Topics in Discrete Mathematics
Part 2: Introduction to Graph Theory

Lecture 5

Graph Theory and Linear Algebra

- The adjacency matrix
- The spectrum, and that isomorphic graphs are cospectral
- Properties that can be inferred from the spectrum
- Properties that can't be inferred from the spectrum

5.1 The adjacency matrix

So far in this course, we've seen two ways to define a graph. The more formal way is to write down the sets V and E, which give the graph unambiguously. The less formal way is just to draw a picture, which defines a graph up to isomorphisms.

However, suppose you wanted to input the graph to a computer – how would you define it then? One natural way, for a graph with n vertices, would be to store an $n \times n$ array, or table, and place a 1 in position (i, j) to denote an edge ij, and leave the array as 0 otherwise.

In this lecture, we consider this table as a matrix, an algebraic object, which we call the *adjacency matrix*.

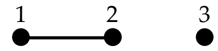
Definition 5.1. For a graph $G = (V, E)$, the *adjacency matrix* $\mathsf{A} = (a_{ij} : i, j \in V)$ of G is defined by

$$a_{ij} = \begin{cases} 1 & \text{if } ij \in E, \\ 0 & \text{if } ij \notin E. \end{cases}$$

For this lecture, we will follows conventions for algebra and label vertices using letters like i and j, rather than the u and v we've used elsewhere.

Note that since $ij = ji$ is the same edge, we have that $a_{ij} = a_{ji}$, so the adjacency matrix $\mathsf{A} = \mathsf{A}^\top$ is symmetric.

Consider, for example $K_2 \cup K_1$.



Since the only edge is $12 = 21$, the adjacency matrix is

$$\mathsf{A} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Alternatively, consider the complete graph K_n. Since ij is now an edge for every distinct $i \neq j$, we see that the adjacency matrix is

$$\mathsf{A} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 0 \end{pmatrix},$$

with 0s down the diagonal and 1s everywhere else.

One use of the adjacency matrix is that it gives us a quick way to calculate the number of walks between given vertices.

Theorem 5.2. *Consider a graph G, and write $W_{ij}(k)$ for the number of walks between vertices i and j of length k. Then $W_{ij}(k) = (\mathsf{A}^k)_{ij}$; that is, the (i, j)th entry of the matrix power A^k.*

Proof. We work by induction on k. The base case $k = 1$ is easy, since there is one path if ij is an edge, and no paths if it isn't.

Now assume the theorem holds for paths of length k. A path from i to j of length $k + 1$ consists of a walk of length k, followed by an edge from the final vertex of the walk to j. Hence, we have

$$W_{ij}(k+1) = \sum_{l \in V : lj \in E} W_{il}(k) = \sum_{l \in V} W_{il}(k) a_{lj},$$

since the a_{lj} ensures that we only count vertices l adjacent to j. Substituting in the indctive hypothesis, we get

$$W_{ij}(k+1) = \sum_{l \in V} (\mathsf{A}^k)_{il} a_{lj} = (\mathsf{A}^k \mathsf{A})_{ij} = (\mathsf{A}^{k+1})_{ij},$$

and we're done. □

5.2 The spectrum

In this lecture, we will be interested in investigating 'spectral graph theory' which involves trying to infer properties of a graph by looking at the eigenvalues of the adjacency matrix, which are called the *spectrum*.

Definition 5.3. The *spectrum* of a graph G is the set of eigenvalues (with multiplicity) of the adjacency matrix of G.

For a graph $G = (V, E)$ with $n = |V|$ vertices, the $n \times n$ adjacency matrix A has n eigenvalues, when counted with multiplicity. Further, since A is symmetric, all n eigenvalues will be real.

For small graphs, the easiest way to find the spectrum is to find the roots of the characteristic polynomial $\chi(x) = \det(x\mathsf{I} - \mathsf{A})$.

