

# Topics in Discrete Mathematics

## Introduction to Graph Theory

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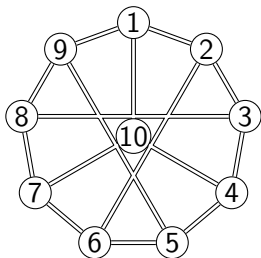
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## Last time...

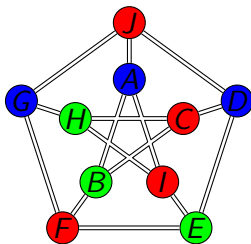
- We wrapped up Hamiltonian cycles by proving Dirac's Theorem;
- We learnt how to recognise trees;
- We played spot the difference, and formalised that idea as *isomorphism*;
- and we introduced adjacency matrices.

## Definition

Let  $G_1 = G(V_1, E_1)$  and  $G_2 = G(V_2, E_2)$  be two graphs. We say that  $G_1$  and  $G_2$  are **isomorphic** if there exists a bijection  $f : V_1 \rightarrow V_2$  such that  $\{v_1, v_2\} \in E_1 \Leftrightarrow \{f(v_1), f(v_2)\} \in E_2$ . Such an  $f$  is called a **graph isomorphism**.

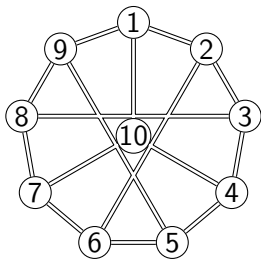


$$V_1 = \{1, \dots, 10\}$$

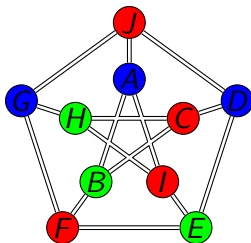


$$V_2 = \{A, \dots, J\}$$

The map  $f$  that sends  $1 \leftrightarrow A, \dots, 10 \leftrightarrow J$  is clearly a bijection, and satisfies  $\{i, j\} \in V_1 \Leftrightarrow \{f(i), f(j)\} \in V_2$ , so is a graph isomorphism.



$$V_1 = \{1, \dots, 10\}$$



$$V_2 = \{A, \dots, J\}$$

The map  $g$  that sends  $10 \leftrightarrow A, \dots, 1 \leftrightarrow J$  is also bijective, but fails to be a graph isomorphism since  $\{10, 4\} \in E_1$  but  $\{A, G\} \notin E_2$ .

## Definition

Let  $G = (V, E)$  be an  $n$ -vertex graph. The **adjacency matrix** of  $G$  is the  $n$ -by- $n$  matrix  $\mathbf{A}$  given by

$$A_{ij} = \begin{cases} 1 & \text{If } \{v_i, v_j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

Let  $\mathbf{A}_1, \mathbf{A}_2$  be adjacency matrices for graphs  $G_1, G_2$ . Then

$G_1, G_2$  are isomorphic  
if and only if

$$\mathbf{A}_1 = \mathbf{P}^{-1}\mathbf{A}_2\mathbf{P} \text{ for some permutation matrix } \mathbf{P}.$$

## Definition

We let  $N_{ij}^{(r)}$  denote the number of walks of length  $r$  from  $v_i$  to  $v_j$ .

## Proposition

If  $\mathbf{A}$  is the adjacency matrix, then

$$N_{ij}^{(r)} = [\mathbf{A}^r]_{ij}.$$

## Proof

- For  $r = 1$ , there is clearly only a walk of length 1 from  $v_i$  to  $v_j$  if  $A_{ij} = 1$ .
- For a path of length  $r + 1$  from  $v_i$  to  $v_j$ , we may follow the edge from  $v_i$  to any neighbour  $v_k$  - that is, for any  $k$  satisfying  $A_{ik} = 1$  - then any length  $r$  path from  $v_k$  to  $v_j$ , of which there are  $N_{kj}^{(r)}$ .
- So, inductively,

$$N_{ij}^{(r+1)} = \sum_{k=1}^n A_{ik} N_{kj}^{(r)} = \sum_{k=1}^n A_{ik} [\mathbf{A}^r]_{kj} = [\mathbf{A} \cdot \mathbf{A}^r]_{ij} = [\mathbf{A}^{(r+1)}]_{ij}$$



