Adjacency matrices

The Adjacency Matrix

Let G be a graph with vertex set $V = \{v_1, v_2, . . ., v_n\}$.

The adjacency matrix **A** of G, with respect to this listing of the vertices, is the n x n zero–one matrix (бинарная матрица) **A**.

$$a_{ij} = \begin{cases} 1 & \text{if } \{v_i, v_j\} \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

If G is undirected **A** is a symmetric matrix, that is, $\mathbf{A}^T = \mathbf{A}$.
By definition, the indices of the non-zero entries of the ith row of **A** correspond to the neighbors of vertex v_i.

Similarly, the non-zero indices of the ith column of **A** are the neighbors of vertex v_i.

The Adjacency Matrix

The adjacency matrix of a graph which can be used to obtain structural properties of a graph.

In particular, the eigenvalues and eigenvectors of the adjacency matrix can be used to infer properties such as bipartiteness, degree of connectivity, and many others.

This approach to graph theory is therefore called spectral graph theory.

Some notations

The identity matrix will be denoted by **I** and the matrix whose entries are all ones will be denoted by **J**.

For example, the 3×3 identity matrix and the 4×4 all ones matrix are shown bellow

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{J} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

The transpose of a matrix M will be denoted by $\mathbf{M}^{T}$.

Recall that a matrix

$\mathbf{M}$ is symmetric if $\mathbf{M}^{T} = \mathbf{M}$.

The (i, j) entry of a matrix $\mathbf{M}$ will be denoted by $\mathbf{M}(i, j)$.

It follows that the degree of v_i is the sum of the ith row (or ith column) of **A**, that is,

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

If we denote the column vector of all 1 by **e** = (1, 1, .., 1), then

$$\mathbf{Ae} = \begin{bmatrix} \deg(v_1) \\ \deg(v_2) \\ \vdots \\ \deg(v_n) \end{bmatrix}.$$

We will call **Ae** the degree vector of *G*.
We note that, after a possible permutation of the vertices, **Ae** is equal to the degree sequence of *G*.

One of the first applications of the the adjacency matrix of a graph G is to count paths in G.

A closed path of length 3 in a graph G implies that G contains $K_3 = C_3$ as a subgraph.
For obvious reasons, K_3 is called a triangle.

Counting Paths

Theorem 1: For any graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, the (i, j) entry of $\mathbf{A}^k$ is the number of paths from v_i to v_j of length k.

Proof. The proof is by induction on k.

For $k = 1$, $\mathbf{A}(i, j) = 1$ implies that v_i and v_j are adjacent and then clearly there is a paths of length $k = 1$ from v_i to v_j.

If on the other hand $\mathbf{A}(i, j) = 0$ then v_i and v_j are not adjacent and then clearly there is no path of length $k = 1$ from v_i to v_j.

Now assume that the claim is true for some $k \geq 1$ and consider the number of paths of length $k + 1$ from v_i to v_j.

Any path of length $k + 1$ from v_i to v_j contains a path of length k from v_i to a neighbor of v_j.

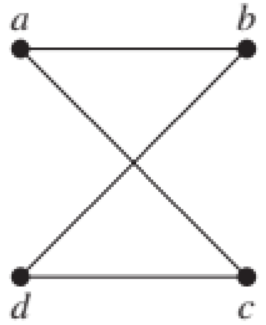
If $v_p \in N(v_j)$ then by induction the number of paths of length k from v_i to v_p is $\mathbf{A}^k(i, p)$.

Hence, the total number of paths of length $k + 1$ from v_i to v_j is

$$\sum_{v_p \in N(v_j)} \mathbf{A}^k(i,p) = \sum_{\ell=1}^{n} \mathbf{A}^k(i,\ell)\mathbf{A}(\ell,j) = \mathbf{A}^{k+1}(i,j).$$

EXAMPLE 1

How many paths of length 4 are there from a to d in the simple graph G in Figure bellow?