Example 5.4. Earlier, we saw that the adjacency matrix of $K_2 \cup K_1$ was

$$\mathsf{A} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Finding roots of the characteristic polynomial, we get

$$0 = \chi(\lambda) = \begin{pmatrix} \lambda & -1 & 0 \\ -1 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} = \lambda(\lambda^2) + 1(-\lambda) = \lambda^3 - \lambda = \lambda(\lambda - 1)(\lambda + 1).$$

Hence, we see that the spectrum is $\lambda = 1, 0, -1$.

For large but structured graphs, it can be easier to find the spectrum by guessing the eigenvectors.

Example 5.5. Consider K_n, which we saw had adjacency matrix

$$\mathsf{A} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 0 \end{pmatrix}.$$

First, applying A to the all-1 vector $\mathbf{1} = (1, 1, 1, \dots, 1)$, we see that $\mathsf{A}\mathbf{1} = (n-1)\mathbf{1}$. Hence $\lambda = n - 1$ is an eigenvector.

Second, consider taking a vector $\mathbf{x}$ orthogonal to $\mathbf{1}$, so that

$$\mathbf{x} \cdot \mathbf{1} = \sum_{i=1}^{n} x_i = 0.$$

We then see that

$$\mathsf{A} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} x_2 + x_3 + \cdots + x_n \\ x_1 \quad + x_3 + \cdots + x_n \\ x_1 + x_2 \quad + \cdots + x_n \\ \vdots \\ x_1 + x_2 + x_3 + \cdots \end{pmatrix} = \begin{pmatrix} \sum_i x_i - x_1 \\ \sum_i x_i - x_2 \\ \sum_i x_i - x_3 \\ \vdots \\ \sum_i x_i - x_n \end{pmatrix} = \begin{pmatrix} -x_1 \\ -x_2 \\ -x_3 \\ \vdots \\ -x_n \end{pmatrix},$$

so $\lambda = -1$ is an eigenvalue also. The subspace of vectors $\mathbf{x}$ such that $\sum_i x_i = 0$ has dimension $n - 1$, so the eigenvalue $\lambda = -1$ has multiplicity $n - 1$ also.

We now have n eigenvalues (counted with multiplicity) so there are no others. Hence, we see that the spectrum of K_n is $\lambda = n - 1$ with multiplicity 1 and $\lambda = -1$ with multiplicity $n - 1$.

Usefully, it turns out that isomorphic graphs have the same spectrum – reinforcing the view we've taken throughout the course that isomorphic graphs can be considered equal.

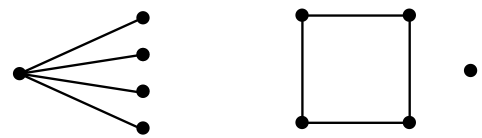
(If you'd worried earlier that our definition of the adjacency matrix could be argued to depend on an ordering put on the vertices, then this should put your mind at rest.)

Definition 5.6. Graphs with the same spectrum – that is, with adjacency matrices having the same eigenvalues with the same multiplicities – are called *cospectral*.

Theorem 5.7. *Isomorphic graphs are cospectral.*

Proof. Let G and G' be isomorphic graphs, and let A and A' be their respective adjacency matrices. Since an isomorphism is just a relabelling of vertices, we see that $\mathsf{A}' = \mathsf{P}^{-1}\mathsf{A}\mathsf{P}$ for some permutation matrix P, so A' and A are similar matrices. But similar matrices have the same eigenvalues with the same multiplicities, so we are done. □

Unfortunately, the converse to this theorem is not true. Consider the two graph $K_{1,4}$ and $C_4 \cup K_1$.



These graphs are clearly nonisomorphic, but you can check that they both have the characteristic polynomial $\chi(x) = x^3(x - 2)(x + 2)$, so have the common spectrum $\lambda = 2, 0, 0, 0, -2$.

5.3 Properties that can be inferred from the spectrum

We will now consider some properties of a graph that can be deduced from its spectrum.

1 Number of vertices

We saw earlier that the number of eigenvalues of the adjacency matrix was equal to the number of vertices.

