Adjacency Matrices and Graph Eigenvalues

MATH 3V03
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Abstract

The following is a note from MATH 3V03: Graph Theory at McMaster University which I taught in Fall, 2019. These notes are presented as-is and may contain errors. You have been warned.

1 Linear algebra review

1.1 Eigenvalues and eigenvectors

Let A denote a $n \times n$ matrix with real entries, where n is some positive integer. A number λ is an *eigenvalue* of A if there exists a nonzero $n \times 1$ column vector $\mathbf{x}$ such that

$$A\mathbf{x} = \lambda\mathbf{x}.$$

A vector $\mathbf{x} \neq 0$ with this property is an *eigenvector* of A for the eigenvalue λ. The set of all eigenvalues of A is the *spectrum* of A, sometimes denoted *spec*(A).

The *characteristic polynomial of* A is

$$p_A(x) := \det(xI - A)$$

which is a polynomial of degree n in the variable x. A number λ is an eigenvalue of A if and only if it is a root of p_A. The *algebraic multiplicity* of an eigenvalue λ is the multiplicity of λ as a root of p_A, denoted $m_{alg}(\lambda)$. By the Fundamental Theorem of Algebra,

$$\sum_{\lambda \in spec(A)} m_{alg}(\lambda) = n.$$

It is worth noting that in general the eigenvalues of A may be complex numbers. However, we will not need to deal with complex numbers in this course.

1.2 Orthogonal matrices and the spectral theorem

A $n \times n$ matrix S with real entries is *orthogonal* if $SS^T = I$. Equivalently, the columns of S form an orthonormal basis of $\mathbb{R}^n$. One of the main properties of orthogonal matrices is that for any $n \times n$ matrix A,

$$\det(SAS^T) = \det(A).$$

It follows that the characteristic polynomials of A and SAS^T are the same since

$$\det(xI - SAS^T) = \det(S(xI - A)S^T) = \det(xI - A).$$

A matrix $A \in M_n(\mathbb{R})$ is *orthogonally diagonalizable* if there exists an orthogonal matrix, S, and a diagonal matrix with real entries, D, such that

$$A = SDS^T.$$

If A is orthogonally diagonalizable and the diagonal entries of D are $d_1, \ldots, d_n$ (possibly with repetition), then

$$p_A(x) = p_D(x) = \prod_{i=1}^{n}(x - d_i)$$

In particular, if A is orthogonally diagonalizable, then A has n real eigenvalues, counting algebraic multiplicity.

Not all $n \times n$ matrices with real entries are orthogonally diagonalizable. Recall that a matrix A is *symmetric* if $A = A^T$. The following theorem is arguably one of the most important results in linear algebra.

Theorem 1.1 (The Spectral Theorem)**.** *Every symmetric matrix is orthogonally diagonalizable.*

2 Adjacency matrices

Let $G = (V, E)$ be a finite simple graph of order n. An *enumeration of the vertices of* G is a bijection $V \leftrightarrow \{1, \ldots, n\}$. Given a choice of enumeration of the vertices of G, we may refer to the ith vertex and denote it by v_i. Note that there are many different ways to enumerate the vertices of a graph.

Definition 2.1 (Adjacency matrix)**.** For a given choice of enumeration of the vertices of G, we can define an *adjacency matrix*, the $n \times n$ matrix $A(G)$ with entries

$$a_{i,j} = \begin{cases} 1 & \text{if the } i\text{th vertex is adjacent to the } j\text{th vertex} \\ 0 & \text{else.} \end{cases}$$

Example 2.2. Simple example: P_2.

We note the following facts about adjacency matrices:

- The adjacency matrix contains all the information about G; it is possible to completely reconstruct G from $A(G)$.
- $A(G)$ depends on the choice of enumeration of the vertices of G. In general, two different enumerations for the same graph will give different adjacency matrices. Thus, even though $A(G)$ encodes all the information of G, it is not an isomorphism invariant of graphs: it encodes too much information!
- Since simple graphs don't have loops, the diagonal entries of $A(G)$ are all 0.
- One could make a similar definition of adjacency matrices for multigraphs or pseudographs. In this case, entries of $A(G)$ could be any non-negative integer and in the latter case the diagonal entries might be nonzero. One could also define adjacency matrices for graphs with weighted edges, where $a_{i,j} = w(e_{i,j})$, in which case the entries could be whatever numbers are allowed as weights.
- For all $1 \leq i \leq n$, it follows from the definition that

  $$\sum_{j=1}^{n} a_{i,j} = \sum_{j=1}^{n} a_{j,i} = \deg(v_i).$$

  Thus, one can recover the degree sequence of G from $A(G)$ by summing all the rows or columns.

