MATH 8237

LECTURE Mar. 17, 2021

SPECTRAL GRAPH THEORY

Spectral graph theory studies relations between the spectra of matrices associated with graphs and the properties of the graphs themselves.

There are many ways to associate a matrix with a graph. The most common matrices are:

- adjacency;
- Laplacian;
- signless Laplacian;
- the normalized Laplacian;
- incidence matrix;
- distance matrix, etc.

Our focus will be on the adjacency matrix.

THE ADJACENCY MATRIX

Let G be a graph of order n and assume that $V(G) = \{1, 2, \ldots, n\}$.

Definition Define the **adjacency matrix** $A(G)$ of G as an $n \times n$ matrix $[a_{i,j}]$ by the following formula for its entries

$$a_{i,j} := \begin{cases} 1, & \text{if } \{i,j\} \in E(G); \\ 0, & \text{otherwise.} \end{cases}$$

Examples:

$$A(K_2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad A(\overline{K}_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$A(K_{1,2}) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad A(K_3) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

PROPERTIES OF THE ADJACENCY MATRIX

There are a few general properties of the adjacency matrix that should be spelled out right away:

- - all entries of $A(G)$ are 0 or 1; hence $A(G)$ is nonnegative;
- - $A(G)$ is **symmetric**, because $\{i,j\} \in E(G)$ if and only $\{j,i\} \in E(G)$;
- - the diagonal entries of $A(G)$ are zero, because the sets $\{i,i\}$ are not edges;
- - the ith row of $A(G)$ is the indicator function of the set $N_G(i)$.
- If the vertices of G are renumbered then both the rows and columns of $A(G)$ get renumbered in the same way

A FEW OBSERVATIONS

If $A(G)$ is given, the graph G is determined up to isomorphism.

- Every square, symmetric, $(0,1)$-matrix with zero diagonal is the adjacency matrix of some graph.

- The sum of all entries of the adjacency matrix of a graph G is twice the number the edges of G.

- The adjacency matrix of the edgeless graph is a zero matrix.

- The adjacency matrix of a disconnected graph is a direct sum of the adjacency matrices of its components.

- The adjacency matrix of a path is a tri-diagonal matrix.

EIGENVALUES OF A SQUARE MATRIX

Let $A := [a_{i,j}]$ be a square matrix of size $n \times n$. Recall the following definition:

Definition An **eigenvalue** is a number λ such that the linear equation

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

has a solution for some nonzero vector $\mathbf{x}$, called an **eigenvector** to λ.

Remark All nonzero multiples of an eigenvector to λ are also eigenvectors. An eigenvalue can have linearly independent eigenvectors as well. By contrast, an eigenvector cannot corresponds to a distinct eigenvalues.

Letting $\mathbf{x} := (x_1, \ldots, x_n)$, note that the above equation expands to

$$\begin{aligned} a_{1,1}x_1 + \cdots + a_{1,n}x_n &= \lambda x_1 \\ &\cdots \\ a_{n,1}x_1 + \cdots + a_{n,n}x_n &= \lambda x_n. \end{aligned}$$

Write I_n for the $n \times n$ identity matrix (the diagonal matrix with ones along the diagonal.)

Note that the equation

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

is equivalent to

$$(\lambda I_n - A)\,\mathbf{x} = 0.$$

Hence, λ is an eigenvalue of A if and only if the equation

$$(\lambda I_n - A)\,\mathbf{x} = 0$$

has a nonzero solution $\mathbf{x}$, which happens if and only if

$$\det(\lambda I_n - A) = 0.$$

THE CHARACTERISTIC POLYNOMIAL OF A

We can introduce a real (or complex) variable x and consider the expression

$$\det(xI_n - A)$$

or in expanded form

$$\det \begin{bmatrix} x - a_{1,1} & \cdots & -a_{1,n} \\ \cdots & \cdots & \cdots \\ -a_{n,1} & \cdots & x - a_{n,n} \end{bmatrix}.$$

Hence, $\det(xI_n - A)$ turns out to be a polynomial of degree n, with leading coefficient 1.

This polynomial is called the **characteristic polynomial** of A and its roots are the eigenvalues of the matrix A.

THE EIGENVALUES OF A GRAPH

Let G be a graph of order n with adjacency matrix A.

Since A is symmetric, all its eigenvalues are real (why?)

Moreover, we can choose a real eigenvector to each eigenvalue.

Definition The **eigenvalues** of G are the eigenvalues of its adjacency matrix.

Since the characteristic polynomial of A is of degree n, a graph of order n has n eigenvalues, which are real.

Note that not all eigenvalues of G must be distinct.

