An Introduction to Algebraic Graph Theory

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Preface

Welcome to an Introduction to Algebraic Graph Theory!

If you find any typos or errors in these notes, no matter how small, please email me a short description (with a page number) of the typo/error. Suggestions and comments on how to improve the notes are also welcomed.

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Chapter 1

Graphs

1.1 What is a graph?

Before we give the definition of a graph, we introduce the following useful notation. For any set S we denote by $\binom{S}{2}$ the set of all two-element subsets of S, that is,

$$\binom{S}{2} = \big\{\{u, v\} \,|\, u, v \in S,\ u \neq v\big\}.$$

If S is finite and contains $n = |S| \geq 1$ elements then the number of elements of $\binom{S}{2}$ is

$$\binom{n}{2} = \frac{n!}{2!(n-2)!} = \frac{n(n-1)}{2}.$$

For instance, if $S = \{v_1, v_2, v_3, v_4\}$ then

$$\binom{S}{2} = \big\{ \{v_1, v_2\}, \{v_1, v_3\}, \{v_1, v_4\}, \{v_2, v_3\}, \{v_2, v_4\}, \{v_3, v_4\} \big\}.$$

and the number of elements of $\binom{S}{2}$ is $\binom{4}{2} = \frac{4 \cdot 3}{2} = 6$. We are now ready to define a graph.

Definition 1.1.1: Graph

A **graph** G consists of two sets V and E where E is some subset of $\binom{V}{2}$. The set V is called the **vertex set** of G and E is called the **edge set** of G. In this case we write $G = (V, E)$.

Let $G = (V, E)$ be a graph. The elements of V are called the **vertices** of G and the elements of E are called the **edges** of G. We will frequently use the notation $V(G)$ and $E(G)$ to denote the vertex set and edge set, respectively, of G. If V is a finite set, then G is called a **finite graph**. In this book, we consider only finite graphs.

A graph can be used to encode some relationship of interest between entities. The entities are represented by the vertices and two vertices u and v form an edge $\{u, v\}$ in the graph if u and v are "related". The condition for being "related" might be that u and v are friends in a social network, or u and v are subway stations that are directly linked by a train, or u and v are cells in a biological network that are biologically linked in some energy transfer, etc.

Sometimes, it is useful to think of a graph as a collection of points connected by lines (or curves) in the 2D-plane. One can visualize a graph $G = (V, E)$ by drawing a point on the 2D plane for each vertex and then connecting vertices u and v with a line if and only if $\{u, v\} \in E$. As an example, a visual representation of the graph G with vertex set $V = \{x, y, z, w\}$ and edge set $E = \{\{x, y\}, \{x, z\}, \{y, z\}, \{z, w\}\}$ is shown in Figure 1.1. Although a visual representation of a small graph might be useful, it is important to remember that a graph is **just a pair of sets V and E where $E \subset \binom{V}{2}$**.

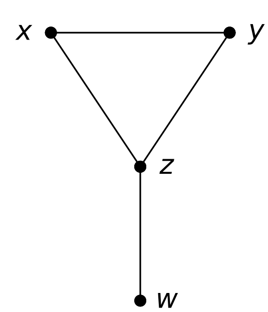


Figure 1.1: Visual representation of the graph $G = (V, E)$ with vertex set $V = \{x, y, z, w\}$ and edge set $E = \{\{x, y\}, \{x, z\}, \{y, z\}, \{z, w\}\}$

Example 1.1. Consider the graph G shown in Figure 1.2. Based on this graphical representation of G, what is $V(G)$ and $E(G)$?

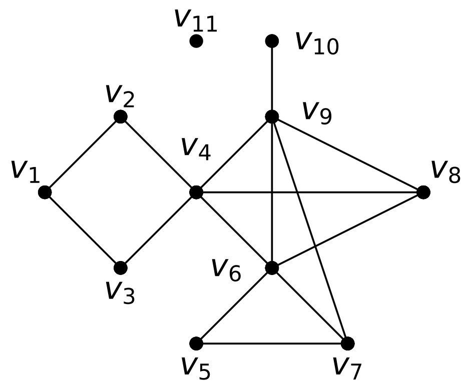


Figure 1.2: For this graph G, what is $V(G)$ and $E(G)$?

Example 1.2. Let $G = (V, E)$ be the graph with vertex set $V = \{2, 3, \dots, 10\}$ and edge set

$$E = \{\{u, v\} \mid \gcd(u, v) \geq 2\}.$$

What is the edge set E and how many edges does G have? Draw a visual representation of G.

Example 1.3. Check-out the Wiki page on Graph theory.

1.1.1 Exercises

Exercise 1.1. Let $G = (V, E)$ be the graph with vertex set $V = \{2, 3, \dots, 10\}$ and edge set

$$E = \{\{u, v\} \mid \gcd(u, v) = 1\}.$$

Write out the edge set E and draw the graph G. How many edges does G have? Aside from having the same vertex set, what is the relationship between the graph in this exercise and the graph in Example 1.2?

Exercise 1.2. Let V be the set of 3-dimensional binary vectors. In other words, an element of V is of the form $\mathbf{b} = (b_1, b_2, b_3)$ where b_i is either zero or one. Let $G = (V, E)$ be the graph with edge set E consisting of edges formed by two binary vectors that differ at only a single entry. For example, if $\mathbf{b}_1 = (1, 0, 1)$ and $\mathbf{b}_2 = (1, 0, 0)$ then $\{\mathbf{b}_1, \mathbf{b}_2\}$ is an edge of G since $\mathbf{b}_1$ and $\mathbf{b}_2$ differ only in the third entry, whereas if $\mathbf{b}_1 = (0, 1, 1)$ and $\mathbf{b}_2 = (1, 0, 0)$ then $\{\mathbf{b}_1, \mathbf{b}_2\}$ is note an edge of G. Do the following:

(a) Explicitly write out the vertex set V. How many vertices are there?

(b) Explicitly write out the edge set E. How many edges are there?

(c) Make a visual representation of G in the 2D plane. (Do not read part (d) yet!)

(d) Now make a visual representation of G in a 3D coordinate system by drawing each vertex $\mathbf{b} = (b_1, b_2, b_3)$ as a point in $\mathbb{R}^3$.

Exercise 1.3. Consider the following list $\sigma = (5, 2, 6, 1, 7, 3, 4)$ and let $V = \{1, 2, \ldots, 7\}$. Let $G = (V, E)$ be the graph such that $\{i, j\} \in E$ if and only if the numbers i and j appear in reverse order in σ. For example, $\{1, 3\} \notin E$ because 1 appears before 3 and so are in correct order, whereas $\{3, 6\} \in E$ because 6 appears before 3 in σ and so are in reverse order. Write out the edge set E and draw a visual representation of G.

Exercise 1.4. What are some real-world systems that can be modeled as graph? What are the vertices and when would two vertices form an edge?

1.2 The rudiments of graph theory

Let us now introduce same basic terminology associated with a graph. The **order** of a graph G is the cardinality of the vertex set V and the **size** of G is the cardinality of the edge set. Usually, we use the variables $n = |V|$ and $m = |E|$ to denote the order and size of G, respectively.

Given two vertices $u, v \in V$, we say that u and v are **adjacent** or **neighbors** if $\{u, v\} \in E$. In this case, we will write $u \sim v$ to denote adjacency and, whenever it is convenient to do so, we will denote the 2-element set $\{u, v\}$ by simply uv. Given an edge $e = uv \in E$, we will simply say that u and v are the vertices of the edge e. If $u \in e$ we say that u is **incident** with e and that

e is incident with u. The **neighborhood** of $v \in V$, denoted by $N(v)$, is the set of all vertices adjacent to v, in other words

$$N(v) = \{u \in V \mid u \sim v\} = \{u \in V \mid \{u, v\} \in E\}.$$

The **degree** of a vertex v, denoted by $\deg(v)$, is the cardinality of $N(v)$, that is, the number of neighbors of v. It is clear that $0 \leq \deg(v) \leq n - 1$ for all $v \in V(G)$. A vertex v with $\deg(v) = n-1$ is called a **dominating vertex** and if $\deg(v) = 0$ then v is called an **isolated** vertex. The **maximum/minimum degree** of a graph G is the maximum/minimum degree among all vertices of G. The maximum degree of G is denoted by $\Delta(G)$ and the minimum degree is denoted by $\delta(G)$, in other words

$$\Delta(G) = \max \{\deg(v) \mid v \in V\}$$

and

$$\delta(G) = \min \{\deg(v) \mid v \in V\}.$$

It is clear that $0 \leq \delta(G) \leq \Delta(G) \leq n - 1$. The **degree sequence** of a graph G, denoted by $d(G)$, is the sequence of the vertex degrees of G listed in decreasing order. Hence, if $n = |V(G)|$ then the degree sequence of G is of the form $d(G) = (d_1, d_2, \ldots, d_n)$ where $d_1 \geq d_2 \geq d_3 \geq \cdots \geq d_n$.

Example 1.4. Consider again the graph G in Figure 1.2.

(a) What is the order n and size m of G?

(b) Find $N(v_4)$, $N(v_6)$, $N(v_{10})$ and $\deg(v_4), \deg(v_6)$, and $\deg(v_{10})$.

(c) Find $\Delta(G)$ and $\delta(G)$.

(d) Find the degree sequence $d(G)$.

(e) Find $\sum_{i=1}^{n} \deg(v_i)$ and compare it with m.

The last part of the previous example is known as the Handshaking Lemma.

Lemma 1.2.1: Handshaking Lemma

For any graph $G = (V, E)$ it holds that

$$\sum_{v \in V} \deg(v) = 2|E|.$$

Consequently, in any graph the number of vertices with odd degree is even.

Proof. The degree of v counts the number of edges incident with v. Since each edge is incident with exactly two vertices, the sum $\sum_{v\in V} \deg(v)$ counts each edge twice, and therefore $\sum_{v\in V} \deg(v) = 2|E|$. It follows then that the number of vertices v with odd degree $\deg(v)$ is even. □

Another property of the degree sequence is the following.

Lemma 1.2.2

In any graph G there are at least two vertices with equal degree.

Proof. Let G be any graph of order n with degree sequence

$$d(G) = (d_1, d_2, \ldots, d_n).$$

We consider two mutually exclusive cases. In the first case, if $\delta(G) = 0$ then $\Delta(G) \leq n - 2$. Hence, $0 \leq d_i \leq n - 2$ for every $i = 1, 2, \ldots, n$, and then by the pigeon-hole principle there is at least two degrees that are equal. On the other hand, if $\delta(G) \geq 1$ then $1 \leq d_i \leq n-1$ for every $i = 1, 2, \ldots, n$, and then again by the pigeon-hole principle there are at least two equal degrees. □

Example 1.5. Explain why in every social gathering there are at least two persons who are friends with the same number of persons.

Let V be a finite set with cardinality $n = |V|$. How many distinct graphs are there with vertex set V? Let us first consider two extreme cases. The

empty graph on V, which we will denote by E_n, is the graph whose edge set is the empty set, that is, $E(E_n) = \emptyset$. A visual representation of the empty graph consists of n points in the plane with no edges among the vertices. At the other extreme, the **complete graph**, which we will denote by K_n, is the graph in which each vertex is adjacent to all other vertices. Hence, in the complete graph K_n, every possible edge is present. The total number of possible edges in a graph with n vertices is $M = \binom{n}{2}$. For example, if $V = \{v_1, v_2, v_3, v_4\}$ then the set of all 2-element subsets of V is

$$\binom{V}{2} = \{\, \{v_1, v_2\}, \{v_1, v_3\}, \{v_1, v_4\}, \{v_2, v_3\}, \{v_2, v_4\}, \{v_3, v_4\} \,\}$$

and in this case $\binom{4}{2} = 6$, which is the cardinality of $\binom{V}{2}$. Now, recall that by definition of a graph, the edge set is a **subset** of $\binom{V}{2}$. Hence, the total number of distinct graphs with vertex set V is equal to the number of subsets of $\binom{V}{2}$. The number of subsets of a set with M elements is 2^M. Applying this to the set $\binom{V}{2}$ we conclude that the number of graphs with vertex set V is therefore $2^M = 2^{\binom{n}{2}}$ where $n = |V|$.

Lemma 1.2.3

If V is a set with n elements then the number of distinct graphs with vertex set V is $2^{\binom{n}{2}}$.

Example 1.6. How many graphs are there with vertex set $V = \{1, 2, 3\}$? Draw all of them and group them by the number of edges in the graph.

Example 1.7. Let V be a finite set with cardinality $n = |V|$. How many graphs are there on V that have exactly m edges? Note that necessarily $0 \le m \le \binom{n}{2}$. Use your result to obtain a formula for $2^{\binom{n}{2}}$.