- Combining the previous fact with the Degree-Sum Theorem,

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{i,j} = \sum_{i=1}^{n} \deg(v_i) = 2|E|.$$

- $A(G)$ is symmetric. It follows from the Spectral Theorem that $A(G)$ has n real eigenvalues, counting multiplicities. It is often useful to denote these eigenvalues by $\lambda_1, \dots, \lambda_n$ (possibly with repetitions) such that

$$\lambda_1 \leq \cdots \leq \lambda_n.$$

- Since the diagonal entries of $A(G)$ are all 0, the trace of $A(G)$ is also 0. It follows from the "sum of eigenvalues equals trace" identity that

$$\sum_{i=1}^{n} \lambda_i = \mathrm{Tr}(A(G)) = 0.$$

- Suppose $\{i_1, \dots, i_k\} \subset \{1, \dots, n\}$, with $i_1 < i_2 < \cdots < i_k$. Let H be the induced subgraph of G with vertices $v_{i_1}, \dots, v_{i_k}$. The adjacency matrix of H corresponding to the enumeration $v_{i_1}, \dots, v_{i_k}$ is the $k \times k$ matrix $A(H)$ such that

$$A(H)_{p,q} = A(G)_{i_p,i_q} \qquad \forall 1 \leq p, q \leq k.$$

  In other words, $A(H)$ is the square submatrix of $A(G)$ with rows and columns $i_1, \dots, i_k$. To summarize:

  "The adjacency matrix of an induced subgraph is the corresponding submatrix of the adjacency matrix."

Example 2.3. Fix any enumeration of the vertices of K_n. Then $A(K_n)$ is the $n \times n$ matrix whose diagonal entries are 0 and whose off-diagonal entries are 1. For example

$$A(K_4) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Example 2.4. Recall that $K_{n,m}$ is the complete bipartite graph on n and m vertices. The vertices of $K_{n,m}$ are divided into two subsets: red and blue. There are n red vertices and m blue vertices and two vertices in $K_{n,m}$ are adjacent if and only if one is red and the other is blue.

Fix an enumeration of the vertices of $K_{n,m}$ such that the first n vertices are red and the last m vertices are blue. Then $A(G)$ is the $(n+m) \times (n+m)$-matrix that can written in a block-form

$$A(K_{n,m}) = \begin{pmatrix} 0_{n\times n} & 1_{n\times m} \\ 1_{m\times n} & 0_{m\times m} \end{pmatrix}$$

where $0_{j\times k}$ denotes the $j \times k$-matrix whose entries are all 0, and $1_{j\times k}$ denotes the $j \times k$-matrix whose entries are all 1. For example,

$$A(K_{2,3}) = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Example 2.5. For certain enumerations of the vertices of C_5 and P_5,

$$A(C_5) = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}, \qquad A(P_5) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Lemma 2.6. *Let $G = (V, E)$ be a finite simple graph of order n. Suppose that A and A' are adjacency matrices of G corresponding to different enumerations of V. Then there exists an orthonormal matrix S such that*

$$A = SA'S^T.$$

Proof. The enumerations of V used to define A and A' are related by a permutation of the set $\{1, \ldots, n\}$. It follows that A is related to A' by applying that permutation to both the rows and columns of A'. Applying a permutation to the rows of A' is equivalent to left multiplication by the corresponding permutation matrix, P. Applying the same permutation to the columns of A' is equivalent to multiplication on the right by P^T. Thus,

$$A = PA'P^T.$$

Finally, note that any permutation matrix P is orthogonal since the columns of P are an orthonormal basis (they're simply a reordering of the standard basis). $\square$

It follows from this lemma that the characteristic polynomial (and therefore also the eigenvalues) of an adjacency matrix of G does not depend on the choice of enumeration of the vertices of G. Thus we can make the following definition:

Definition 2.7. Let G be a finite simple graph.

- The *characteristic polynomial* of G is

$$p_G(x) := p_A(x)$$

  where A is any adjacency matrix of G.

- A number λ is an *eigenvalue* of G if it is an eigenvalue of the adjacency matrices of G.

- The *spectrum* of G is

$$spec(G) := spec(A)$$

  where A is any adjacency matrix of G.

The following theorem tells us that if $G_1 \cong G_2$, then $spec(G_1) = spec(G_2)$. In other words, characteristic polynomial and spectrum are isomorphism invariants of graphs.

Theorem 2.8. *Let G_1 and G_2 be finite simple graphs of order n. If G_1 and G_2 are isomorphic, then their characteristic polynomials are equal (i.e. $p_{G_1}(x) = p_{G_2}(x)$).*

Proof. We already showed in Lemma 2.6 that the characteristic polynomial of a graph doesn't depend on the choice of enumeration/adjacency matrix. It is therefore sufficient to show the following: if G_1 and G_2 are isomorphic, then for a particular choice of enumeration of the vertices for both graphs, $A(G_1) = A(G_2)$.

Let $f\colon V_1 \to V_2$ be a bijection that defines a graph isomorphism between $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. Fix a choice of enumeration of V_1 (i.e. a bijection $\{1, \ldots, n\} \leftrightarrow V_1$) and let $A(G_1)$ be the adjacency matrix determined by this enumeration.