## Some Linear Algebra

- $\lambda$  is an **eigenvalue** of  $\mathbf{A}$  if there exists  $\mathbf{v} \neq \mathbf{0}$  such that  $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ ; such a  $\mathbf{v}$  is an **eigenvector**.
- The **characteristic polynomial** of  $\mathbf{A}$  is  $\Phi_A(x) = \det(x\mathbf{I} - \mathbf{A})$ ; its roots are precisely the eigenvalues of  $\mathbf{A}$ .
- The **spectrum** of  $\mathbf{A}$  is the list of eigenvalues of  $\mathbf{A}$ , with their multiplicities (as roots of  $\Phi_A$ ).

## Lemma

*If  $\mathbf{A}$  is a real symmetric matrix, and  $\mathbf{u}, \mathbf{v}$  are eigenvectors of  $\mathbf{A}$  with distinct eigenvalues, then  $\mathbf{u}$  and  $\mathbf{v}$  are orthogonal.*

Let  $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$ ,  $\mathbf{A}\mathbf{v} = \tau\mathbf{v}$ . Then

$$\mathbf{u}^T \mathbf{A}\mathbf{v} = \mathbf{u}^T \mathbf{A}^T \mathbf{v} = (\mathbf{v}^T \mathbf{A}\mathbf{u})^T = (\mathbf{v}^T \lambda\mathbf{u})^T = \lambda \mathbf{u}^T \mathbf{v}$$

But  $\mathbf{u}^T \mathbf{A}\mathbf{v}$  is also equal to  $\tau \mathbf{u}^T \mathbf{v}$  so  $(\tau - \lambda)\mathbf{u}^T \mathbf{v} = 0$ . As  $\tau \neq \lambda$ , we conclude

$$\mathbf{u}^T \mathbf{v} = 0.$$

## Lemma

*The eigenvalues of a real symmetric matrix  $\mathbf{A}$  are real numbers.*

Let  $\lambda$  be an eigenvalue of  $\mathbf{A}$  with eigenvector  $\mathbf{v} \neq 0$ , so  $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ .

Then

$$\overline{\lambda\mathbf{v}} = \overline{\lambda\mathbf{v}} = \overline{\mathbf{A}\mathbf{v}} = \overline{\mathbf{A}\mathbf{v}} = \mathbf{A}\overline{\mathbf{v}}$$

so  $\overline{\lambda}$  is an eigenvalue of  $\mathbf{A}$  with eigenvector  $\overline{\mathbf{v}}$ .

By the previous lemma, if  $\lambda \neq \overline{\lambda}$  then  $\mathbf{v}^T\overline{\mathbf{v}} = 0$ , but  $\mathbf{v}^T\overline{\mathbf{v}} = |\mathbf{v}| > 0$ .

Hence  $\lambda = \overline{\lambda}$ , so  $\lambda \in \mathbb{R}$ .

Let  $G$  be a graph with adjacency matrix  $\mathbf{A}$ . We may define the **spectrum of  $G$** ,  $\text{spec}(G)$ , to be that of  $\mathbf{A}$ .

### Lemma

*The spectrum of  $G$  is well-defined.*

We need to show that the spectrum is a **graph invariant**: that is, that isomorphic graphs have the same spectrum, so it doesn't matter which adjacency matrix we pick as representative.

Suppose  $\mathbf{A}$  is the adjacency matrix of  $G$ , and  $\mathbf{A}'$  the adjacency matrix of some  $G'$  such that  $G \cong G'$ . Then there exists  $\mathbf{P}$  such that  $\mathbf{A}' = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ .

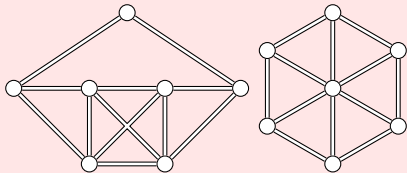
$$\begin{aligned}\Phi_{\mathbf{A}'}(x) &= \det(x\mathbf{I} - \mathbf{A}') = \det(x\mathbf{I} - \mathbf{P}^{-1}\mathbf{A}\mathbf{P}) \\ &= \det(\mathbf{P}^{-1}x\mathbf{I}\mathbf{P} - \mathbf{P}^{-1}\mathbf{A}\mathbf{P}) \\ &= \det(\mathbf{P}^{-1}(x\mathbf{I} - \mathbf{A})\mathbf{P}) \\ &= \det(\mathbf{P}^{-1})\det(x\mathbf{I} - \mathbf{A})\det(\mathbf{P}) \\ &= \frac{1}{\det(\mathbf{P})}\Phi_{\mathbf{A}}(x)\det(\mathbf{P}) \\ &= \Phi_{\mathbf{A}}(x)\end{aligned}$$

## Definition

We say that two graphs with the same spectrum are **cospectral**.

## Cospectral $\neq$ Isomorphic!

By the previous lemma, we have that isomorphic graphs are cospectral. But non-isomorphic graphs can also be cospectral!  
The graphs



both have  $\Phi(x) = (x + 2)(x + 1)^2(x - 1)^2(x^2 - 2x - 6)$  and spectrum

$$\{-2, -1^{(2)}, 1^{(2)}, 1 \pm \sqrt{7}\}$$

but are not isomorphic.

Now, let's denote by  $C_r$  the number of closed walks of length  $r$  (that is, containing  $r$  edges) in a graph.

Note: we count  $v_1 \rightarrow v_2 \rightarrow v_3 \rightarrow v_1$ ,  $v_2 \rightarrow v_3 \rightarrow v_1 \rightarrow v_2$  and  $v_1 \rightarrow v_3 \rightarrow v_2 \rightarrow v_1$  as distinct walks of length 3.

### Proposition

Let  $\mathbf{A}$  be the adjacency matrix of an  $n$ -vertex graph. Let the eigenvalues of  $\mathbf{A}$ , counted with multiplicity, be  $\lambda_1, \dots, \lambda_n$ . Then the number of closed walks of length  $r$  is

$$C_r = \sum_{i=1}^n \lambda_i^r.$$

## Some More Linear Algebra

If an  $n \times n$  matrix  $A$  has eigenvalues  $\lambda_1, \dots, \lambda_n$ , then it is **diagonalisable** if there exists non-singular  $\mathbf{Q}$  such that  $\mathbf{A} = \mathbf{Q}\mathbf{D}\mathbf{Q}^{-1}$  with

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{n-1} & 0 \\ 0 & \cdots & 0 & 0 & \lambda_n \end{pmatrix}$$



## Some More Linear Algebra

More generally, we have the **Jordan Normal Form Theorem**: there *always* exists a nonsingular  $\mathbf{Q}$  such that  $\mathbf{A} = \mathbf{Q}\mathbf{J}\mathbf{Q}^{-1}$ , where  $\mathbf{J}$  is upper triangular and block diagonal,

$$\mathbf{J} = \begin{pmatrix} \mathbf{J}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{J}_p \end{pmatrix}$$

and each “Jordan block”  $\mathbf{J}_i$  is an upper triangular square matrix of the form

$$\mathbf{J}_i = \begin{pmatrix} \lambda_i & 1 & 0 & \cdots & 0 \\ 0 & \lambda_i & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_i & 1 \\ 0 & \cdots & 0 & 0 & \lambda_i \end{pmatrix}$$

and each diagonal entry  $\lambda_i$  an eigenvalue of  $\mathbf{A}$ .

- The number of times an eigenvalue  $\lambda$  appears on the diagonal of  $\mathbf{J}$  is its **algebraic multiplicity**  $am(\lambda)$ , i.e., its multiplicity as a root of  $\Phi_A(x)$ .
- So the diagonal entries of  $\mathbf{J}$ , with multiplicity, are the eigenvalues of  $\mathbf{A}$ , with multiplicity (i.e., the spectrum).

- $$\sum_{i=1}^d am(\lambda_i) = n.$$

- The number of blocks containing  $\lambda$  on the diagonal is its **geometric multiplicity**.
- $gm(\lambda) \leq am(\lambda)$  and  $\mathbf{A}$  is diagonalisable if and only if

$$\sum_{i=1}^d gm(\lambda_i) = n.$$

- If  $\mathbf{A}$  is diagonalisable then every Jordan block is a  $1 \times 1$  block containing some eigenvalue of  $\mathbf{A}$ .