The **complement** of a graph $G = (V, E)$ is the graph $\overline{G}$ with the same vertex set as G and whose edge set consists of all edges not present in G. In other words, $E(\overline{G}) = \binom{V}{2} \backslash E(G)$. It follows then that $|E(G)| + |E(\overline{G})| = \binom{n}{2}$.

Example 1.8. Let $G = (V, E)$ be the graph with $V(G) = \{1, 2, 3, 4, 5, 6\}$ and

$$E(G) = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{2, 6\}, \{3, 4\}, \{4, 5\}, \{4, 6\}\}.$$

What is $E(\overline{G})$? Draw both G and $\overline{G}$.

Example 1.9. If G is a graph of order $n = 17$ and $\deg_G(v) = 9$ then what is $\deg_{\overline{G}}(v)$? Here we are using the notation $\deg_G(v)$ to denote the degree of v in the graph G and $\deg_{\overline{G}}(v)$ the degree of v in $\overline{G}$. In general, what is $\deg_{\overline{G}}(v)$ in terms of $n = |V|$ and $\deg_G(v)$?

A graph G is said to be k-**regular** if every vertex in G has degree k. If G is k-regular then clearly $k = \delta(G) = \Delta(G)$. Conversely, given any graph G if $\delta(G) = \Delta(G)$ then G is a regular graph.

Example 1.10. Prove that if G is k-regular then $\overline{G}$ is also regular. What is the degree of each vertex in $\overline{G}$?

Example 1.11. Draw a 3-regular graph on $n = 6$ vertices.

Example 1.12. Is there a k-regular graph on n vertices if $n = 11$ and $k = 3$? To answer this question, prove that if G is a k-regular graph on n vertices then nk must be even. Hint: Use the Handshaking lemma.

A graph $H = (V(H), E(H))$ is said to be a **subgraph** of $G = (V(G), E(G))$ if $V(H) \subset V(G)$ and $E(H) \subset E(G)$. For any subset of vertices $W \subset V(G)$, the **subgraph induced** by W, denoted by $G[W]$, is the subgraph of G with vertex set W and edge set

$$E(G[W]) = E(G) \cap \binom{W}{2}.$$

In other words, the subgraph $G[W]$ contains all edges of G whose end-vertices are in W. The following example will make clear the difference between a subgraph and an induced subgraph.

Example 1.13. Consider again the graph in Figure 1.2. You can verify that the graph H with $V(H) = \{v_2, v_3, v_4, v_6, v_8, v_9\}$ and edge set $E(H) = \{v_2v_4, v_3v_4, v_4v_9, v_4v_6, v_8v_9\}$ is a subgraph of G. However, it is not an *induced* subgraph. The subgraph of G induced by the vertices $W = \{v_2, v_3, v_4, v_6, v_8, v_9\}$ (that is, the graph $G[W]$) has edge set

$$E(G[W]) = \{v_2v_4, v_3v_4, v_4v_6, v_4v_8, v_4v_9, v_6v_8, v_6v_9, v_8v_9\}.$$

A subgraph $H = (V(H), E(H))$ of G is called a **path** in G if we can order the vertices of H, say $(w_0, w_1, \ldots, w_r)$, such that $w_{i-1} \sim w_i$ for $i = 1, 2, \ldots, r$. We also say that H is a path from the vertex w_0 to w_r and that the length of the path H is r. As an example, $(v_1, v_3, v_4, v_8, v_7, v_6, v_9)$ is a path of length six in the graph in Figure 1.2. A graph G is said to be **connected** if for any distinct vertices $u, v \in V(G)$ there exists a path from u to v, and is called **disconnected** otherwise. A **connected component** of a graph G is an induced subgraph $H = G[W]$ such that H is connected and H is not a proper subgraph of a connected subgraph of G. From these definitions, it is straightforward to show that a graph G is connected if and only if it contains only one connected component.

Example 1.14. Draw a graph on $n = 8$ vertices with $m = 5$ edges having 3 connected components.

Example 1.15. Prove that if G is disconnected then $\overline{G}$ is connected. Give an example of a connected graph G such that $\overline{G}$ is also connected. Hint: There is one for $n = 4$ and several for $n = 5$.

Having defined the length of a path, we define the distance between vertices.

Definition 1.2.4: Distance

The **distance** between vertices $u, v \in G$ is the length of a shortest path from u to v (or equivalently from v to u). We denote the distance between u and v as $d_G(u, v)$, and if the graph G is understood simply by $d(u, v)$.

If there is no path in G from u to v then $d(u,v)$ is not defined.

Example 1.16. Let H be a connected subgraph of the connected graph G and let u and v be vertices of H. Prove that $d_G(u,v) \leq d_H(u,v)$.

Lastly, the **diameter** of a connected graph G, denoted by $\operatorname{diam}(G)$, is the maximum distance among all the vertices in G, in other words

$$\operatorname{diam}(G) = \max\{d(u,v) \mid u,v \in V(G),\, u \neq v\}.$$

Example 1.17. If H is a connected subgraph of a connected graph G, what is the relationship between $\operatorname{diam}(H)$ and $\operatorname{diam}(G)$? To answer this question consider the following.

(a) Give an example of H and G such that $\operatorname{diam}(H) = \operatorname{diam}(G)$.
(b) Give an example of H and G such that $\operatorname{diam}(H) < \operatorname{diam}(G)$.
(c) Give an example of H and G such that $\operatorname{diam}(H) > \operatorname{diam}(G)$.
(d) Suppose that $d_H(u,v) = d_G(u,v)$ for all vertices $u,v \in V(H)$. Prove that $\operatorname{diam}(H) \leq \operatorname{diam}(G)$.

1.2.1 Exercises

Exercise 1.5. How many graphs are there with vertex set $V = \{1,2,\ldots,8\}$? How many of these have $m = 14$ edges?

Exercise 1.6. Let G be a graph with $n = |V(G)|$ and $m = |E(G)|$. Show that

$$\delta(G) \leq \tfrac{2m}{n} \leq \Delta(G).$$

What statistical measure of the vertex degrees is $\frac{2m}{n}$?

Exercise 1.7. Let V be the set of all Hollywood actors and let $G = (V,E)$ be the graph where $\{u,v\} \in E$ if and only if u and v have appeared in the same Hollywood film.

(a) For $v \in V$, what does $\deg(v)$ represent?

(b) If v is such that $\deg(v) = 0$, what can we say about the actor v and the film(s) v has appeared in?

(c) If v is such that $\deg(v) = 1$, what can we say about the actor v and the film(s) v has appeared in?

(d) What does $\Delta(G)$ represent?

Exercise 1.8. If G has degree sequence $d(G) = (d_1, d_2, \ldots, d_n)$, what is the degree sequence of $\overline{G}$?

Exercise 1.9. Draw a graph with degree sequence $d = (4, 4, 4, 4, 1, 1, 1, 1)$.

Exercise 1.10. For each case, decide whether or not a graph can have the given degree sequence. Justify your answers.

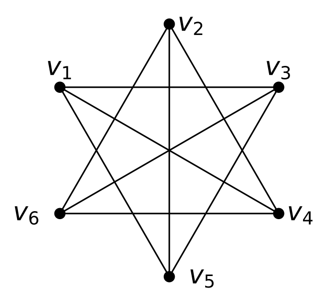
(a) $d = (3, 3, 2, 1)$

(b) $d = (3, 2, 1, 0)$

(c) $d = (4, 4, 2, 1)$

(d) $d = (2, 2, 2, 2)$

Exercise 1.11. Draw the complement of the graph G shown below:



Exercise 1.12. For the graph shown in Figure 1.3 with vertex set $V = \{v_1, v_2, \ldots, v_{11}\}$, decide if the given subgraph $H = (V(H), E(H))$ is induced. Explain your answer.

(a) $V(H) = \{v_1, v_2, v_3, v_5, v_6, v_7, v_{10}\}$, $E(H) = \{v_1v_3, v_2v_3, v_5v_6, v_6v_7, v_7v_{10}\}$

(b) $V(H) = \{v_5, v_6, v_7, v_8, v_9\}$, $E(H) = \{v_5v_6, v_5v_8, v_6v_7, v_7v_9\}$

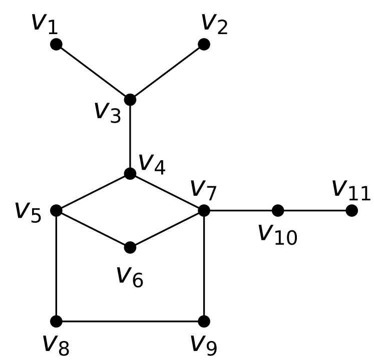


Figure 1.3: Graph for Exercises 1.12 and 1.13

Exercise 1.13. For the graph G in Figure 1.3, determine a path from v_2 to v_9. What is the length of the path? Do the same for vertices v_8 to v_{11}. What is $\text{diam}(G)$?

Exercise 1.14. How many edges in a graph guarantee that it is connected? To answer this question, show the following.

(a) Let G be a graph with $n \geq 2$ vertices and m edges. Show that if $m \geq \binom{n-1}{2} + 1$ then G is connected. HINT: Try this for small n.

(b) Show that for each $n \geq 1$, there exists a graph with $m = \binom{n-1}{2}$ edges that is disconnected.

(c) Conclude that $\binom{n-1}{2} + 1$ is the least number of edges that guarantee that G is connected.

(d) Give an example of a connected graph G with fewer than $\binom{n-1}{2}$ edges.

Exercise 1.15. Show by example that if G is connected then $\overline{G}$ can be disconnected.

Exercise 1.16. Prove that if $\delta(G) \geq \frac{n-1}{2}$ then G is a connected graph, where as usual $n = |V(G)|$. Prove also that $\text{diam}(G) \leq 2$.

1.3 Permutations

In this section, we pause our introduction to graph theory so that we can introduce some background material on permutations. We will need to be fluent with the rudiments of permutations in the next section when we consider the very important notion of graph isomorphisms and automorphisms.

The set of permutations on a set is an example of a **group**. Usually, groups are denoted with the letters G or H but since these are usually the letters used for graphs, we will use instead the symbol Γ to denote a generic group. Let us recall the definition of a group.

Definition 1.3.1: Group

A **group** is a set Γ and a binary operation defined on Γ, denoted by $\star : \Gamma \times \Gamma \to \Gamma$, that satisfies the following:

(i) For all $a, b, c \in \Gamma$ it holds that $(a \star b) \star c = a \star (b \star c)$ (associativity)

(ii) There is an element $e \in \Gamma$ such that $a \star e = a$ and $e \star a = a$ for every $a \in \Gamma$. The element e is called the **identity element**.

(iii) For each $a \in \Gamma$ there exists an element $b \in \Gamma$ such that $a \star b = e$ and $b \star a = e$. Usually, b is denoted instead by a^{-1} so that $a \star a^{-1} = a^{-1} \star a = e$, and a^{-1} is called an **inverse** of a.

In many cases, the group operation $a \star b$ is a sort of product operation in which case the product $a \star b$ is denoted simply as ab. Sometimes, however, the group operation is a sort of addition operation and so in that case $a \star b$ would be denoted by $a + b$. The essential feature, however, is that $a \star b$ is a binary operation that satisfies the listed properties (i)-(iii). Before we give examples of groups, we give the following definition.

Definition 1.3.2: Abelian group

A group Γ with group operation $\star : \Gamma \times \Gamma \to \Gamma$ is said to be an **abelian** group if the group operation is commutative, that is, if $a \star b = b \star a$ for every $a, b \in \Gamma$.

Example 1.18. The integers $\mathbb{Z}$ with the operation of addition forms a group. Indeed, addition is an associative operation; if $a, b, c \in \mathbb{Z}$ then $(a + b) + c = a + (b + c)$. The identity element of $\mathbb{Z}$ is zero because $a + 0 = 0 + a = a$ for every $a \in \mathbb{Z}$. Lastly, for each $a \in \mathbb{Z}$ its inverse under addition is $-a$, and since $-a \in \mathbb{Z}$ it follows that every $a \in \mathbb{Z}$ has an inverse in $\mathbb{Z}$. Hence, $\mathbb{Z}$ with operation $+$ is a group. Since addition of integers is commutative, the group $(\mathbb{Z}, +)$ is an abelian group.

Example 1.19. The integers $\mathbb{Z}$ with the operation of multiplication is not a group. What property of a group does $\mathbb{Z}$ not satisfy when the operation is multiplication?

Example 1.20. Consider the finite set $\Gamma = \{1, -1, i, -i\}$ where i satisfies $i^2 = -1$. Then Γ is a group under multiplication. Multiplication of real or complex numbers is an associative operation. You can verify that multiplication is a binary operation on Γ, that is, whenever we take two elements in Γ and multiply them we obtain an element back in Γ. The identity element is the number 1. Lastly, every element in Γ has an inverse that is in Γ. For example, the inverse of $i \in \Gamma$ is $-i \in \Gamma$ because $i \cdot (-i) = -i^2 = -(-1) = 1$. As another example, the inverse of $-1 \in \Gamma$ is itself because $-1 \cdot -1 = 1$. Is Γ an abelian group? Draw the multiplication table for Γ.