We can also enumerate V_2 by composing the bijection $\{1, \ldots, n\} \leftrightarrow V_1$ with the map $f\colon V_1 \to V_2$. It follows by definition of graph isomorphism and adjacency matrices that the adjacency matrix $A(G_2)$ determined by this enumeration is the same as $A(G_1)$. $\square$

3 Graph eigenvalues and maximum degree

Definition 3.1. Let $G = (V, E)$ be a finite simple graph. The *maximum degree* of G is

$$\Delta(G) := \max_{v \in V}\{\deg(v)\}.$$

The *minimum degree* of G is

$$\delta(G) := \min_{v \in V}\{\deg(v)\}.$$

Maximum degree and minimum degree are graph invariants similar to the others we defined in lecture 2. They contain less information about a graph than the entire degree sequence. The following theorem gives a relationship between the spectrum of a graph and its maximum degree.

Theorem 3.2. *Let G be a finite simple graph. Then*

$$-\Delta(G) \leq \lambda \leq \Delta(G)$$

for all $\lambda \in spec(G)$.

Proof. Let n denote the order of G. Fix any enumeration of the vertices of G and let A be the corresponding adjacency matrix. Let λ be an arbitrary eigenvalue of G and let

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

be an eigenvector of A for the eigenvalue λ.

Choose an index $1 \leq i \leq n$ such that $|x_i| \geq |x_j|$ for all $1 \leq j \leq n$. Then,

$$\begin{aligned}
|\lambda||x_i| &= |\lambda x_i| \\
&= |(A\mathbf{x})_i| \qquad \text{by definition of eigenvector} \\
&= |\sum_{j=1}^{n} a_{i,j}x_j| \\
&\leq \sum_{j=1}^{n} a_{i,j}|x_j| \qquad \text{by the triangle inequality} \\
&\leq \left(\sum_{j=1}^{n} a_{i,j}\right)|x_i| \qquad \text{by definition of } x_i \\
&= \deg(v_i)|x_i| \qquad \text{by property of adjacency matrices} \\
&\leq \Delta(G)|x_i| \qquad \text{by definition of } \Delta(G).
\end{aligned}$$

Since it is an eigenvector, $\mathbf{x} \neq 0$, so $|x_i| > 0$. The theorem follows by dividing both sides of the inequality above by $|x_i|$. □

4 Counting walks in pseudographs using adjacency matrices

More generally now, suppose we have a finite pseudograph G with vertex set V, and suppose that we want to count the number of walks of a certain length between two vertices.

Fix an enumeration of the set of vertices. We can define an adjacency matrix A for G by defining the i,j-entry to be

$$a_{i,j} = \text{ the number of edges between vertex } i \text{ and vertex } j.$$

Remark 4.1. Note that with this convention, a loop at vertex i contributes $+1$ to the entry $a_{i,i}$. This convention has the disadvantage that the row and column sums of A no longer add up to the degree of the corresponding vertex (recall that when we defined degree of a vertex in pseudographs, we counted loops as $+2$). For this reason, most references adopt the convention that the adjacency matrix of a pseudograph has $+2$ in diagonal entries for each loop.

The utility of this definition is the following theorem.

Theorem 4.2. *Let A be an adjacency matrix of a finite pseudograph G. Then the i,j entry of A^ℓ equals the number of walks in G of length ℓ from vertex i to vertex j.*

Proof. We proceed by induction on ℓ.

Base case: ($\ell = 1$) A walk of length 1 is a sequence $v_i e v_j$ where v_i, v_j are vertices and e is an edge incident to v_i and v_j. The number of such walks is simply the number of edges incident to v_i and v_j. This is the entry of A, by definition.

Induction step: Let $b_{i,j}$ denote the i,j-entry of A^ℓ. Our induction hypothesis is that

$$b_{i,j} = \text{the number of walks of length } \ell \text{ from } v_i \text{ to } v_j.$$

Every walk of length $\ell + 1$ from v_i to v_j has the form

$$A_1 e_1 A_2 e_2 A_3 \dots A_\ell e_\ell A_{\ell+1}, \quad v_i = A_1,\, v_j = A_\ell.$$

By the induction hypothesis, for any vertex v_k, we have that

$$\begin{aligned}
&\text{the number of walks of length } \ell+1 \text{ from } v_i \text{ to } v_j \text{ with } A_\ell = v_k \\
&= (\text{the number of walks of length } \ell \text{ from } v_i \text{ to } v_k) \cdot (\text{the number of walks of length } 1 \text{ from } v_k \text{ to } v_j) \\
&= b_{i,k} a_{k,j}.
\end{aligned}$$

The total number of walks can then be counted in the following way:

$$\begin{aligned}
&\text{the number of walks of length } \ell+1 \text{ from } v_i \text{ to } v_j \\
&= \sum_{k=1}^{\ell} (\text{ the number of walks of length } \ell+1 \text{ from } v_i \text{ to } v_j \text{ with } A_\ell = v_k) \\
&= \sum_{k=1}^{n} b_{i,k} a_{k,j}.
\end{aligned}$$

On the other hand, observe that by associativity of matrix multiplication, $A^{\ell+1} = A^\ell A$. Thus, by definition of matrix multiplication, the i, j-entry of $A^{\ell+1}$ is

$$\sum_{k=1}^{n} b_{i,k} a_{k,j}. \qquad \square$$