SIMPLE PROPERTIES OF EIGENVALUES

Write $\lambda_1, \lambda_2, \ldots, \lambda_n$ for the eigenvalues of G and arrange them in descending order

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

- The eigenvectors corresponding to a given eigenvalue λ, that is, the set of all $\mathbf{x} \in \mathbb{R}^n$ such that

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

is a subspace of $\mathbb{R}^n$, called the **eigenspace** of λ.

- **Proposition** *If λ' and λ'' are distinct eigenvalues of G with eigenvectors x' and x'', then x' and x'' are orthogonal.*

- **Corollary** *The eigenspaces corresponding to distinct eigenvalues are orthogonal.*

Theorem *If G is a graph of order n, then there is an orthogonal basis of R^n consisting of eigenvectors of G.*

Example

The characteristic polynomial of K_2 is

$$\det \begin{bmatrix} x & -1 \\ -1 & x \end{bmatrix} = x^2 - 1.$$

Hence the eigenvalues of K_2 are -1 and 1.

Writing down the system $A\mathbf{x} = \mathbf{x}$, we get

$$\begin{aligned} -x_1 + x_2 &= 0 \\ x_1 - x_2 &= 0 \end{aligned}$$

and we find that $\left(1/\sqrt{2},\ 1/\sqrt{2}\right)$ is a unit eigenvector to 1. Likewise we find that $\left(1/\sqrt{2},\ -1/\sqrt{2}\right)$ is a unit vector to -1.

THE EIGENEQUATIONS OF A GRAPH

The expanded form of the equation $A\mathbf{x} = \lambda\mathbf{x}$, can be written conveniently as

$$\lambda x_k = \sum_{i \in N(k)} x_i \qquad k = 1, \ldots, n. \tag{1}$$

Definition Equations (1) are called the **eigenequations** of G.

Proposition *If* G *is a graph with* $\Delta(G) = \Delta$*, then* $|\lambda| \leq \Delta$ *for every eigenvalue of* G.

Indeed, let $(x_1, \ldots, x_n)$ be an eigenvector to λ and suppose that $|x_k| = \max\{|x_1|, \ldots, |x_k|\}$. Then, taking the kth eigenequation, we find that

$$|\lambda x_k| = \left| \sum_{i \in N(k)} x_i \right| \leq \sum_{i \in N(k)} |x_i| \leq \sum_{i \in N(k)} |x_k| \leq \Delta |x_k|$$

and the assertion follows, because $|x_k| > 0$.

FURTHER USES OF EIGENEQUATIONS

Proposition *If G is an r-regular graph, then r is an eigenvalue of G with eigenvector of all ones.*

Indeed, let n be the order of G and let $\mathbf{j}_n$ denote the n-vector $(1, \ldots, 1)$. For $k = 1, \ldots, n$, we see that

$$r \cdot 1 = \sum_{i \in N(k)} 1,$$

and so r *is an eigenvalue of* G.

Corollary *If G is an r-regular graph, then $\lambda_1 = r$.*

Indeed, $\Delta(G) = r$, so $\lambda_1 \leq r$.

On the other hand, r is an eigenvalue of G, hence $\lambda_1 \geq r$, yielding $\lambda_1 = r$.

THE SUM OF THE EIGENVALUES

Looking at the characteristic polynomial of $n \times n$ matrix $\left[a_{i,j}\right]$

$$\det \begin{bmatrix} x - a_{1,1} & \cdots & -a_{1,n} \\ \cdots & \cdots & \cdots \\ -a_{n,1} & \cdots & x - a_{n,n} \end{bmatrix},$$

we see that its expanded form is a sum of the term

$$(x - a_{1,n}) \cdots (x - a_{n,n})$$

plus $n! - 1$ other terms all of degree $n - 2$.

Hence the coefficient to x^{n-1} is equal to the negative of the **trace** of the matrix $\left[a_{i,j}\right]$

$$a_{1,1} + \cdots + a_{n,n}.$$

By the Vieta formula, *the sum of the eigenvalues of a square matrix is equal to its trace.*

THE SUM OF THE EIGENVALUES OF GRAPH

Proposition *The sum of the eigenvalues of any graph is* 0.

- Hence, unless all eigenvalues of a graph G are 0, G has both positive and negative eigenvalues.

- *How large and how small the eigenvalues of a graph of order* n *can be?*

- Further answers to this question require that we view eigenvalues from a different angle.