Example 1.21. Denote by $GL(n)$ the set of $n \times n$ invertible matrices. Then $GL(n)$ is a group with matrix multiplication being the group operation. Recall that matrix multiplication is associative, that is, if $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are matrices then $\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}$, and thus property (i) is satisfied. The identity element of $GL(n)$ is the $n \times n$ identity matrix $\mathbf{I}$ (the matrix with ones along the diagonal and all other entries are zero). By definition, each $\mathbf{A} \in GL(n)$ has an inverse $\mathbf{A}^{-1}$ and $\mathbf{A}^{-1} \in GL(n)$ because $\mathbf{A}^{-1}$ is itself invertible (its inverse is $\mathbf{A}$). Hence, $GL(n)$ satisfies all the properties of a group. Note that matrix multiplication is not commutative and thus $GL(n)$ is not an abelian group for $n \geq 2$.

For our purposes, the most important group is the group of bijections on a finite set. Recall that bijections are one-to-one and onto mappings, and are therefore invertible. To be concrete, we will consider the finite set $V = \{1, 2, \ldots, n\}$ where $n \in \mathbb{N}$ is fixed. A **permutation** on V is a bijection $\sigma : V \to V$. The set of all permutations on the set V is called the **symmetric group on** V, and it is usually denoted by S_n. We now show that S_n is indeed a group. First of all, the candidate binary operation on S_n will be function composition. Recall that if σ_1 and σ_2 are functions from V to V then the composite function $\sigma_1 \circ \sigma_2$ is the new function defined by $(\sigma_1 \circ \sigma_2)(k) = \sigma_1(\sigma_2(k))$ for each $k \in V$. Given $\sigma_1, \sigma_2 \in S_n$ the composite function $\sigma_1 \circ \sigma_2$ is also a bijection on V and thus $\sigma_1 \circ \sigma_2 \in S_n$. Hence, function composition is a binary operation on S_n. Now we verify that each property of a group is satisfied for S_n with group operation being function composition:

(i) Function composition is associative; if $\sigma_1, \sigma_2, \sigma_3 \in S_n$ then $(\sigma_1 \circ \sigma_2) \circ \sigma_3 = \sigma_1 \circ (\sigma_2 \circ \sigma_3)$. Associativity of function composition is not only true for bijections but for any functions.

(ii) The identity element of S_n is the **identity permutation** $\mathrm{id} : V \to V$ defined as $\mathrm{id}(k) = k$ for every $k \in V$. In other words, the function id fixes each element of V. For any $\sigma \in S_n$ we have that $(\sigma \circ \mathrm{id})(k) = \sigma(\mathrm{id}(k)) = \sigma(k)$ and so $\sigma \circ \mathrm{id} = \sigma$. Similarly, $(\mathrm{id} \circ \sigma)(k) = \mathrm{id}(\sigma(k)) = \sigma(k)$, and therefore $\mathrm{id} \circ \sigma = \sigma$. Hence, the identity permutation is the identity element of S_n.

(iii) Lastly, by definition of S_n each $\sigma \in S_n$ has an inverse σ^{-1} and because σ^{-1} is itself invertible (its inverse is σ) then $\sigma^{-1} \in S_n$. By definition of an inverse function, we have that $\sigma \circ \sigma^{-1} = \mathrm{id}$ and $\sigma^{-1} \circ \sigma = \mathrm{id}$.

If $V = \{1, 2, \ldots, n\}$ then the number of permutations on V is $n!$, and therefore $|S_n| = n!$. As n increases, S_n becomes a very big set. The group S_n is perhaps one of the most important groups in all of mathematics (Permutation group).

A permutation $\sigma : V \to V$ can be represented as array in the following way:

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma(1) & \sigma(2) & \sigma(3) & \cdots & \sigma(n) \end{pmatrix}.$$

The array representation indicates that the number $i \in V$ is mapped to $\sigma(i) \in V$. For example, if $V = \{1, 2, 3, 4\}$ and σ is the permutation $\sigma(1) = 3, \sigma(2) = 4, \sigma(3) = 1$, and $\sigma(4) = 2$ then the array representation of σ is

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \end{pmatrix}.$$

The array representation indicates that a permutation σ is a rearrangement of the ordered list $(1, 2, 3, \ldots, n)$ into the list $(\sigma(1), \sigma(2), \ldots, \sigma(n))$. Since σ is one-to-one and onto, every integer in $\{1, 2, \ldots, n\}$ will appear once and only once in the list $(\sigma(1), \sigma(2), \ldots, \sigma(n))$.

Example 1.22. Let $V = \{1, 2, 3\}$ so that $|S_n| = 3! = 6$. Using array representations, write out all 6 permutations on V.

Another more common way to represent a permutation is via its **cycle decomposition**. As an example, consider the permutation on $n = 8$ defined as

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 4 & 8 & 5 & 3 & 1 & 6 & 7 & 2 \end{pmatrix}.$$

Then $\sigma(1) = 4$, and $\sigma(4) = 3$, and $\sigma(3) = 5$, and $\sigma(5) = 1$ which is where we started. We then say that the sequence of integers $(1\ 4\ 3\ 5)$ is a **cycle** of σ because σ cycles through the list $(1, 4, 3, 5)$ mapping one integer to the next until reaching the end of the list which is mapped to the first integer. Now take the lowest integer not in the cycle $(1\ 4\ 3\ 5)$, in this case it is 2. Then $\sigma(2) = 8$ and $\sigma(8) = 2$ which is where we started. Hence $(2\ 8)$ is another cycle of σ. Now select the next integer that does not appear in any of the previous cycles, in this case it is 6. Now $\sigma(6) = 6$ and so (6) is another cycle of σ. Lastly, $\sigma(7) = 7$. Hence, σ **fixes** the integers 6 and 7 and thus the cycles for these are both singleton cycles. The permutation σ can therefore be represented as the product of the cycles

$$\sigma = (1\ 4\ 3\ 5)(2\ 8)(6)(7).$$

This is called the **cycle decomposition** of σ. From the cycle decomposition we can read directly what σ does to each integer. For example, to find $\sigma(4)$ we simply find 4 in the cycle decomposition and pick out the integer to the right of 4, in this case $\sigma(4) = 3$. As another example, $\sigma(5) = 1$ because 5 is at the end of a cycle and so this means 5 is mapped to the beginning of the cycle, which is 1. The **length** of a cycle is the number of integers appearing in the cycle. Therefore, $(1\ 4\ 3\ 5)$ is a cycle of length 4, $(2\ 8)$ is a cycle of length 2, and (6) and (7) are cycles of length 1. By convention, cycles of length one are not displayed in the cycle decomposition of σ. In this case, the cycle decomposition of σ would be written as $\sigma = (1\ 4\ 3\ 5)(2\ 8)$ and it is understood that the remaining integers not displayed are fixed by σ (in this case 6 and 7).

Example 1.23. Let $n = 10$ and let $\sigma \in S_n$ be defined by

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 3 & 6 & 1 & 8 & 5 & 9 & 2 & 10 & 7 & 4 \end{pmatrix}.$$

Find the cycle decomposition of σ and determine the lengths of the cycles.

Example 1.24. Suppose that σ is a permutation on $n = 9$ and it has the cycle decomposition

$$\sigma = (1\ 7\ 9\ 4)(2\ 6\ 5)$$

Write the array representation of σ.

Example 1.25. Let $\sigma_1, \sigma_2 \in S_6$ have cycle decomposition $\sigma_1 = (1\ 3)(2\ 5\ 6)$ and $\sigma_2 = (2\ 3)(4\ 5\ 1)$. Find the array representation of the composition $\sigma_1 \circ \sigma_2$ and then write out the cycle decomposition of $\sigma_1 \circ \sigma_2$. Do the same for $\sigma_2 \circ \sigma_1$. Try writing the cycle decomposition of $\sigma_1 \circ \sigma_2$ and $\sigma_2 \circ \sigma_1$ directly using the cycle decompositions of σ_1 and σ_2 without first writing their array representations.

Example 1.26. Let $n = 10$ and let $\sigma \in S_n$ be defined by

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 5 & 7 & 6 & 10 & 9 & 3 & 4 & 8 & 1 & 2 \end{pmatrix}.$$

Write out the cycle decomposition of σ and then find the cycle decomposition of σ^{-1}. Compare the cycle decompositions of σ and σ^{-1}. Do you see how to quickly find the cycle decomposition of σ^{-1} once you know the cycle decomposition of σ?

By the **order** of a permutation σ we mean the least integer $k \geq 1$ such that

$$\sigma^k = \underbrace{\sigma \circ \sigma \circ \cdots \circ \sigma}_{k\text{-times}} = \text{id}.$$

If the cycle decompsotion of σ has r cycles each having length $k_1, k_2, \ldots, k_r \geq 2$ then the order of σ is the least common multiple (lcm) of $k_1, k_2, \ldots, k_r$.

Example 1.27. Let $\sigma = (1\ 5)(2\ 3\ 6\ 4)$ be a permutation in S_6. The length of the cycles of σ are $k_1 = 2$ and $k_2 = 4$. Hence, the order of σ is $\text{lcm}(2, 4) = 4$. Find $\sigma^2, \sigma^3, \sigma^4$ and verify that σ^4 is the identity permutation.

Example 1.28. Let Γ be a group such that every element $\sigma \in \Gamma$ has order $k = 2$. Prove that Γ is an abelian group, that is, that $\sigma_1\sigma_2 = \sigma_2\sigma_1$ for all $\sigma_1, \sigma_2 \in \Gamma$.

Finally, a **transposition** is a permutation that fixes all but two elements. Hence, if τ is a transposition then its cycle decomposition is of the form $\tau = (a\ b)$ and thus $\tau(a) = b$ and $\tau(b) = a$ and τ fixes all other integers. Clearly, the order of τ is two. In particular, if $\sigma = \tau_1 \circ \tau_2 \circ \cdots \circ \tau_r$ is a product of **disjoint** transpositions (by disjoint we mean that the cycles in all the τ_i's are mutually disjoint and by product we mean function composition because composition is the product operation in S_n) then σ is also of order two. For example, the permutation $\sigma = (1\ 7)(2\ 5)(3\ 8)$ in S_9 has order 2. The converse also holds; if $\sigma \in S_n$ has order two then σ can be written as a product of disjoint transpositions.

1.3.1 Exercises

Exercise 1.17. Write a Python function that takes as input a permutation represented as a list and returns the cycle decomposition of the permutation as a list of lists. Call your function `cycleDecomposition`. For example, consider the permutation

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 2 & 4 & 1 & 3 & 7 & 6 & 5 \end{pmatrix}.$$

We can represent σ as a list as $\sigma = [2, 4, 1, 3, 7, 6, 5]$. However, recall that Python uses **zero-based** indexing and thus as a Python list we have $\sigma = [1, 3, 0, 2, 6, 5, 4]$. The cycle decomposition of σ as a list of lists is therefore $\sigma = [[0, 1, 3, 2], [4, 6], [5]]$. Hence, your function would produce:

```
cycleDecomposition([1,3,0,2,6,5,4])
        [[0,1,3,2], [4,6], [5]]
```

Apply your function to the following permutations (using zero-based indexing):

$$\sigma = [2, 0, 1, 5, 7, 10, 11, 4, 8, 9, 3, 6]$$

$$\sigma = [2, 6, 7, 8, 1, 3, 11, 4, 9, 10, 0, 5]$$

$$\sigma = [13, 7, 0, 8, 18, 2, 17, 9, 1, 3, 14, 15, 12, 5, 16, 11, 6, 10, 4]$$

To test your function further, the Python module `itertools` has a function called `permutations` that returns a generator that produces permutations of a given iterable such as a list or a string. WARNING: Generating all permutations for even small values of n can take a long time; for this reason use $n \leq 10$.