Solution: The adjacency matrix of G (ordering the vertices as a, b, c, d) is

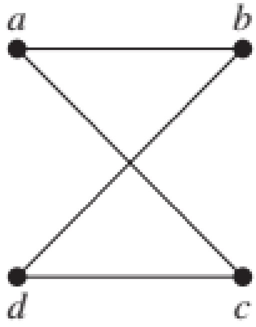
$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

Hence, the number of paths of length 4 from a to d is the $(1, 4)$th entry of $\mathbf{A}^4$.

Because there are exactly 8 paths of length 4 from a to d.

By inspection of the graph, we see that a, b, a, b, d; a, b, a, c, d; a, b, d, b, d; a, b, d, c, d; a, c, a, b, d; a, c, a, c, d; a, c, d, b, d; and a, c, d, c, d are the 8 paths of length 4 from a to d.

$$\mathbf{A}^4 = \begin{bmatrix} 8 & 0 & 0 & 8 \\ 0 & 8 & 8 & 0 \\ 0 & 8 & 8 & 0 \\ 8 & 0 & 0 & 8 \end{bmatrix},$$



The trace of a matrix **M** is the sum of its diagonal entries and will be denoted by *tr*(**M**):

$$\mathrm{tr}(\mathbf{M}) = \sum_{i=1}^{n} \mathbf{M}(i,i).$$

Since all the diagonal entries of an adjacency matrix **A** are all zero we have $\mathrm{tr}(\mathbf{A}) = 0$.

Corollary 2

Let G be a graph with adjacency matrix **A**.

Let m be the number of edges in G,

let t be the number of triangles in G,

and let q be the number of 4-cycles in G.

Then

$$\mathrm{tr}(\mathbf{A}^2) = 2m$$

$$\mathrm{tr}(\mathbf{A}^3) = 6t$$

$$\mathrm{tr}(\mathbf{A}^4) = 8q - 2m + 2\sum_{i=1}^{n} \deg(v_i)^2$$

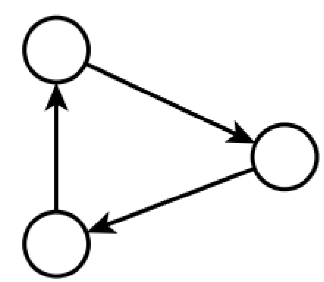
Proof. **1.** The entry $\mathbf{A}^2(i, i)$ is the number of closed paths from v_i of length k =2.

A closed path of length k = 2 counts 1 edge. Hence, $A^2(i, i) = \deg(v_i)$ and therefore

$$\operatorname{tr}(\mathbf{A}^2) = \sum_{i=1}^{n} \mathbf{A}^2(i, i) = \sum_{i=1}^{n} \deg(v_i) = 2m.$$

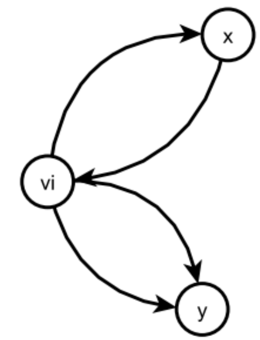
2. To prove the second statement, we begin by noting that a closed path can be traversed in 2 different ways.
Hence, for each vertex v in a triangle, there are 2 walks of length k = 3 that start at v and traverse the triangle.
And since each triangle contains 3 distinct vertices, each triangle in a graph accounts for 6 paths of length k = 3.

Since $\sum_{i=1}^{n} \mathbf{A}^3(i, i)$ counts all walks in G of length 3 we ha



$$\operatorname{tr}(\mathbf{A}^3) = \sum_{i=1}^{n} \mathbf{A}^3(i, i) = 6t.$$

3. Now consider $\mathrm{tr}(\mathbf{A}^4) = \sum_{i=1}^{n} \mathbf{A}^4(i,i)$.



We count the number of closed paths of length $k = 4$ from v_i.

There are 3 types of such walks:

(1) closed paths of the form (v_i, x, v_i, y, v_i) where $x, y \in N(v_i)$.

