are less than D, and $D - d_{kj} = D - d_{lj} = 1 \mod 2$. Thus $D - d_{kj} - 1 = D - d_{lj} - 1 = 0 \mod 2$, which implies that a^{D-1}_{kj}, $a^{D-1}_{lj} > 0$ by Lemma 0.2. But k is adjacent to l. Thus, there must be a walk of length D between vertices k, j and l, j and thus $a^D_{kj}, a^D_{lj} > 0$ which contradicts the orthogonality of r_i and r_j. A similar contradiction is obtained if one assumes that $k, l \in V_2$ are adjacent. ∎

Proposition 0.8 *Let G be a connected, non-bipartite graph, then the index γ of G exists and satisfies $D \leq \gamma \leq 2D$.*

Proof Clearly, $D \leq \gamma$, since if $\gamma < D$ then, by definition of the index γ of G, A^γ has no zero elements. Thus $A^\gamma + A^{\gamma-1}$ has no zero elements but this would contradict Theorem 0.4. Thus $D \leq \gamma$. We will now show that A^{2D} has no zero elements. Suppose, for contradiction that the $(i,j)^{th}$ entry of A^{2D} is 0. Then $a_{ij}^{2D} = A_{ij}^{2D} = A_{ij}^D A_{ij}^D = \sum_{h=1}^n a_{ih}^D a_{hj}^D = \sum_{h=1}^n a_{hi}^D a_{hj}^D = 0$. This implies that the i^{th} and j^{th} columns of A^D, a_i and a_j are orthogonal. But this implies that G is bipartite by the previous lemma, contradicting the premise that G is non-bipartite. Thus since A^{2D} has no zero entries. By the minimality of $\gamma, \gamma \leq 2D$. ∎

Proposition 0.9 *Let G be bipartite. Then the index γ of G does not exist.*

Proof Let G be bipartite, and let V_1, V_2 be the partitions. Then, for $i, j \in V_1$, all walks between i and j must contain an odd number of (not-necessarily distinct) vertices. Thus all walks between i and j must be of even length. Also, for $k \in V_1, l \in V_2$, all walks between k and l must contain an even number of (not necessarily distinct) vertices. Thus all walks between k and l must be of odd length. Thus for γ odd, the $(i,j)^{th}$ entry of A^γ is zero, and for γ even, the $(k,l)^{th}$ entry of A^γ is zero. Thus A^γ always has a zero entry. ∎

Using the above two propositions, we obtain the following corollary:

Corollary 0.10 *G is non-bipartite if and only if $D \leq \gamma \leq 2D$.* ∎

The following Mathematica function will compute the index γ of a non-bipartite graph:

```
GraphIndex[M_] := Module[{d := 1, M1 := M},
                   While [HasZeros[M1], d++; M1 = M1.M]; d]
```

The following algorithm will determine whether a graph G is bipartite by testing the powers of $A = A(G)$, between D and $2D$, as described in the above corollary:

```
isBipartite[G_] := Module[{d = Diam[A], result = True, m},
                    m = MatrixPower[A, d];
                    For [i = d, i <= 2d, i++,
                          If[HasZeros[m], m = m.G,
                               result = False; Break]]; result]
```

The Walk Matrix of a Graph

We will now digress and describe an interesting result that relates the number of main eigenvalues to the rank of a matrix known as the Walk Matrix of the graph. We will denote the all ones vector by $\mathbf{j} = (1, 1, \ldots, 1)^{\top}$.

Definition 0.4 *An eigenvalue is said to be non-main if it has an associated eigenvector* $\mathbf{x}$ *the sum of whose entries is not equal to 0, i.e,* $\mathbf{x}.\mathbf{j} \neq 0$

Definition 0.5 *Let G be a graph with adjacency matrix A. The walk matrix $W = W_p(A)$ of G is the $n \times p$ matrix $(j, Aj, A^2j, \ldots, A^{p-1}j)$, where p is the smallest value such that the walk matrix $W_p(A)$ attains maximum rank.*

The columns of the walk matrix define an A-cyclic subspace $U = \{a_j, \quad i \in N\}$. Since U is a subspace of R^n, it is finite dimensional, having dimension p, and it can be shown that U is generated by the basis $(j, Aj, A^2j, \ldots, A^{p-1}j)$. Thus the above definition is well defined, and p can be defined to be the smallest value such that $Rank(W_p(A)) = Rank(W_{p+1}(A)) = p$.