1.4 Graph isomorphisms

In this section, we study in detail what it means for two graphs to be "equivalent" but not necessarily equal. The basic idea is that since the essential structure of a graph is contained entirely in the make-up of the edge set, or how the vertices are connected, the vertex set can be seen as an arbitrary choice of labels for the vertices. If two graphs have the same edge structure then we will declare them to be equivalent even though the vertices might be distinct or differ by a rearrangement. For example, consider the two graphs G_1 and G_2 given by

$$\begin{aligned} V(G_1) &= \{v_1, v_2, v_3, v_4\} & V(G_2) &= \{x, y, z, w\} \\ E(G_1) &= \{v_1v_2, v_1v_3, v_2v_3, v_3v_4\} & E(G_2) &= \{zy, zw, yw, xw\}. \end{aligned}$$

It is clear that G_1 and G_2 are distinct graphs because $V(G_1) \neq V(G_2)$. In each graph, there is one dominating vertex; in G_1 it is v_3 and in G_2 it is w. Each graph has one vertex with degree one; in G_1 it is v_4 and in G_2 it is x. In both graphs, the remaining two vertices are adjacent and each have the same degree. Hence, in both graphs the manner in which the vertices are connected is the same and the only feature that distinguishes the graphs are the actual names or labels of the vertices. Specifically, our analysis has shown that there exists a bijection between the vertices of G_1 and G_2 that shows that these graphs are structurally equivalent (but not equal). To be more precise, the bijection $\sigma : V(G_1) \to V(G_2)$ defined by $\sigma(v_3) = w$, $\sigma(v_4) = x$, $\sigma(v_2) = y$, and $\sigma(v_1) = z$ leaves the adjacency property of vertices invariant. Let us now be more rigorous with the definition of equivalent graphs.

Definition 1.4.1: Graph Isomorphisms

The graph $G_1 = (V_1, E_1)$ is **isomorphic** to the graph $G_2 = (V_2, E_2)$ if there exists a bijection $\sigma : V_1 \to V_2$ such that if $\{u, v\}$ is an edge in G_1 then $\{\sigma(u), \sigma(v)\}$ is an edge in G_2 and if $\{u, v\}$ is not an edge in G_1 then $\{\sigma(u), \sigma(v)\}$ is not an edge in G_2. In this case, we say that σ is an

isomorphism from G_1 to G_2 and we write $G_1 \cong G_2$.

In other words, σ is an isomorphism from G_1 to G_2 if σ maps an edge in G_1 to an edge in G_2 and maps a non-edge in G_1 to a non-edge in G_2, in other words

$$E_2 = \sigma(E_1) := \{\{\sigma(u), \sigma(v)\} \mid \{u, v\} \in E_1\}.$$

Before we proceed, we note that if G_1 is isomorphic to G_2 then G_2 is isomorphic to G_1 (why?). Hence, we can without ambiguity say that G_1 and G_2 are isomorphic. Clearly, if $G_1 \cong G_2$ then necessarily $|V_1| = |V_2|$ since there is no bijection between sets of distinct cardinality. Moreover, if σ is a bijection, the condition that $\sigma(E_1) = E_2$ implies that also $|E_1| = |E_2|$. A mathematical way to say this is that the order and size of a graph are **invariants**, that is, quantities (or objects, sub-structures, etc.) that are preserved by an isomorphism. Later on we will identify further invariants of graphs.

Example 1.29. Verify that the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ shown in Figure 1.4 are distinct. Then prove that G_1 and G_2 are isomorphic. To do this, you need to explicitly find a bijection $\sigma : V \to V$ that satisfies the definition of a graph isomorphism. Here $V = V_1 = V_2 = \{v_1, v_2, v_3, v_4, v_5\}$. Once you have an isomorphism σ, pick any non-edge in G_1 and show that it is mapped under σ to a non-edge in G_2.

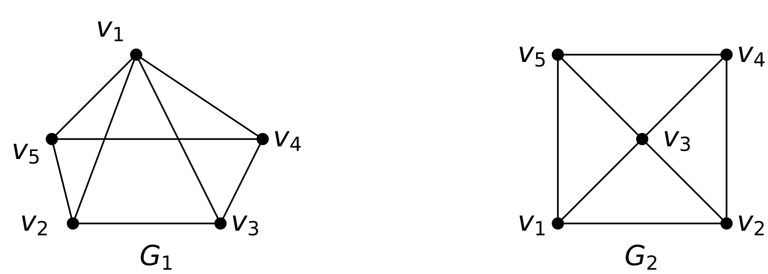


Figure 1.4: Are these graphs isomorphic?

Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, if $|V_1| \neq |V_2|$ then as discussed above G_1 and G_2 cannot be isomorphic. Hence, if G_1 and G_2 are graphs with $n = |V_1| = |V_2|$, then when investigating whether G_1 and G_2 are isomorphic we can without loss of generality rename the vertex sets of G_1 and G_2 so that the new relabelled graphs both have the same vertex set. It is convenient to let the common vertex set be $V = \{v_1, v_2, \ldots, v_n\}$ or even $V = \{1, 2, , \ldots, n\}$.

Example 1.30. Consider the graphs $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ where $V = \{1, 2, 3, 4\}$ and

$$E_1 = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}\}$$
$$E_2 = \{\{3, 4\}, \{2, 4\}, \{2, 3\}, \{1, 2\}\}.$$

Consider the permutation $\sigma = (1\ 4)(2\ 3)$ (this is the cycle decomposition). Verify that σ is an isomorphism from G_1 to G_2 and thus $G_1 \cong G_2$. Draw both graphs to see what is happening.

Example 1.31. Suppose that $\sigma : V(G_1) \to V(G_2)$ is an isomorphism from G_1 to G_2. Prove that for every vertex $v \in V(G_1)$ it holds that $\deg(v) = \deg(\sigma(v))$. In other words, an isomorphism must preserve the degree of each vertex. Conclude that the degree sequence of isomorphic graphs are equal. In other words, the degree sequence of a graph is an invariant.

Example 1.32. Consider the graphs $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ with vertex set $V = \{1, 2, \ldots, 6\}$ and edge sets

$$E_1 = \{\{3, 5\}, \{4, 6\}, \{2, 6\}, \{1, 5\}, \{3, 6\}, \{1, 4\}, \{3, 4\}\}$$
$$E_2 = \{\{1, 2\}, \{1, 5\}, \{2, 4\}, \{5, 6\}, \{6, 4\}, \{1, 3\}, \{5, 2\}\}.$$

The degree sequences of G_1 and G_2 are $d(G_1) = d(G_2) = (3, 3, 3, 2, 2, 1)$. Thus, there is a possibility that G_1 and G_2 are isomorphic. With the help of a drawing of G_1 and G_2, conclude that $G_1 \cong G_2$ and determine an isomorphism from G_1 to G_2.

Lemma 1.4.2

Suppose that $\sigma : V(G_1) \to V(G_2)$ is an isomorphism of the graphs G_1 and G_2. If $(w_0, w_1, \ldots, w_r)$ is a path in G_1 then $(\sigma(w_0), \sigma(w_1), \ldots, \sigma(w_r))$ is a path in G_2.

Proof. First of all, since σ is a bijection, all vertices in the list

$$(\sigma(w_0), \sigma(w_1), \ldots, \sigma(w_r))$$

are distinct. Since $\{w_{i-1}, w_i\} \in E(G_1)$ and σ is an isomorphism then

$$\{\sigma(w_{i-1}), \sigma(w_i)\} \in E(G_2),$$

for $i = 1, \ldots, r$. Thus, $(\sigma(w_0), \sigma(w_1), \ldots, \sigma(w_r))$ is a path in G_2. $\square$

Example 1.33. Recall that the **distance** between vertices u and v in a graph G, denoted by $d_G(u, v)$, is the length of a shortest path in G from u to v, and if there is no path from u to v then $d(u, v)$ does not exist. Prove that if $\sigma : V(G_1) \to V(G_2)$ is an isomorphism from G_1 to G_2 then $d_{G_1}(u, v) = d_{G_2}(\sigma(u), \sigma(v))$ for all vertices $u, v \in V(G_1)$.

Example 1.34. Prove that if G_1 and G_2 are isomorphic then their complements $\overline{G}_1$ and $\overline{G}_2$ are isomorphic.

Example 1.35. Suppose that $G_1 \cong G_2$. Prove that G_1 is connected if and only if G_2 is connected.

Given two graphs $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$, how do we decide if they are isomorphic? Well, first of all it must hold that $|E_1| = |E_2|$ otherwise the graphs are not isomorphic. If we select a specific permutation $\sigma : V \to V$ and if it is true that $\{u, v\} \in E_1$ if and only if $\{\sigma(u), \sigma(v)\} \in E_2$, for all $u, v \in V$, then G_1 and G_2 are isomorphic. Hence, it is computationally easy to verify whether or not a specific permutation is an isomorphism from one graph to the other. If a specific permutation σ is not an isomorphism from G_1 to G_2, then we proceed by choosing another permutation $\tilde{\sigma}$ and perform the same test and if $\tilde{\sigma}$ is not an isomorphism then we proceed to another permutation, etc. In principle, we would have to perform an exhaustive test through all $n!$ permutations on V to decide if G_1 and G_2 are isomorphic. This brute-force search is computationally intractable when n is large; in fact it is already computationally non-trivial even when say $n \approx 20$. In general, the existence of an efficient algorithm that decides whether two given graphs G_1 and G_2 are isomorphic is still unknown and is a long-standing unsolved problem in mathematics and computer science (Graph isomorphism problem).

You may have already noticed that being isomorphic defines an **equivalence relation** on the set of all graphs with n vertices. To be concrete, let $V = \{1, 2, \ldots, n\}$ and let $\mathcal{G}_n$ be the set of all graphs with vertex set V, that is,

$$\mathcal{G}_n = \left\{ (V, E) \mid E \subset \binom{V}{2} \right\}.$$

Recall that the cardinality of $\mathcal{G}_n$ is $|\mathcal{G}_n| = 2^{\binom{n}{2}}$. We say that two graphs G_1 and G_2 are **equivalent** if G_1 and G_2 are isomorphic. To see that this is indeed an equivalence relation, we first note that $G \cong G$ by taking the identity permutation since $\mathrm{id}(E) = E$ (this shows reflexivity); next if $G_1 \cong G_2$ and σ is the isomorphism such that $\sigma(E_1) = E_2$ then $G_2 \cong G_1$ with isomorphism σ^{-1} since $\sigma^{-1}(E_2) = E_1$ (this shows symmetry); and finally to show transitivity if $G_1 \cong G_2$ with isomorphism σ and $G_2 \cong G_3$ with isomorphism ρ then $\rho \circ \sigma$ is an isomorphism from G_1 to G_3 since $(\rho \circ \sigma)(E_1) = \rho(\sigma(E_1)) = \rho(E_2) = E_3$. Hence, for fixed $V = \{1, 2, \ldots, n\}$, we can partition the set of all graphs $\mathcal{G}_n$ into equivalences classes.

Definition 1.4.3: Graph Isomorphism Classes

Let $G = (V, E)$ be a graph on the vertex set $V = \{1, 2, \ldots, n\}$. The **isomorphism class** of G is the set of all graphs with vertex set V that are isomorphic to G. We will denote the isomorphism class of G by $[G]$. Explicitly,

$$[G] = \big\{(V, \sigma(E)) \mid \sigma \in S_n\big\}.$$

The number of distinct isomorphism classes on V will be denoted by $\zeta(n)$.

An isomorphism class can be thought of as a graph with unlabelled vertices. The following exercise illustrates this point.

Example 1.36. Let $n = 4$. If we draw all $2^{\binom{n}{2}} = 64$ graphs on the vertex set $V = \{v_1, v_2, v_3, v_4\}$, and remove the labels of the vertices, then each graph will look like one of those shown in Figure 1.5. Therefore, there are $\zeta(4) = 11$ isomorphism classes for $n = 4$. Alternatively, we say that there are $\zeta(4) = 11$ non-isomorphic graphs on $n = 4$ vertices.

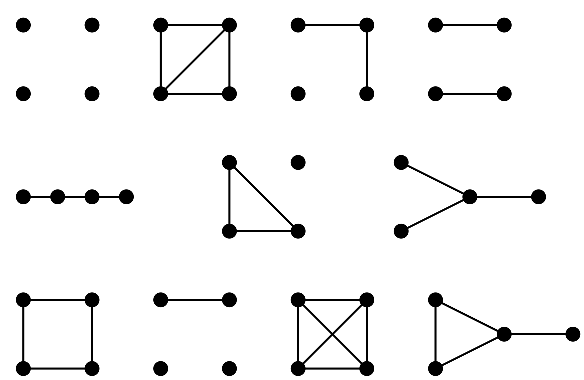


Figure 1.5: The graph isomorphism classes for $n = 4$

Given a graph $G = (V, E)$, one can generate by brute-force the individual members of the isomorphism class $[G]$ by computing $\sigma(E)$ for every permutation $\sigma \in S_n$. One expects $[G]$ to contain $n!$ graphs (one for each element of S_n) and in many (most) cases this is indeed true. In general, however, the isomorphism class $[G]$ will contain less than $n!$ graphs as the next example shows.

Example 1.37. Consider the graph $G = (V, E)$ where $V = \{1, 2, 3, 4\}$ and

$$E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}\}.$$

There are a total of $4! = 24$ permutations in S_4. Any graph $\tilde{G}$ isomorphic to G is of the form $\tilde{G} = (V, \sigma(E))$ for some permutation $\sigma \in S_n$. Consider the permutations $\sigma_1 = (1\ 4)(2\ 3)$ and $\sigma_2 = (1\ 3\ 2\ 4)$, both in their cycle decomposition. Clearly, these permutations are distinct. Verify however that $\sigma_1(E) = \sigma_2(E)$ and thus σ_1 and σ_2 generate the same graph isomorphic to G. This shows that the set $[G]$ contains less than $4!$ graphs. In fact, one can show that in this case $[G]$ contains only 12 graphs.