The number of such paths is $\deg(v_i)^2$ since we have $\deg(v_i)$ choices for x and $\deg(v_i)$ choices for;

(2) closed paths of the form (v_i, v_j, x, v_j, v_i) where $v_j \in N(v_i)$ ber

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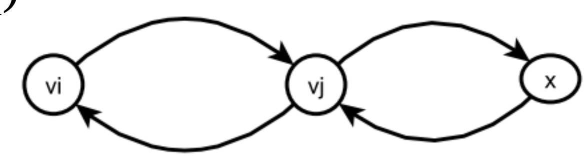
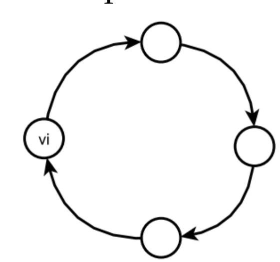
$\sum_{v_j \sim v_i} (\deg(v_j) - 1)$



(3) closed paths along 4-cycles from v_i and there are 2 such paths for each cycle v_i is contained in, say q_i. Hence,

$$\mathbf{A}^4(i,i) = 2q_i + \deg(v_i)^2 + \sum_{v_j \sim v_i} (\deg(v_j) - 1)$$



$$
\begin{aligned}
\operatorname{tr}(\mathbf{A}^4) &= \sum_{i=1}^{n} \left(2q_i + \deg(v_i)^2 + \sum_{v_j \sim v_i} (\deg(v_j) - 1) \right) \\
&= 8q + \sum_{i=1}^{n} \left(\deg(v_i)^2 - \deg(v_i) + \sum_{v_j \sim v_i} \deg(v_j) \right) \\
&= 8q - 2m + \sum_{i=1}^{n} \deg(v_i)^2 + \sum_{i=1}^{n} \sum_{v_j \sim v_i} \deg(v_j) \\
&= 8q - 2m + \sum_{i=1}^{n} \deg(v_i)^2 + \sum_{i=1}^{n} \deg(v_i)^2 \\
&= 8q - 2m + 2\sum_{i=1}^{n} \deg(v_i)^2
\end{aligned}
$$

$\square$

Corollary 3
A graph G with $n \geq 2$ vertices is connected $\Leftrightarrow$ the off-diagonal entries of the matrix $\mathbf{B} = \mathbf{A} + \mathbf{A}^2 + \cdot\cdot\cdot + \mathbf{A}^{n-1}$ are all positive.

In fact, $d(v_i, v_j) = \min\{k \mid \mathbf{A}^k(i, j) > 0\}$.

Proof. We first note that for any $k \geq 1$, all the entries of $\mathbf{A}^k$ are non-negative and therefore

if $\mathbf{A}^k(i, j) > 0$ for some $k \in \{1, 2, . . . , n - 1\}$ then $\mathbf{B}(i, j) > 0$.

=> Assume first that G is connected.

Then for distinct vertices $v_i \neq v_j$ we have that $1 \leq d(v_i, v_j) \leq n - 1$ since there is path from v_i to v_j.

Therefore,
if $k = d(v_i, v_j)$ then $\mathbf{A}^k(v_i, v_j) > 0$ and then also $\mathbf{B}(i, j) > 0$.

Hence, all off-diagonal entries of $\mathbf{B}$ are positive.

<= Now assume that all off-diagonal entries of **B** are positive.

Let v_i and v_j be arbitrary distinct vertices.

Since **B**$(i, j) > 0$ then there is a **minimum** $k \in \{1, . . . , n- 1\}$ such that $\mathbf{A}^k(i, j) > 0$.

Therefore, there is a path of length k from v_i to v_j.

We proved in the previous lecture that every such path is a **simple** path.

This proves that G is connected.

Below we give a relationship between the adjacency matrices of G and G' (complement of G).

Lemma 4
For any graph G it holds that
$\mathbf{A}(G) + \mathbf{A}(G') + \mathbf{I} = \mathbf{J}$.