**Proof that**  $C_r = \sum_{i=1}^n \lambda_i^r$

We have

$$C_r = \sum_{i=1}^n N_{ii}^{(r)} = \sum_{i=1}^n A_{ii}^r = \text{Tr}(\mathbf{A}^r).$$

By JNF,

$$\begin{aligned} \text{Tr}(\mathbf{A}^r) &= \text{Tr}([\mathbf{Q}\mathbf{J}\mathbf{Q}^{-1}]^r) \\ &= \text{Tr}(\mathbf{Q}\mathbf{J}^r\mathbf{Q}^{-1}) \\ &= \text{Tr}(\mathbf{J}^r\mathbf{Q}^{-1}\mathbf{Q}) \\ &= \text{Tr}(\mathbf{J}^r) \\ &= \sum_{i=1}^n \lambda_i^r. \end{aligned}$$

## Corollary

Let  $\mathbf{A}$  be the adjacency matrix of an  $n$ -vertex graph  $G = (V, E)$   
Let the eigenvalues of  $\mathbf{A}$ , counted with multiplicity, be  $\lambda_1, \dots, \lambda_n$ .  
Then

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

For every  $e_{ij} \in E$  we have a closed walk of length 2 from  $i$  to  $i$ , and another from  $j$  to  $j$ ; and this is the only way to have a closed walk of length 2. So  $C_2 = 2|E|$ , but  $C_2 = \sum \lambda_i^2$  by the previous proposition.

## Corollary

Let  $\mathbf{A}$  be the adjacency matrix of an  $n$ -vertex graph  $G = (V, E)$   
Let the eigenvalues of  $\mathbf{A}$ , counted with multiplicity, be  $\lambda_1, \dots, \lambda_n$ .  
Then the number of triangles in  $G$  is

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

For every triangle of vertices  $i, j, k$ , there are six closed walks of length 3 ( $ijk, ikj, jki, jik, kij, kji$ ); and it is impossible to have a closed walk of length 3 that isn't on a triangle of vertices. So  $C_3 = 6|E|$ , but  $C_3 = \sum \lambda_i^3$  by the previous proposition.

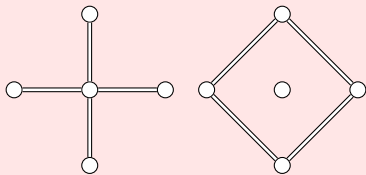
## Cycles $\neq$ Closed Walks

A closed walk of length 3 is necessarily a triangle, which is a cycle of length 3. But a closed walk of length 4 does not have to be a cycle of length 4. So we cannot count squares by counting closed walks of length 4.

A closed walk of length 3 is necessarily a triangle, which is a cycle of length 3. But a closed walk of length 4 does not have to be a cycle of length 4. So we cannot count squares by counting closed walks of length 4.

Worse, we can't count squares using only spectral information, as there are cospectral graphs with different numbers of squares:

## Cycles $\neq$ Closed Walks



These both have  $\Phi_A(x) = x^5 - 4x^3$  and hence

$$\text{spec}(\mathbf{A}) = \{2, -2, 0^{(3)}\},$$

but only one contains squares.

## Summary

The spectrum of a graph  $G = (V, E)$  is an invariant of its isomorphism class, and we've seen that it can tell us:

- $|V|$ ;
- $|E|$ ;
- The number of triangles in  $G$ ;
- The number of closed walks of length  $r$  in  $G$ ;
- and that  $G'$  is not isomorphic to  $G$  if they have different spectra.

There are many other (rather more sophisticated) properties that can be deduced from the spectrum.



## Summary

However, the existence of cospectral graphs means that, as we have seen, it cannot tell us:

- The number of squares in  $G$  (so in general, we cannot count cycles);
- The degrees of the vertices of  $G$ ;
- Whether  $G$  is connected;
- That  $G$  and  $G'$  are isomorphic, just because they have the same spectrum.