Example 1.38. Let $G_1 = (V, E_1)$ be the graph shown in Figure 1.6. Let $\sigma_1 = (1\ 3)(2\ 4)(5\ 6)$ and let $\sigma_2 = (1\ 2)(3\ 4)$. Verify that $\sigma_1(E_1) = E_1$ and $\sigma_2(E_1) = E_1$. Hence, the equivalence class of G_1 contains fewer than $6!$ graphs. On the other hand, for the graph $G_2 = (V, E_2)$, one can verify that for all non-identity permutations $\sigma \in S_6$, it holds that $\sigma(E_2) \neq E_2$.

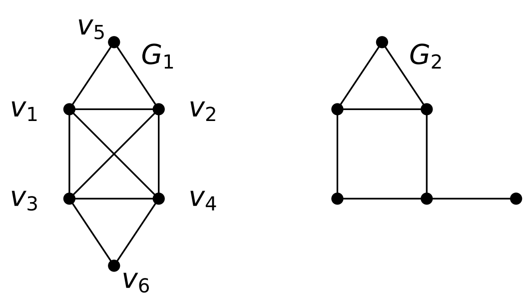


Figure 1.6: Two graphs on $n = 6$ vertices

The previous examples illustrate that for some graphs there are permutations that preserve the adjacency property of vertices. This leads us to the following definition.

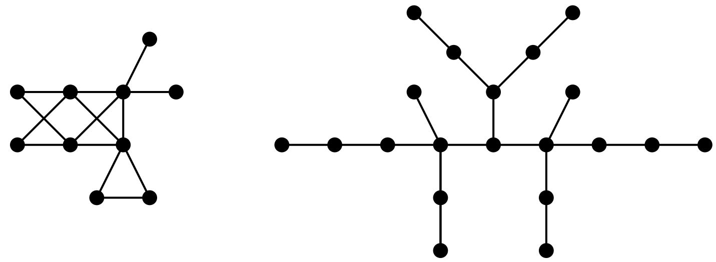


Figure 1.7: Finding automorphisms using a visual representation for small graphs

Definition 1.4.4: Automorphisms

An **automorphism** of a graph $G = (V, E)$ is an isomorphism of G onto itself, that is, a bijection $\sigma : V \to V$ such that $\{u, v\}$ is an edge in G if and only if $\{\sigma(u), \sigma(v)\}$ is an edge in G. In other words, if $\sigma(E) = E$. The set of all automorphisms of a graph G is called the **automorphism group** of G, and will be denoted by $\mathrm{Aut}(G)$.

As the name suggests, the automorphism group is a group, and more specifically, it is a subgroup of the symmetric group. For any graph G, the identity permutation is an automorphism of G. If, however, G has only the identity permutation as an automorphism then we say that G is **asymmetric** otherwise we say that G is **symmetric**. We verified that the graph G_1 in Figure 1.6 is a symmetric graph while graph G_2 in the same figure is asymmetric. For small graphs, automorphisms may be found by identifying the "geometric symmetries" from a visual representation of the graph. In general, however, this approach is futile for finding automorphisms for large graphs and serves only to illustrate the idea of an automorphism.

Example 1.39. Find at least two automorphisms for each graph in Figure 1.7. You will first need to label the vertices of the graph.

Example 1.40. The complete graph K_n on the vertex set $V = \{1, 2, \ldots, n\}$

has every permutation on V as an automorphism. Thus, $\mathrm{Aut}(K_n) = S_n$. Verify this for K_3.

When n is very small, a typical graph will have an automorphism other than the identity permutation, that is, when n is small a typical graph will have at least one symmetry. In fact, an exhaustive search reveals that it is not until $n = 6$ that asymmetric graphs appear. It is natural to ask what the trend is as $n \to \infty$. As before, let $\zeta(n)$ denote the number of graph isomorphism classes on n vertices. We have seen that some graphs have a non-trivial automorphism group and therefore there are isomorphism classes that contain fewer than $n!$ graphs. Therefore,

$$2^{\binom{n}{2}} < n!\zeta(n)$$

from which it follows that

$$\frac{2^{\binom{n}{2}}}{n!} < \zeta(n).$$

It can be shown [2] that in fact $\zeta(n)$ asymptotically converges to $\frac{2^{\binom{n}{2}}}{n!}$ (see Figure 1.8), that is,

$$\lim_{n\to\infty} \frac{\zeta(n)}{\frac{2^{\binom{n}{2}}}{n!}} = 1.$$

From this fact one can deduce that as $n \to \infty$, the proportion of graphs that are asymmetric tends to one. These facts were proved by P. Erdös and A. Réyni [1] and summarized below.

Theorem 1.4.5: Symmetric Graphs Are Rare

For each $n \in \mathbb{N}$, let $a(n)$ be the number of asymmetric non-isomorphic graphs on n vertices. Then

$$\lim_{n\to\infty} \frac{a(n)}{\zeta(n)} = 1,$$

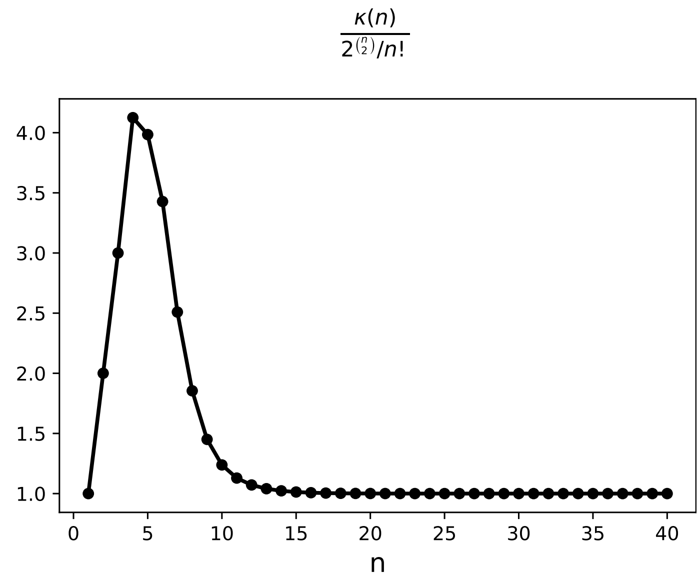


Figure 1.8: The ratio $\frac{\zeta(n)n!}{2^{\binom{n}{2}}}$ for $n \in \{1, 2, \ldots, 40\}$. The values of $\zeta(n)$ were obtained from the On-Line Encyclopedia of Integer Sequences https://oeis.org/A000088.

that is, the proportion of graphs that are asymmetric for each n tends to 1 as $n \to \infty$.

Another way of saying this is that **almost all graphs are asymmetric** (Asymmetric graphs). Although symmetry in graphs is mathematically rare, many real-world graph models have many symmetries.

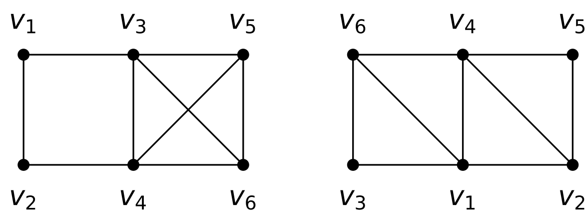
1.4.1 Exercises

Exercise 1.18. A subset of vertices $W \subset V(G)$ of a graph G is called a **clique** if all vertices in W are mutually adjacent. In other words, W is a clique if the induced subgraph $G[W]$ is a complete graph. Prove that if σ is an isomorphism from G to H then if W is a clique in G then $\sigma(W)$ is a clique in H.

Exercise 1.19. Prove that if $G_1 \cong G_2$ then $\text{diam}(G_1) = \text{diam}(G_2)$.

Exercise 1.20. Two vertices $u, v \in V(G)$ are said to be **twin vertices** if $N(u)\backslash\{v\} = N(v)\backslash\{u\}$. In other words, u and v are twins if they have the same neighbors (other than possibly themselves). Prove that u and v are twin vertices if and only if the transposition that permutes u and v, and fixes all other vertices, is an automorphism of G.

Exercise 1.21. Are these graphs isomorphic? If not explain why, and if yes then provide an isomorphism.



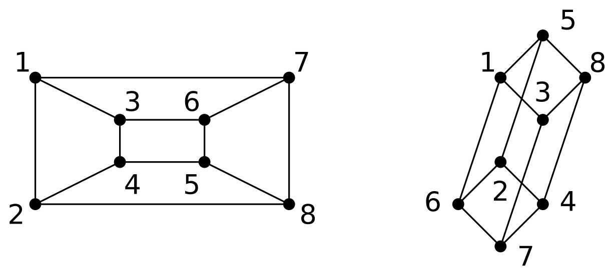
Exercise 1.22. We know that the degree sequence of a graph is an isomorphism invariant.

(a) Show by example that two graphs with the same degree sequence need not be isomorphic. Your graphs should be non-regular graphs.

(b) Do the same as in part (a) but now the two graphs must be regular.

For each case, explain why they are non-isomorphic. Your explanation should not be "because the pictures of the graph look different".

Exercise 1.23. Are these graphs isomorphic? If not explain why, and if yes then provide an isomorphism.



Exercise 1.24. The **eccentricity** of a vertex $v \in V(G)$, denoted by $\mathrm{ecc}_G(v)$, is the maximum distance from v to any other vertex in G. In other words,

$$\mathrm{ecc}_G(v) = \max_{u \in V} d(v, u).$$

The **radius** of a graph G, denoted by $\mathrm{rad}(G)$, is the minimum eccentricity among all vertices of G. The **center** of G is the subset of vertices v such that $\mathrm{ecc}_G(v) = \mathrm{rad}(G)$. Suppose that σ is an isomorphism from G_1 to G_2. Prove that

(a) $\mathrm{ecc}_{G_2}(\sigma(v)) = \mathrm{ecc}_{G_1}(v)$ for every $v \in V(G_1)$,

(b) $\mathrm{rad}(G_1) = \mathrm{rad}(G_2)$, and

(c) the center of G_1 is mapped onto the center of G_2 under σ.

Exercise 1.25. Prove that the number of connected components in a graph is an invariant. In other words, if G has connected components $G_1, G_2, \ldots, G_k$, and H has connected components $H_1, H_2, \ldots, H_\ell$ then if $G \cong H$ then $k = \ell$. To get you started, prove the following: Suppose that $\sigma : V(G) \to V(H)$ is an isomorphism from G to H. If G_i is a connected component of G then the graph in H induced by the vertices $\sigma(V(G_i))$ is a connected component in H.

1.5 Special graphs and graph operations

In this section, we present a small catalog of graphs that appear frequently in graph theory and also present some standard operations on graphs.

We have already discussed the **complete** graph on n vertices, denoted by K_n, which is the graph where all vertices are mutually adjacent. The complement of the complete graph is the **empty** graph, denoted by $E_n = \overline{K_n}$.

Fix a vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The **path** graph on V, denoted by P_n, is the graph with edge set

$$E(P_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\}.$$

Hence, P_n is a path of length $n-1$ from v_1 to v_n. The **cycle** graph on V, denoted by C_n, is the graph with edge set

$$E(C_n) = \{v_1v_2, v_2v_3, v_3v_4, \ldots, v_{n-1}v_n, v_nv_1\} = E(P_n) \cup \{v_1, v_n\}.$$

Hence, C_n can be obtained by connecting the end-vertices of P_n. In Figure 1.9, we illustrate P_2, P_3, P_4, and C_3, C_4, C_5.

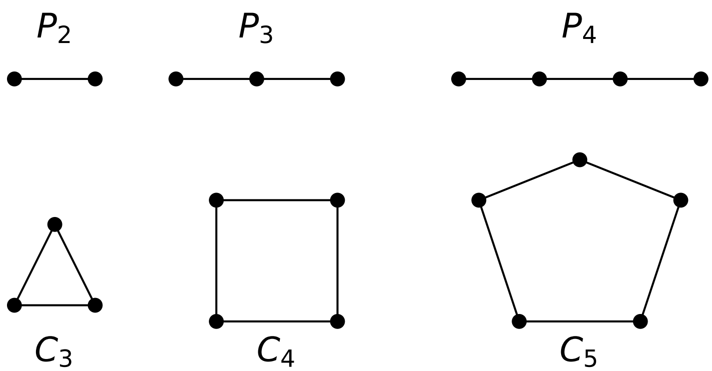


Figure 1.9: Some path and cycle graphs

Example 1.41. A graph G is called **self-complementary** if G is isomorphic to its complement.