Proof. Let $\mathbf{A} = \mathbf{A}(G)$ and let $\mathbf{A}' = \mathbf{A}(G')$.

For $i \neq j$, if $\mathbf{A}(i, j) = 0$ then $\mathbf{A}'(i, j) = 1$, and vice-versa.

Therefore, $\mathbf{A}(i, j) + \mathbf{A}'(i, j) = 1$ for all $i \neq j$.

On the other hand, $\mathbf{A}(i, i) = \mathbf{A}'(i, i) = 0$ for all i.

Thus $\mathbf{A}(G) + \mathbf{A}'(G) + \mathbf{I} = \mathbf{J}$ as claimed.

2.3	The characteristic polynomial and spectrum of a graph

Now we will consider the characteristic polynomial and spectrum of a graph and prove some of their basic properties.
Before we begin, we recall some basic facts from linear algebra.
Recall that λ is an eigenvalue of the matrix **M** if there exists a vector **x** such that $\mathbf{M}\mathbf{x} = \lambda\mathbf{x}$.
In this case, **x** is called an eigenvector of **M** corresponding to the eigenvalue λ.
To find the eigenvalues of **M**, we find the zeros of the characteristic polynomial of **M**:
$p(t) = \det(t\mathbf{I} - \mathbf{M})$.

If **M** is an $n \times n$ matrix, then the characteristic polynomial $p(t)$ is an nth order polynomial and

$p(\lambda) = 0 \Leftrightarrow \lambda$ is an eigenvalue of **M**.

From the Fundamental Theorem of Algebra, $p(t)$ has n eigenvalues, possibly repeated and complex.

However, if **M** is a symmetric matrix, then an important result in linear algebra is that the eigenvalues of **M** are all real numbers and we may therefore order them from say smallest to largest:
$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.

Also, if **M** is symmetric and **x** and **y** are eigenvectors of **M** corresponding to distinct eigenvalues then **x** and **y** are orthogonal, that is,

$$\langle \mathrm{x}, \mathrm{y} \rangle = \sum_{i=1}^{n} x_i y_i = 0.$$

Moreover, if **M** is symmetric, there exists an orthonormal basis $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, x_n\}$ of R^n consisting of eigenvectors of **M**.

Recall that $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_\mathbf{n}\}$ is an orthonormal basis of R^n if $\|\mathbf{x}_i\| = 1$ and $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = 0$ if $i \neq j$,

that is, the vectors in β are unit vectors and are mutually orthogonal.

Definition : Spectrum of a Graph

The characteristic polynomial of a graph G with adjacency matrix $\mathbf{A}$ is $p(t) = \det(t\mathbf{I} - \mathbf{A})$.

The spectrum of G, denoted by spec(G), is the list of the eigenvalues of $\mathbf{A}$ in increasing order

$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$:

spec(G) = $(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

Example 2 Show by direct computation that the characteristic polynomial of P_3 is $p(t) = t^3 - 2t$ and find the eigenvalues of P_3.

Example 3 The adjacency matrix of the empty graph E_n is the zero matrix and therefore the characteristic polynomial of E_n is $p(x) = x^n$.

Hence, E_n has spectrum $\mathrm{spec}(E_n) = (0, 0, \ldots, 0)$.

Example 2.8. The adjacency matrix of K_4 is

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Consider the vectors $\mathbf{x}_1 = (1, -1, 0, 0)$, $\mathbf{x}_2 = (1, 0, -1, 0)$, and $\mathbf{x}_3 = (1, 0, 0, -1)$.
It is not hard to see that $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ are linearly independent.
A direct computation yields $\mathbf{Ax}_1 = (-1, 1, 0, 0) = -\mathbf{x}_1$ and therefore $\lambda_1 = -1$ is an eigenvalue of $\mathbf{A}$.
Similarly, a direct computation yields that $\mathbf{Ax}_2 = -\mathbf{x}_2$ and $\mathbf{Ax}_3 = -\mathbf{x}_3$.
Hence, $\lambda_2 = \lambda_3 = -1$.
Finally, we have that $\mathbf{Ae} = (3, 3, 3, 3) = 3\mathbf{e}$, and therefore $\lambda_4 = 3$ is an eigenvalue of $\mathbf{A}$.