- We introduced eigenvalues algebraically, but they can also be introduced analytically, as solutions to constraint optimization problems.

l_p-NORMS AND UNIT SPHERES

For any real $p \geq 1$, write $|\mathbf{x}|_p$ for the l_p-norm of a (complex) vector $\mathbf{x}$, that is, if $\mathbf{x} := (x_1, \ldots, x_n)$, then

$$|\mathbf{x}|_p := \left(|x_1|^p + \cdots + |x_n|^p\right)^{1/p}.$$

The set of all n-vectors $\mathbf{x}$ such that $|\mathbf{x}|_p = 1$ is called the **unit sphere** in l_p^n and is denoted by $\mathbb{S}_p^{n-1}$, that is,

$$\mathbb{S}_p^{n-1} := \left\{\mathbf{x} : \mathbf{x} \in \mathbb{R}^n \text{ and } |\mathbf{x}|_p = 1\right\}.$$

Note that $\mathbb{S}_p^{n-1}$ can be equivalently defined also as (avoiding the $1/p$ exponent)

$$\mathbb{S}_p^{n-1} := \{(x_1, \ldots, x_n) : (x_1, \ldots, x_n) \in \mathbb{R}^n,\ \ |x_1|^p + \cdots + |x_n|^p = 1\}.$$

Likewise, $\mathbb{S}_{p,+}^{n-1}$ is often used to denote the set

$$\mathbb{S}_{p,+}^{n-1} := \left\{(x_1, \ldots, x_n) : (x_1, \ldots, x_n) \in \mathbb{S}_p^{n-1} \text{ and } x_i \geq 0,\ \ i = 1, \ldots, n\right\}.$$

QUADRATIC FORMS

Given an $n \times n$ matrix $A := [a_{i,j}]$ and a vector variable $\mathbf{x} := (x_1, \ldots, x_n)$, the **quadratic form** of A is a function

$$P_A(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$$

defined as

$$P_A(\mathbf{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} x_j x_i.$$

Using the inner product notation, we get a more compact form for $P_A(\mathbf{x})$:

$$P_A(\mathbf{x}) = \langle A\mathbf{x}, \mathbf{x} \rangle.$$

Remark The quadratic form of the adjacency matrix A of a graph G can be written down as

$$P_A(\mathbf{x}) = 2 \sum_{\{i,j\} \in E(G)} x_i x_j.$$

QUADRATIC FORM AND UNIT EIGENVECTORS

Let G be a graph and λ be an eigenvalue of G with unit eigenvector $(x_1, \dots, x_n)$.

- Recall the eigenequations
$$\lambda x_i = \sum_{j \in N(i)} x_j \qquad i \in V(G).$$

- Multiply the ith equation by x_i and add all obtained equations. We get
$$\lambda = \sum_{i \in V(G)} \lambda x_i^2 = 2 \sum_{\{i,j\} \in E(G)} x_i x_j.$$

- **Proposition** *If G is a graph and λ is an eigenvalue of G with unit eigenvector $(x_1, \dots, x_n)$, then*
$$\lambda = 2 \sum_{\{i,j\} \in E(G)} x_i x_j.$$

THE RAYLEIGH PRINCIPLE

Theorem (Rayleigh-Ritz) *Let $A = [a_{i,j}]$ be an $n \times n$ real symmetric matrix.*

If λ and $\lambda_{\min}$ are the largest and the smallest eigenvalues of A, then

$$\lambda = \max_{|\mathbf{x}|_2=1} \langle A\mathbf{x}, \mathbf{x} \rangle, \qquad \lambda_{\min} = \min_{|\mathbf{x}|_2=1} \langle A\mathbf{x}, \mathbf{x} \rangle.$$

Moreover, $\lambda_1 = \max_{|\mathbf{x}|_2=1} \langle A\mathbf{x}, \mathbf{x} \rangle$ if and only if $\mathbf{x}$ is a unit eigenvector to λ_1, and the same holds for $\lambda_{\min}$.

Let us spell out the Rayleigh principle for a graph G:

$$\lambda_1 = 2 \max_{|\mathbf{x}|_2=1} \sum_{\{i,j\} \in E(G)} x_i x_j, \qquad \lambda_n = 2 \min_{|\mathbf{x}|_2=1} \sum_{\{i,j\} \in E(G)} x_i x_j.$$

The Rayleigh principle is extremely powerful statement and it makes graph eigenvalues widely applicable to extremal problems in graph theory.