(a) Verify that P_4 is self-complementary.

(b) Prove that if G is self-complementary then $|E(G)| = \frac{\binom{n}{2}}{2}$, and thus G has half the number of edges of the complete graph.

(c) Deduce that $n \equiv 0$ or $n \equiv 1 \pmod 4$.

A graph G is called **bipartite** if there exists two non-empty disjoint subsets X and Y of $V(G)$ such that $X \cup Y = V(G)$ and every edge in G has one end-vertex in X and the other in Y. The sets X and Y are called the **parts** of the **bipartition** $\{X, Y\}$. Bipartite graphs are usually drawn with the vertices from X on one side and the vertices from Y on the other side. An example of a bipartite graph, drawn in two different ways, is shown in Figure 1.10.

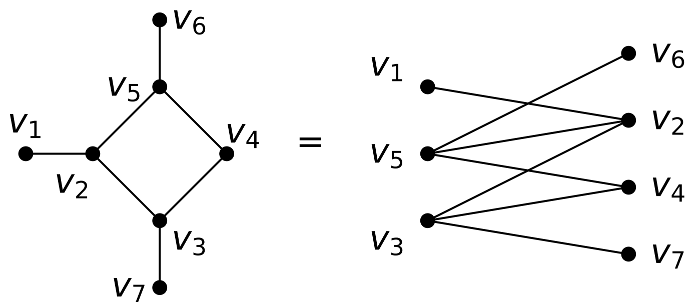


Figure 1.10: A bipartite graph

Example 1.42. Suppose that G is a connected bipartite graph. Prove that G has a unique bipartition. In other words, prove that if $\{X, Y\}$ and $\{A, B\}$ are bipartitions of G then $\{A, B\} = \{X, Y\}$. Give an example of a disconnected bipartite graph that does not have a unique bipartition.

The **complete bipartite** graph of regularity (n_1, n_2), denoted by K_{n_1,n_2}, is a bipartite graph with parts X and Y such that $n_1 = |X|$ and $n_2 = |Y|$ and every vertex in X is adjacent to all vertices in Y (and hence all vertices in Y are adjacent to X). Figure 1.11 illustrates $K_{2,3}$ and $K_{1,4}$.

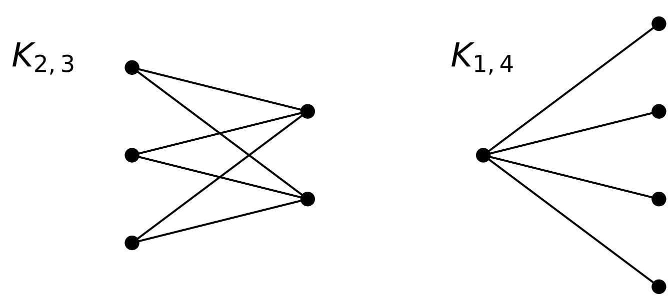


Figure 1.11: The complete bipartite graphs $K_{2,3}$ and $K_{1,4}$.

We now give a characterization of bipartite graphs.

Theorem 1.5.1: Bipartite Graphs

A graph G is bipartite if and only if it does not contain cycles of odd length.

Proof. Suppose first that G is bipartite with parts X and Y, and let $\gamma = (w_0, w_1, \ldots, w_k)$ be a cycle in G of length k, and thus $w_0 = w_k$. Assume without loss of generality that $w_0 \in X$. Since G is bipartite, $w_i \in X$ for all even i and $w_j \in Y$ for all odd j. Since $w_k = w_0 \in X$, it follows that k is even and thus the cycle γ has even length.

Now we prove the converse statement. The statement is trivial if $|V(G)| \leq 2$ so suppose that $n \geq 3$. We can assume that G is connected, otherwise we apply the forthcoming arguments to each connected component of G. Let $v \in V(G)$ be an arbitrary but fixed vertex and define

$$X = \{x \in V(G) \mid d(v, x) \text{ is even}\}$$

and let $Y = V(G) \backslash X$. Hence, Y contains vertices whose distance to v is odd. It is clear that X and Y are disjoint. Since G is connected, $X \cup Y = V(G)$. Assume that G is not bipartite. Then at least one of X or Y contains two adjacent vertices. Suppose without loss of generality that X contains two vertices a and b that are adjacent. Then neither a nor b equals v by definition of X. Let $\gamma_1 = (a_0, a_1, a_2, \ldots, a_{2k})$ be a path of minimum length from v to a and let $\gamma_2 = (b_0, b_1, b_2, \ldots, b_{2j})$ be a path of minimum length from v to b. Both paths γ_1 and γ_2 contain $v = a_0 = b_0$ as a common vertex. In general, if γ_1 and γ_2 contain a common vertex v' then $v' = a_i = b_i$ for some i. Indeed, if $v' = a_i$ and $v' = b_\ell$ for say $i < \ell$ then there exists a path from v to b that has length less than γ_2 which is a contradiction. Let i be the largest integer such that $a_i = b_i$. Then $(a_i, a_{i+1}, \ldots, a_{2k}, b_{2j}, b_{2j-1}, \ldots, b_i)$ is a cycle of length $(2k - i) + (2j - i) + 1$, which is odd. Hence, we have proved that if G is not bipartite then G has a cycle of odd length. Thus, if G has no cycles of odd length then G is bipartite. □

Example 1.43. Label the cycle graph C_6 and find a bipartition for it.

Given two graphs G and H with disjoint vertex sets, we define the **union** of G and H, denoted by $G \oplus H$, as the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. The **join** of G and H, denoted by $G \vee H$, is the graph obtained from $G \oplus H$ by connecting every vertex in G to every vertex in H. Explicitly,

$$E(G \vee H) = E(G) \cup E(H) \cup \{\{v, w\} \mid v \in V(G),\ w \in V(H)\}.$$

It is not hard to show that $\oplus$ and $\vee$ are commutative and associative operations, in other words,

$$\begin{aligned} G_1 \oplus G_2 &= G_2 \oplus G_1 & (G_1 \oplus G_2) \oplus G_3 &= G_1 \oplus (G_2 \oplus G_3) \\ G_1 \vee G_2 &= G_2 \vee G_1 & (G_1 \vee G_2) \vee G_3 &= G_1 \vee (G_2 \vee G_3). \end{aligned}$$

for all graphs G_1, G_2, G_3. It is clear that $G_1 \oplus G_2$ is a disconnected graph while $G_1 \vee G_2$ is connected.

Example 1.44. Draw the graphs $(P_2 \vee (P_2 \oplus P_2) \vee P_2) \vee K_1$ and $((P_2 \vee P_2) \oplus (P_2 \vee P_2)) \vee K_1$.

Example 1.45. Suppose that G is disconnected and has components $G_1, G_2, \ldots, G_k$. Then $G = G_1 \oplus G_2 \oplus \cdots \oplus G_k$.

Example 1.46. Suppose that $G = G_1 \vee G_2$. Prove that $\operatorname{diam}(G) \leq 2$. What if $\operatorname{diam}(G) = 1$?

Example 1.47. Recall that $K_{|X|,|Y|}$ is the bipartite graph with parts X and Y such that every vertex in X is adjacent to every vertex in Y. Prove that $K_{|X|,|Y|} = E_{|X|} \vee E_{|Y|}$, where recall that E_n is the empty graph on n vertices.

Given a graph G and $v \in V(G)$, we denote by $G - v$ the graph obtained from G by removing the vertex v and all edges incident with v. More generally, for $S \subset V(G)$, the graph $G - S$ is the graph obtained from G by removing all vertices S and all edges incident with a vertex in S. Formally,

$$G - S = G[S^c]$$

where $S^c = V(G)\backslash S$. Similarly, if $e \in E(G)$ then $G - e$ is the graph obtained from G by removing the edge e, and more generally, for $\Omega \subset E(G)$, the graph $G - \Omega$ is obtained from G by removing all edges in Ω, in other words, $E(G - \Omega) = E(G)\backslash\Omega$.

Let G be a connected graph. A vertex $v \in V(G)$ is called a **cut vertex** if $G - v$ is disconnected. More generally, a subset S of vertices is called a **vertex cut set** if $G - S$ is disconnected. The minimum cardinality over all vertex cut sets is called the **connectivity** of G and denoted by $\kappa(G)$. If G is disconnected we define $\kappa(G) = 0$ and $\kappa(K_n) = n - 1$ for $n \geq 1$. Similarly, an edge e is called a **bridge** if $G - e$ is disconnected. A subset $\Omega \subset E(G)$ of edges is called an **edge cut set** if $G - \Omega$ is disconnected. The minimum cardinality over all edge cut sets is called the **edge connectivity** of G and denoted by $e(G)$.

Lemma 1.5.2

For any connected graph G we have $\kappa(G) \leq e(G) \leq \delta(G)$.

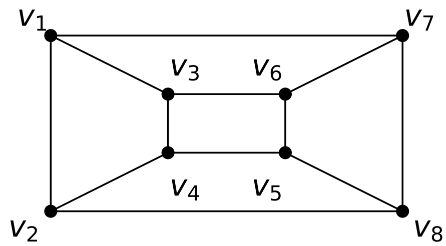
Proof. If v is a vertex with $\deg(v) = \delta(G)$ then removing all edges incident with v leaves v isolated and therefore G is disconnected. Hence, $e(G) \leq \delta(G)$. The other inequality is left as an exercise. □

Example 1.48. The **girth** of a graph G, denoted by $g(G)$, is the length of the shortest cycle in G. Prove that $g(G) \leq 2\,\mathrm{diam}(G) + 1$ for any graph G with at least one cycle. Assume G is connected.

1.5.1 Exercises

Exercise 1.26. Is the graph given below bipartite? If yes, find a bipartition for it.

Exercise 1.27. Consider the complete bipartite graph K_{n_1,n_2}.



(a) Find the number of edges of K_{n_1,n_2} in terms of n_1 and n_2.

(b) Is there a complete bipartite graph with $n = 11$ vertices and 25 edges? Explain.

(c) Is there a complete bipartite graph with $n = 11$ vertices and 24 edges? Explain.

Exercise 1.28. Draw the graph $K_{1,n-1}$ for $n = 5$, $n = 7$, and $n = 9$. What celestial objects do these graphs resemble?

Exercise 1.29. For each $n \geq 4$, let $W_n = C_{n-1} \vee K_1$. Draw W_n for $n \in \{4, 5, 9, 12\}$. What name would you give these graphs?

Exercise 1.30. Draw the graph $K_1 \vee (E_2 \oplus C_3)$.

Exercise 1.31. Let G_1 and G_2 be graph.

(a) Prove that if $G_1 \vee G_2$ is a regular graph then both G_1 and G_2 are regular.

(b) Suppose that G_1 is k_1-regular, with n_1 vertices, and G_2 is k_2-regular, with n_2 vertices. Under what conditions on k_1, k_2, n_1, and n_2 is $G_1 \vee G_2$ a regular graph? Give a proof of your condition.

(c) Give an example of regular graphs G_1 and G_2 such that $G_1 \vee G_2$ is not regular.

Exercise 1.32. Consider the following recursively defined sequence of graphs:

$$
\begin{aligned}
G_1 &= K_1 \\
G_2 &= G_1 \vee K_1 \\
G_3 &= G_2 \oplus K_1 \\
G_4 &= G_3 \vee K_1 \\
G_5 &= G_4 \oplus K_1
\end{aligned}
$$

and in general $G_k = G_{k-1} \oplus K_1$ if $k \geq 3$ is odd and $G_k = G_{k-1} \vee K_1$ if $k \geq 2$ is even.

(a) Draw G_8 and label the vertices so that the vertex added at step j is labelled v_j.

(b) Prove by induction that if k is even then

$$d(G_k) = \left(k-1, k-2, \ldots, \tfrac{k}{2}, \tfrac{k}{2}, \tfrac{k}{2} - 1, \ldots, 2, 1\right).$$

In other words, the degree sequence has only one repeated value, namely $\frac{k}{2}$.

Exercise 1.33. Let G be a graph with $\delta(G) \geq k$.

(a) Prove that G has a path of length at least k.

(b) Prove that if $k \geq 2$ then G has a cycle of length at least $k+1$.

Exercise 1.34. Prove that if $\delta(G) \geq \frac{n}{2} + 1$ then adjacent vertices have a common neighbor, that is, for every $\{u, v\} \in E(G)$ there exists $w \in V(G)$ such that $\{u, w\} \in E(G)$ and $\{v, w\} \in E(G)$.

Exercise 1.35. The **complete multipartite graph** of regularity $(n_1, n_2, \ldots, n_k)$, denoted by $K_{n_1,n_2,\ldots,n_k}$, is the graph

$$K_{n_1,n_2,\ldots,n_k} = E_{n_1} \vee E_{n_2} \vee \cdots \vee E_{n_k}.$$

In other words, there is a partition $X_1, X_2, \ldots, X_k$ of the vertex set V such that for each distinct X_i and X_j, each vertex of X_i is adjacent to every vertex of X_j. Find the order and size of $K_{n_1,n_2,\ldots,n_k}$ in terms of $n_1, n_2, \ldots, n_k$.