Therefore, the spectrum of K_n is spec(K_4) = (-1, -1, -1, 3)

and therefore the characteristic polynomial of K_4 is $p(t) = (t - 3)(t + 1)^3$.

In general, one can show that spec(K_n) = (-1, -1, . . ., -1, n - 1)

and therefore the characteristic polynomial of K_n is

$p(t) = (t - (n - 1))(t + 1)^{n-1}$.

The following result, and the previous example, shows that $\Delta(G)$ is a sharp bound for the magnitude of the eigenvalues of G.

Proposition 5
For any eigenvalue λ of G it holds that $|\lambda| \leq \Delta(G)$.

Proposition 6

Let spec(G) = ($\lambda_1, \lambda_2, \ldots, \lambda_n$) and let

$d_{\text{avg}} = \frac{2|E(G)|}{n}$ denote the average degree of G.

Then $d_{\text{avg}} \leq \lambda_n \leq \Delta(G)$.

Proposition 7

A graph G is k-regular if ⇔ $\mathbf{e} = (1, 1, . . . , 1)$ is an eigenvector of G with eigenvalue $\lambda = k$.

Proof. Recall that

$\mathbf{Ae} = (\deg(v_1), \deg(v_2), . . ., \deg(v_n))$.

If G is k-regular then $\deg(v_i) = k$ for all v_i and therefore

$\mathbf{Ae} = (k, k, . . . , k) = k\mathbf{e}$.

Thus, k is an eigenvalue of $\mathbf{A}$ with corresponding eigenvector $\mathbf{e}$.

On the other hand, if $\mathbf{e}$ is an eigenvector of G with eigenvalue k then

$\mathbf{Ae} = k\mathbf{e} = (k, k, . . . , k)$

and thus $\deg(v_i) = k$ for all v_i and then G is k-regular.

Cospectral graphs

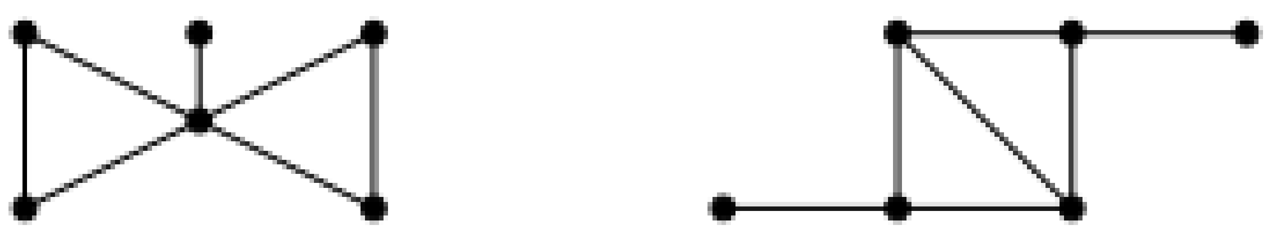
Let us consider now the question of whether it is possible to uniquely determine a graph from its spectrum.

To that end, we say that 2 graphs G_1 and G_2 are cospectral if they have the same (adjacency) eigenvalues.
Proposition 8 **: Spectrum of Isomorphic Graphs**
If G_1 and G_2 are isomorphic then $\mathrm{spec}(G_1) = \mathrm{spec}(G_2)$.

It is now natural to ask whether non-isomorphic graphs can have the same eigenvalues.

The answer turns out to be yes, and in fact it is not too difficult to find non-isomorphic graphs that have the same eigenvalues.

The smallest connected non-isomorphic cospectral graphs are shown bellow



Smallest connected non-isomorphic cospectral graphs