A FEW APPLICATIONS OF THE RAYLEIGH PRINCIPLE

Theorem *If G is a graph of order n and m edges, then*

$$\lambda_1 \geq \frac{2m}{n}.$$

Proof Indeed, let $\mathbf{y}$ be the n-vector

$$n^{-1/2}\mathbf{j}_n = \left(\frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}}\right).$$

Obviously

$$|\mathbf{y}|_2^2 = n\left(\frac{1}{\sqrt{n}}\right)^2 = 1.$$

Hence, the Rayleigh principle implies that

$$\begin{aligned}\lambda_1 &= 2 \max_{|\mathbf{x}|_2=1} \sum_{\{i,j\}\in E(G)} x_i x_j \\ &\geq 2 \sum_{\{i,j\}\in E(G)} \frac{1}{\sqrt{n}} \cdot \frac{1}{\sqrt{n}} = \frac{2m}{n}.\end{aligned}$$

Theorem *If G is a graph of order $n \geq 2$ and has at least one edge, then*

$$\lambda_n \leq -1.$$

Proof Indeed, let $\{u, v\} \in E(G)$ and $\mathbf{y}$ be the n-vector

$$y_i := \begin{cases} 1/\sqrt{2}, & \text{if } i = u; \\ -1/\sqrt{2}, & \text{if } i = v; \\ 0, & \text{if } i \neq u \text{ and } i \neq v. \end{cases}.$$

We see that

$$|\mathbf{y}|_2^2 = \left(1/\sqrt{2}\right)^2 + \left(-1/\sqrt{2}\right)^2 = 1.$$

Hence, the Rayleigh principle implies that

$$\lambda_n = 2 \min_{|\mathbf{x}|_2=1} \sum_{\{i,j\} \in E(G)} x_i x_j \leq 2\left(1/\sqrt{2}\right)\left(-1/\sqrt{2}\right) = -1.$$

THE SPECTRAL RADIUS OF A GRAPH

If G is a graph of order n with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, a legitimate question is:

Question *Is is possible that* $|\lambda_k| > \lambda_1$ *for* $2 \leq k \leq n$?

Rayleigh's principle helps to answer this question in the negative.

First note that if

$$\mathbf{x} = (x_1, \ldots, x_n)$$

is a unit eigenvector to λ_1, then

$$\mathbf{x}' = (|x_1|, \ldots, |x_n|)$$

is also a unit eigenvector to λ_1, because $|\mathbf{x}'|_2 = 1$, and

$$\lambda_1 = 2 \sum_{\{i,j\} \in E(G)} x_i x_j \leq 2 \sum_{\{i,j\} \in E(G)} |x_i| |x_j| \leq \lambda_1.$$

That is, λ_1 always has a nonnegative eigenvector, and therefore

$$\lambda_1 = 2 \max_{\mathbb{S}_{2,+}^{n-1}} \sum_{\{i,j\} \in E(G)} x_i x_j.$$

Now, if λ_k is an eigenvalue with unit eigenvector $(y_1, \ldots, y_n)$, we know that

$$\lambda_k = 2 \sum_{\{i,j\} \in E(G)} y_i y_j$$

Hence, we find that

$$|\lambda_k| = 2 \left| \sum_{\{i,j\} \in E(G)} y_i y_j \right| \leq 2 \sum_{\{i,j\} \in E(G)} |y_i| \left| y_j \right| \leq \lambda_1.$$

Hence, λ_1 has maximal absolute value among all eigenvalues of a graph.

Definition The largest absolute value of an eigenvalue of a matrix A is called the **spectral radius** of A.

Corollary *If G is a graph, then the spectral radius of $A(G)$ is equal to $\lambda_1(G)$.*

HOFMEISTER'S BOUND ON λ_1

So far we have determined that if G is a graph of order n with m edges, and with $\Delta(G) = \Delta$, then

$$\frac{2m}{n} \leq \lambda_1 \leq \Delta \leq n - 1.$$

The lower bound on λ_1 can be improved by invoking the square of $A(G)$.

Observation Let $A = A(G)$ and λ be an eigenvalue of A with eigenvector $\mathbf{x}$. We see that

$$A^2\mathbf{x} = A(A\mathbf{x}) = A(\lambda\mathbf{x}) = \lambda A\mathbf{x} = \lambda^2\mathbf{x}.$$

Proposition *If G is a graph of order n with adjacency matrix A, then the eigenvalues of A^2 are $\lambda_1^2, \lambda_2^2, \ldots, \lambda_n^2$.*

Letting $A^2 = [b_{i,j}]$ and taking the n-vector

$$\left(\frac{1}{\sqrt{n}}, \ldots, \frac{1}{\sqrt{n}}\right),$$

the Rayleigh principle implies that

$$\lambda_1^2 \geq \sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j}\frac{1}{\sqrt{n}} \cdot \frac{1}{\sqrt{n}} = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j}.$$

It is not hard to see that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j} = \sum_{j=1}^{n} d_i^2.$$

Therefore, we get the following bound:

Theorem (Hofmeister) *If G is a graph of order n with degrees* $d_1, \ldots, d_n$, then

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{j=1}^{n} d_i^2}.$$

THANK YOU