Exercise 1.36. Prove that the center of a complete bipartite graph K_{n_1,n_2}, with $n_1, n_2 \geq 2$, is the entire vertex set. (See Exercise 1.24 for the definition of the center of a graph.)

1.6 Trees

We begin at the beginning.

Definition 1.6.1: Trees

A graph G is called a **tree** if it is connected and does not contain any cycles. A **forest** is the union of trees.

It follows by definition and Theorem 1.5.1 that a tree is a bipartite graph. By definition, K_1 is a tree, and the only trees on $n = 2$ and $n = 3$ vertices are P_2 and P_3, respectively. Some trees are shown in Figure 1.12.

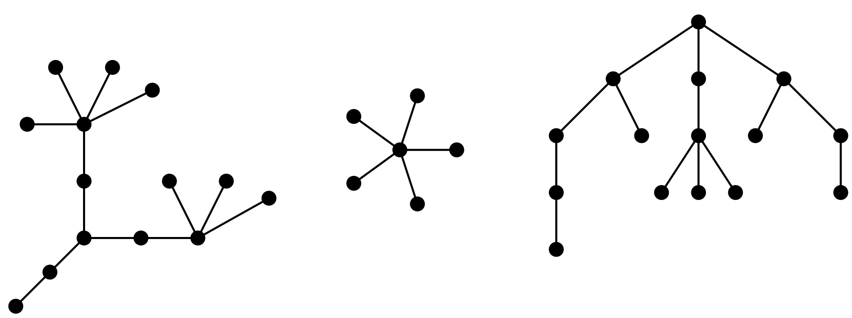


Figure 1.12: Some tree graphs

Example 1.49. There are 2 trees on $n = 4$ vertices and 3 trees on $n = 5$ vertices. Draw them.

Proposition 1.6.2: Paths in Trees

Let G be a connected graph. Then G is a tree if and only if there is a unique path between any two given vertices.

Proof. We first prove that if G is a tree then for any distinct vertices u and v there is only one path from u to v. We prove the contrapositive. Suppose that there are two distinct paths $\gamma_1 = (x_0, x_1, \ldots, x_k)$ and $\gamma_2 = (y_0, y_1, \ldots, y_\ell)$

from u to v, and thus $u = x_0 = y_0$ and $x_k = y_\ell = v$. Since the paths are distinct, there is a minimal $i \geq 1$ such that $x_i \neq y_i$ and $x_{i-1} = y_{i-1}$. Since the paths have at least one vertex in common after u (namely v), there is a minimal $j > i$ such that $x_j = y_m$ for some $m \leq \ell$. Hence, $\tilde{\gamma} = (x_{i-1}, x_i, \ldots, x_j, y_{m-1}, y_{m-2}, \ldots, y_i, y_{i-1})$ is a cycle in G, and thus G is not a tree.

Now suppose that G is not a tree and let $\gamma = (u, w_1, w_2, \ldots, w_k, u)$ be a cycle in G. Then for $1 \leq i < k$, $\gamma_1 = (u, w_1, \ldots, w_i)$ and $\gamma_2 = (u, w_k, w_{k-1}, \ldots, w_i)$ are two paths in G from u to w_i. Hence, if in G there is only one path between any two given vertices then G has no cycles, that is, G is a tree. □

A vertex v of a tree G is called a **leaf** or a **pendant vertex** if $\deg(v) = 1$. If G is a tree and $\deg(v) = 1$ then $G - v$ is connected and contains no cycles. Therefore, $G - v$ is a tree whenever $\deg(v) = 1$. Before we continue, we need the following more-or-less obvious fact.

Lemma 1.6.3

If G is a connected graph of order $n \geq 3$ then there exists $v \in V(G)$ such that $\deg(v) \geq 2$.

Proof. If $\deg(v) = 1$ for all $v \in V(G)$ then G is the disjoint union of copies of P_2 and thus G is not connected. □

We now describe what happens to a tree when we remove a non-leaf.

Theorem 1.6.4: Removing a Non-Leaf from a Tree

If G is a tree with $n \geq 3$ vertices then $G - v$ is a forest for any $v \in V(G)$ having $\deg(v) \geq 2$. In fact, the number of components of $G - v$ is $\deg(v)$.

Proof. Let $v \in V(G)$ be such that $\deg(v) \geq 2$ and consider $G - v$. Let x, y be neighbors of v in G. If $G - v$ is connected, then there exists a path in $G - v$ from

x to y, say $\gamma = (x, w_1, w_2, \ldots, w_{k-1}, y)$. Then $\tilde{\gamma} = (x, w_1, w_2, \ldots, w_{k-1}, y, v, x)$ is a cycle in G which is a contradiction since G is a tree. Hence, $G - v$ is disconnected. Our proof also shows that each neighbor of v is contained in a distinct component of $G - v$, and hence $G - v$ contains at least $\deg(v)$ components. It is clear, however, that $G - v$ can have no more than $\deg(v)$ components for if H is a component of $G - v$ that does not contain any of the neighbors of v in G then G contains H as a connected component which contradicts the connectivity of G. Finally, if any component of $G - v$ contains a cycle then clearly so does G which is a contradiction. Hence, $G - v$ is a forest containing $\deg(v)$ trees. □

Proposition 1.6.5: Minimum Number of Leaves in a Tree

Every tree with $n \geq 2$ vertices contains at least two leaves.

Proof. The proof is by strong induction on n. For $n = 2$ and $n = 3$, the only trees are P_2 and P_3, respectively, and both contain two leaves. Now assume that the claim is true for all trees having no more than $n \geq 2$ vertices and let G be a tree of order $n + 1$. Since $n + 1 \geq 3$, Lemma 1.6.3 applies and thus G has a vertex v with $\deg(v) \geq 2$. If v is adjacent to two or more leaves then we are done. If v is adjacent to one leaf, say x, then $G - x$ is a tree of order n and therefore it has at least two leaves, say y and z. This implies that G has at least two of x, y, z as leaves. If v is not adjacent to any leaves, then $G - v$ contains at least two components G_1 and G_2 each containing at least 2 vertices. By the induction hypothesis, G_1 contains at least two leaves, say x_1 and y_1, and G_2 contains at least two leaves x_2 and y_2. Hence, G contains at least two of x_1, y_1, x_2, y_2 as leaves. □

The following gives a characterization of trees in terms of the number of edges.

Theorem 1.6.6: Number of Edges in a Tree

Suppose that G is a connected graph with n vertices. Then G is a tree if and only if G has $n-1$ edges.

Proof. We first prove that if G is a tree with n vertices then it has $n-1$ edges. The case $n=1$ is trivial. Assume by induction that every tree with n vertices contains $n-1$ edges. Let G be a tree with $n+1$ vertices. Let v be a leaf of G. Then $G-v$ is a tree with n vertices and therefore by the induction hypothesis has $n-1$ edges. Since G and $G-v$ differ only by one edge, G has $(n-1)+1=n$ edges.

Now we prove that every connected graph with n vertices and $n-1$ edges is a tree. The case $n=1$ is trivial. Assume by induction that every connected graph with n vertices and $n-1$ edges is a tree. Let G be a connected graph with $n+1$ vertices and n edges. We claim that there is at least one vertex v with $\deg(v)=1$. If not, then $\sum_{i=1}^{n+1}\deg(v_i)\geq 2(n+1)$, while by the Handshaking lemma we have $\sum_{i=1}^{n+1}\deg(v_i)=2n$, which is a contradiction. Let then $v\in V(G)$ be such that $\deg(v)=1$. Then $G-v$ is a connected graph with n vertices and $n-1$ edges. By induction, $G-v$ is a tree. Since $\deg(v)=1$, it is clear that G is also a tree.

$\square$

We obtain the following corollary.

Corollary 1.6.7: Number of Edges in a Forest

If G is a forest of order n containing k components then G has $n-k$ edges.

We now describes what happens in a tree when an edge is removed.

Proposition 1.6.8: Removing Edges in a Tree

Let G be a tree. Then every edge in G is a bridge. Moreover, $G - e$ is a forest with two components for any edge $e \in E(G)$.

Proof. Let G be a connected graph. Assume that no edge of G is a bridge. Hence, if $e = \{u, v\}$ is an edge in G then $G - e$ is connected. Thus, there exists a path in $G - e$ from u to v. Adding the edge e at the end of this path creates a cycle in G, and hence G is not a tree. Hence, if G is a tree then every edge is a bridge.

To prove the second claim, let $G_1, G_2, \ldots, G_k$ be the components of $G - e$. Since G is a tree, each component G_i contains no cycles and therefore G_i is a tree. Hence, the total number of edges in $G - e$ is $n - k$. On the other hand, G has $n - 1$ edges and therefore $G - e$ has $n - 2$ edges. This implies $k = 2$. □

1.6.1 Exercises

Exercise 1.37. Is there a forest with $k = 2$ components having $n = 15$ vertices and $m = 12$ edges? If no, explain why, and if yes provide one. Repeat with $k = 3$.

Exercise 1.38. Suppose that G is a tree. Prove that if e is not an edge of G then $G + e$ has a cycle.

Exercise 1.39. Let a be the average degree of a tree G with n vertices. Find an expression for n in terms of a.

Exercise 1.40. Let G be a tree. Prove that if $d(u, v) = \text{diam}(G)$ then u and v are both leaves. Recall that $\text{diam}(G)$ is the length of the longest path in G.

Exercise 1.41. Let G be a tree.

(a) Prove that G has at least $\Delta(G)$ leaves.

(Hint: Theorem 1.6.4 and Proposition 1.6.5 might be useful here.)

(b) Give an example of a tree that has exactly $\Delta(G)$ leaves.

Exercise 1.42. Let G be a tree of order $n \geq 2$. Prove that the number of leaves in G is

$$2 + \sum_{\deg(v_i) \geq 3} (\deg(v_i) - 2).$$

Chapter 2

The Adjacency Matrix

In this chapter, we introduce 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, structure of the automorphism group, and many others. This approach to graph theory is therefore called **spectral graph theory**.

Before we begin, we introduce some notation. The identity matrix will be denoted by $\mathbf{I}$ and the matrix whose entries are all ones will be denoted by $\mathbf{J}$. For example, the 3×3 identity matrix and the 4×4 all ones matrix are

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

The transpose of a matrix $\mathbf{M}$ 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 $\mathbf{M}(i, j)$.

2.1 The Adjacency Matrix

Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The **adjacency matrix** of G is the $n \times n$ matrix $\mathbf{A} = \mathbf{A}(G)$ whose (i, j) entry is

$$\mathbf{A}(i,j) = \begin{cases} 1, & \text{if } v_i \sim v_j \\ \\ 0, & \text{otherwise.} \end{cases}$$

Since $v_i \sim v_j$ if and only if $v_j \sim v_i$, it follows that $\mathbf{A}(i, j) = \mathbf{A}(j, i)$, and therefore $\mathbf{A}$ 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 $\mathbf{A}$ correspond to the neighbors of vertex v_i. Similarly, the non-zero indices of the ith column of $\mathbf{A}$ are the neighbors of vertex v_i. It follows that the degree of v_i is the sum of the ith row (or ith column) of $\mathbf{A}$, 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 ones by $\mathbf{e} = (1, 1, \ldots, 1)$, then

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

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

Example 2.1. Consider the graph $G = (V, E)$ with $V = \{v_1, v_2, v_3, v_4, v_5\}$ and edge set $E = \{v_1v_2, v_1v_3, v_2v_3, v_3v_4, v_3v_5\}$. The adjacency matrix of G is

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

One of the first applications of the the adjacency matrix of a graph G is to count walks in G. A **walk** from vertex u to vertex v (not necessarily distinct) is a sequence of vertices $(w_0, w_1, \ldots, w_k)$, not necessarily distinct, such that $w_{i-1} \sim w_i$, and $w_0 = u$ and $w_k = v$. In this case, the walk is of length k. In the case that $u = v$, then the walk is said to be a **closed walk**. A walk where all the vertices are distinct is a path and a cycle is a closed walk where the only repeated vertices are the end-vertices of the walk. A closed walk of length three in a graph G implies that G contains $K_3 = C_3$ as a subgraph. For obvious reasons, K_3 is called a **triangle**.