2 Number of closed walks of a given length

Theorem 5.8. *Consider a graph G with spectrum $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$, and write $CW(k)$ for the number of closed walks of length k in G. Then*

$$CW(k) = \sum_{i=1}^{n} \lambda_i^k.$$

Proof. Since the closed walks are precisely the walks that start and end in the same place, we have $CW(k) = \sum_{i \in V} W_{ii}(k)$. Using Theorem 5.2, we have

$$CW(k) = \sum_{i \in V} (\mathsf{A}^k)_{ii} = \operatorname{Tr} \mathsf{A}^k,$$

the trace of A^k.

We know that the trace of a matrix is the sum of its eigenvalues. Further, we know that the eigenvalues of a matrix power are the powers of the eigenvalues of the original matrix. Hence the eigenvalues of A^k are $\lambda_1^k, \lambda_2^k, \dots, \lambda_n^k$, and we have

$$CW(k) = \operatorname{Tr} \mathsf{A}^k = \sum_{i=1}^{n} \lambda_i^n.$$ □

3 Number of edges

Theorem 5.9 (Handshaking lemma for the spectrum)**.** *Consider a graph $G = (V, E)$ with spectrum $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$. Then*

$$\sum_{i=1}^{n} \lambda_i^2 = 2|E|.$$

Proof. Note that the only closed paths of length 2 in a graph go down and back up a single edge. Each edge ij is in two length-2 paths: iji, beginning and ending at one end, i; and jij, beginning and ending at the other end, j. Hence we have $2|E| = CW(2)$, and the result follows by Theorem 5.8. □

4 Number of triangles

Recall that a *triangle* is a subgraph isomorphic to C_3.

Theorem 5.10 (Handshaking lemma for the spectrum)**.** *Consider a graph G with spectrum $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$, and write T for the number of triangles in G. Then*

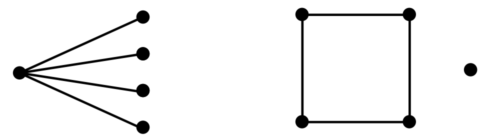
$$T = \frac{1}{6} \sum_{i=1}^{n} \lambda_i^3.$$

Proof. Note that the a closed paths of length 3 cannot repeat an edge, so $CW(3)$ counts precisely the number of 3-cycles in a graph. Note that this counts each triangle six times: starting and ending at each of 1, 2 and 3, going both clockwise and anticlockwise. Hence we have $T = \frac{1}{6} CW(3)$, and the result follows by Theorem 5.8. □

5.4 Properties that can't be inferred from the spectrum

It's also worth noting that their are a number of important properties of graphs that cannot be deduced from the spectrum.

Most of these can be illustrated by the example of the two cospectral graphs we examined earlier, $K_{1,4}$ and $C_4 \cup K_1$.



1 Isomorphism class

Clearly the two graphs above are not isomorphic. (Although, as we noted earlier, it is true that isomorphic graphs are cospectral.)

2 Number of k-cycles, $k \geq 4$

We see that $C_4 \cup K_1$ has one 4-cycle (or rather eight 4-cycles – the same C_4 counted in multiple ways), while $K_{1,4}$ has none. And in fact it can be shown that this extends to longer cycles too.

The reason the earlier proof for triangles does not extend is that it is not possible, only from the spectrum, to tell apart the true cycles from the other closed walks of the same length, when $k \geq 4$.

3 Degree sequence

Since $K_{1,4}$ has degree sequence $(4, 1, 1, 1, 1)$ and $C_4 \cup K_1$ has degree sequence $(2, 2, 2, 2, 0)$. Hence, the spectrum does not identify the degree sequence.

4 Connectivity

Since $K_{1,4}$ is connected and $C_4 \cup K_1$ has two connected components. Hence, the spectrum does not identify whether or not a graph is connected (or the number of connected components).

Next time: *Problems class – think about if you want topics going over again, more examples, or to work through the problem sheet.*

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