The graph-theoretic interpretation of a single column A^rj of the walk matrix, is as follows: the i^{th} entry of A^rj counts the number of walks of length r starting from vertex i. Thus using the above result, the set of these vectors is finitely generated, and every vector A^rj, $p \leq r$ is a linear combination of the vectors $(j, Aj, A^2j, \ldots, A^{p-1}j)$.

Lemma 0.11 *Let $A = A(G)$ be the adjacency matrix of G. Then a set of n orthonormal eigenvectors can be chosen such that for each eigenvalue, at most one corresponding eigenvector is main.*

Proof Suppose there is an eigenvalue λ with multiplicity greater than one, and let $\mathbf{x_1}, \ldots, \mathbf{x_m}$ be an orthonormal basis for the corresponding eigenspace where x_1 is main. Clearly we can assume that that $\mathbf{x_k}.\mathbf{j} \geq 0$ for all k. Now suppose $\mathbf{x_i}$ is another main vector. Then replace $\mathbf{x_i}$ with:

$$\mathbf{x_i'} = \mathbf{x_i} - \frac{\mathbf{x_i}.\mathbf{j}}{\mathbf{x_1}.\mathbf{j}}\mathbf{x_1}$$

and replace $\mathbf{x_1}$ with:

$$\mathbf{x_1'} = \frac{\mathbf{x_i}.\mathbf{j}}{\mathbf{x_1}.\mathbf{j}}\mathbf{x_i} + \mathbf{x_1}$$

and normalize accordingly. Then $\mathbf{x_1'}$ is a main eigenvector, $\mathbf{x_i'}$ is non-main, and the set $\{\mathbf{x_1'}, \mathbf{x_2}, \ldots, \mathbf{x_i'}, \ldots, \mathbf{x_n}\}$ is an orthonormal set of eigenvectors satisfying the required condition. ∎

We can now prove the following theorem relating the rank of the Walk Matrix to the number of main eigenvalues.

Theorem 0.12 *[4] The rank of the walk-matrix of a graph G is equal to the number of its main eigenvalues.*

Proof By the previous lemma, we can choose an orthonormal set of n eigenvectors such that each eigenvalue has at most one corresponding main eigenvector. Let $\mathbf{x_1}, \mathbf{x_2}, \ldots \mathbf{x_m}$ be the set of orthonormal eigenvectors corresponding to the main eigenvalues, $\lambda_1, \ldots, \lambda_m$ of G. As before, we can assume that $a_i = \mathbf{x_i}.\mathbf{j} > 0$ for $i = 1, \ldots, m$. Then $\mathbf{j}$ can be expressed as the linear combination $\mathbf{j} = \sum_{i=1}^{m} a_i \mathbf{x_i}$. Since for any $k \geq 0, A^k\mathbf{j} = \sum_{i=1}^{m} a_i \lambda_i^k \mathbf{x_i}$, then we have that

$$U = \text{Span}(A^k\mathbf{j}, \forall k \geq 0) \subseteq \text{Span}(\mathbf{x_1}, \ldots, \mathbf{x_m})$$

Thus $\dim U =$ rank $W(G) \leq m$. We will now show that U contains a linearly independent set of m vectors, namely $\mathbf{j}, A\mathbf{j}, \ldots, A^{m-1}\mathbf{j}$.

Suppose that $\sum_{j=1}^{m} c_j A^{j-1}\mathbf{j} = 0$ for some constants $c_1, \ldots, c_m$. Then

$$0 = \sum_{j=1}^{m} c_j A^{j-1}\mathbf{j} = \sum_{j=1}^{m} c_j \sum_{i=1}^{m} a_i \lambda_i^{j-1}\mathbf{x_i} = \sum_{i=1}^{m} a_i \sum_{j=1}^{m} c_j \lambda_i^{j-1}\mathbf{x_i}$$

Then since $a_i > 0$ and $\mathbf{x_i}, \quad i = 1, \ldots, m$, are orthonormal, then

$$\sum_{j=1}^{m} c_j \lambda_i^{j-1} = 0, \quad i = 1, \ldots, m$$

But the λ_i's are all distinct, and so we have a polynomial of degree $m-1$ with m distinct roots which is only possible if the polynomial is entirely 0, that is $c_j = 0, \quad j = 1, \ldots, m$. Thus the set $\mathbf{j}, A\mathbf{j}, \ldots, A^{m-1}\mathbf{j}$ is linearly independent and so rank $W(G) = m$. ∎

References

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