Theorem 2.1.1: Counting Walks

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 walks 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 $v_i \sim v_j$ and then clearly there is a walk 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 walk 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 walks of length $k + 1$ from v_i to v_j. Any walk of length $k + 1$ from v_i to v_j contains a walk 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 walks of length k from v_i to v_p is $\mathbf{A}^k(i, p)$. Hence, the total number of walks of length $k + 1$ from v_i to v_j is

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

$\square$

The **trace** of a matrix $\mathbf{M}$ is the sum of its diagonal entries and will be denoted by $\mathrm{tr}(\mathbf{M})$:

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

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

Corollary 2.1.2

Let G be a graph with adjacency matrix $\mathbf{A}$. 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

$$\begin{aligned}
\operatorname{tr}(\mathbf{A}^2) &= 2m \\
\operatorname{tr}(\mathbf{A}^3) &= 6t \\
\operatorname{tr}(\mathbf{A}^4) &= 8q - 2m + 2\sum_{i=1}^{n} \deg(v_i)^2
\end{aligned}$$

Proof. The entry $\mathbf{A}^2(i,i)$ is the number of closed walks from v_i of length $k = 2$. A closed walk of length $k = 2$ counts one edge. Hence, $\mathbf{A}^2(i,i) = \deg(v_i)$ and therefore

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

To prove the second statement, we begin by noting that a closed walk can be traversed in two different ways. Hence, for each vertex v in a triangle, there are two walks of length $k = 3$ that start at v and traverse the triangle. And since each triangle contains three distinct vertices, each triangle in a graph accounts for six walks of length $k = 3$. Since $\sum_{i=1}^{n} \mathbf{A}^3(i,i)$ counts all walks in G of length three we have

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

Now consider $\operatorname{tr}(\mathbf{A}^4) = \sum_{i=1}^{n} \mathbf{A}^4(i,i)$. We count the number of closed walks of length $k = 4$ from v_i. There are 3 types of such walks: (1) closed walks of the form (v_i, x, v_i, y, v_i) where $x, y \in N(v_i)$. The number of such walks is $\deg(v_i)^2$

since we have $\deg(v_i)$ choices for x and $\deg(v_i)$ choices for y; (2) closed walks of the form (v_i, v_j, x, v_j, v_i) where $v_j \in N(v_i)$ and $x \in N(v_j)\backslash\{v_i\}$, the number of such walks is $\sum_{v_j \sim v_i}(\deg(v_j)-1)$; (3) walks along 4-cycles from v_i and there are 2 such walks for each cycle v_i is contained in, say q_i. Hence,

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

Therefore,

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

□

Example 2.2. Show that the total number of walks of length k in a graph G with adjacency matrix $\mathbf{A}$ is $\mathbf{e}^T \mathbf{A}^k \mathbf{e}$.

We also obtain the following as a corollary.

Corollary 2.1.3

A graph G with $n \geq 2$ vertices is connected if and only if the off-diagonal entries of the matrix

$$\mathbf{B} = \mathbf{A} + \mathbf{A}^2 + \cdots + \mathbf{A}^{n-1}$$

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 $k \in \{1, 2, \ldots, n-1\}$ 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 $\mathbf{B}$ are positive. Let v_i and v_j be arbitrary distinct vertices. Since $\mathbf{B}(i, j) > 0$ then there is a minimum $k \in \{1, \ldots, n-1\}$ such that $\mathbf{A}^k(i, j) > 0$. Therefore, there is a walk of length k from v_i to v_j. We claim that every such walk is a path. Assume that $\gamma = (w_0, w_1, \ldots, w_k)$ is a walk (but not a path) from v_i to v_j of length k. If v is a repeated vertex in γ, say $w_a = v$ and $w_b = v$ for $a < b$ then we may delete the vertices $w_{a+1}, w_{a+2}, \ldots, w_b$ from γ and still obtain a walk from v_i to v_j. We can continue this process of deleting vertices from γ to obtain a $v_i - v_j$ walk with no repeated vertices, that is, a $v_i - v_j$ path. This path has length less than k which contradicts the minimality of k. This proves the claim and hence all $v_i - v_j$ walks of length k are paths from v_i to v_j. This proves that G is connected. □

In the proof of the previous corollary we proved the following.

Lemma 2.1.4: Every uv-Walk Contains a uv-Path

Every walk from u to v contains a path from u to v.

Example 2.3. Let $V = \{v_1, v_2, \ldots, v_n\}$. How do you obtain the adjacency matrix of $G - v_i$ given the adjacency matrix of G?

Recall that for a graph G we denote its complement by $\overline{G}$. Below we give a relationship between the adjacency matrices of G and $\overline{G}$.

Lemma 2.1.5

For any graph G it holds that

$$\mathbf{A}(G) + \mathbf{A}(\overline{G}) + \mathbf{I} = \mathbf{J}.$$

Proof. Let $\mathbf{A} = \mathbf{A}(G)$ and let $\bar{\mathbf{A}} = \mathbf{A}(\overline{G})$. For $i \neq j$, if $\mathbf{A}(i,j) = 0$ then $\bar{\mathbf{A}}(i,j) = 1$, and vice-versa. Therefore, $\mathbf{A}(i,j) + \bar{\mathbf{A}}(i,j) = 1$ for all $i \neq j$. On the other hand, $\mathbf{A}(i,i) = \bar{\mathbf{A}}(i,i) = 0$ for all i. Thus $\mathbf{A}(G) + \mathbf{A}(\overline{G}) + \mathbf{I} = \mathbf{J}$ as claimed. □

2.1.1 Exercises

Exercise 2.1. Provide the adjacency matrix for each of the following graphs.

(a) The path graph P_8 where the vertices are labelled in increasing order from one end to the other along the path.

(b) The cycle graph C_7 where the vertices are labelled around the cycle in increasing order.

(c) The complete graph K_n with vertices labelled in any way. (Do this for small n and then write the general form of $\mathbf{A}(K_n)$.)

(d) The graph $(P_2 \vee K_2) \oplus P_2$.

Exercise 2.2. Consider the complete bipartite graph $K_{n,m}$ where X and Y are the parts of the bipartition. Suppose that $X = \{v_1, v_2, \ldots, v_n\}$ and $Y = \{v_{n+1}, v_{n+2}, \ldots, v_{n+m}\}$. What is the form of the adjacency matrix of $K_{n,m}$? Try this for small n, m, say $n = 3$ and $m = 4$, and then generalize.

Exercise 2.3. Consider the following recursively defined sequence of graphs:

$$\begin{aligned}
G_1 &= K_1 \\
G_2 &= G_1 \vee K_1 \\
G_3 &= G_2 \oplus K_1 \\
G_4 &= G_3 \vee K_1 \\
G_5 &= G_4 \oplus K_1
\end{aligned}$$

and in general $G_k = G_{k-1} \oplus K_1$ if $k \geq 3$ is odd and $G_k = G_{k-1} \vee K_1$ if $k \geq 2$ is even.

(a) Consider the graph G_4. Label the vertices of G_4 using v_1, v_2, v_3, v_4 and so that $\deg(v_i) \leq \deg(v_{i+1})$. Using this labelling of the vertices, write out the adjacency matrix of G_4.

(b) Do the same as in part (a) with G_6.

(c) Do the same as in part (a) with G_8.

(d) For general even k, what is the general form of the adjacency matrix of G_k?

Exercise 2.4. For each case, draw the graph with the given adjacency matrix.

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

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

Exercise 2.5. Consider the cycle graph C_6 with vertices $V(C_6) = \{v_1, v_2, \ldots, v_6\}$ and so that $v_i \sim v_{i+1}$ and $v_1 \sim v_6$. Prove that if k is even then $\mathbf{A}^k(v_1, v_4) = 0$. (HINT: C_6 is bipartite.)

Exercise 2.6. Let $\mathbf{A}_1$ and $\mathbf{A}_2$ be the adjacency matrices of G_1 and G_2, respectively.
(a) What is the adjacency matrix of $G_1 \oplus G_2$ in terms of $\mathbf{A}_1$ and $\mathbf{A}_2$?
(b) What is the adjacency matrix of $G_1 \vee G_2$ in terms of $\mathbf{A}_1$ and $\mathbf{A}_2$?
For each case, assume that if $V(G_1) = \{v_1, v_2, \ldots, v_n\}$ and $V(G_2) = \{w_1, w_2, \ldots, w_m\}$ then the order of the vertices of $G_1 \oplus G_2$ and $G_1 \vee G_2$ is $v_1, v_2, \ldots, v_n, w_1, w_2, \ldots, w_m$.

Exercise 2.7. Let $\mathbf{B}_k = \mathbf{A} + \mathbf{A}^2 + \cdots + \mathbf{A}^k$ for $k \geq 1$. Recall that the diameter a graph, denoted by $\operatorname{diam}(G)$, is the maximum distance among all vertices in G. Prove that if G is connected then the smallest integer m such that all the off-diagonal entries of $\mathbf{B}_m$ are positive is the diameter of G.

Exercise 2.8. Let G be a r-regular graph with adjacency matrix $\mathbf{A}$. Prove that the total number of walks of length $k \geq 1$ in G is nr^k.

2.2 The coefficients and roots of a polynomial

As mentioned at the beginning of this chapter, the eigenvalues of the adjacency matrix of a graph contain valuable information about the structure of the graph and we will soon see examples of this. Recall that the eigenvalues of a matrix are the roots of its characteristic polynomial and the coefficients of a polynomial depend in a polynomial way on its roots. For example, expanding the polynomial $g(t) = (t - \lambda_1)(t - \lambda_2)$ we obtain

$$g(t) = t^2 - (\lambda_1 + \lambda_2)t + \lambda_1\lambda_2$$

from which we see that the coefficient of t and the constant term of $g(t)$ are polynomial expressions in the roots λ_1 and λ_2. If we define the polynomials $s_1(x, y) = x + y$ and $s_2(x, y) = xy$ then

$$g(t) = t^2 - s_1(\lambda_1, \lambda_2)t + s_2(\lambda_1, \lambda_2).$$

How about a cubic polynomial? Consider then $g(t) = (t-\lambda_1)(t-\lambda_2)(t-\lambda_3)$ and expand:

$$g(t) = t^3 - (\lambda_1 + \lambda_2 + \lambda_3)t^2 + (\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3)t - \lambda_1\lambda_2\lambda_3.$$

Thus, if define the polynomials $s_1(x,y,z) = x+y+z$, $s_2(x,y,z) = xy+xz+yz$, and $s_3(x,y,z) = xyz$, then

$$g(t) = t^3 - s_1(\lambda_1,\lambda_2,\lambda_3)t^2 + s_2(\lambda_1,\lambda_2,\lambda_3)t - s_3(\lambda_1,\lambda_2,\lambda_3)$$

and again we see that the coefficients of $g(t)$ are polynomial expressions in the roots $\lambda_1, \lambda_2, \lambda_3$. To deal with the general nth order polynomial, let us introduce some terminology and notation.

A **multivariate polynomial** is a polynomial in more than one variable. Examples of polynomials in the variables x, y are

$$f(x,y) = x^2 - xy + 7y^2, \qquad f(x,y) = -8y^5 - xy^2 - 2y^3 + xy^{32}$$

and examples of polynomials in the variables x, y, z are

$$f(x,y,z) = x^2 + xy^2z - 44z^3, \qquad f(x,y,z) = 11xyz.$$

We will only consider polynomials with rational coefficients and we will use $\mathbb{Q}[x_1, x_2, \ldots, x_n]$ to denote the set of all polynomials in the variables $x_1, x_2, \ldots, x_n$ with rational coefficients. For example, the polynomial

$$f(x_1,x_2,x_3,x_4) = 4 - 6x_1^3x_2x_3^2x_4^5 - 33x_1x_2x_3x_4 + \tfrac{5}{2}x_1x^2x_4.$$

is an element of $\mathbb{Q}[x_1, x_2, x_3, x_4]$. We now introduce a set of n particularly important polynomials.

Definition 2.2.1: Elementary Symmetric Polynomials

Let $I = \{1, 2, \ldots, n\}$ and for $1 \le k \le n$ let $\binom{I}{k}$ denote the set of all k-element subsets of I. The k**th elementary symmetric polynomial** in the variables $x_1, x_2, \ldots, x_n$ is defined by

$$s_k(x_1, x_2, \ldots, x_n) = \sum_{\{i_1, i_2, \ldots, i_k\} \in \binom{I}{k}} x_{i_1} x_{i_2} \cdots x_{i_k}.$$

In Definition 2.2.1, the notation $\sum_{\{i_1, i_2, \ldots, i_k\} \in \binom{I}{k}}$ means that the sum is over all k-element subsets of I. The number of elements in $\binom{I}{k}$ is $\binom{n}{k}$ and thus s_k is the sum of $\binom{n}{k}$ monomials of the form $x_{i_1} x_{i_2} \ldots x_{i_k}$. We call s_k the kth elementary symmetric polynomial in n variables. A few examples of s_k are

$$s_1(x_1, x_2, \ldots, x_n) = x_1 + x_2 + x_3 + \cdots + x_n$$

$$s_2(x_1, x_2, \ldots, x_n) = x_1x_2 + x_1x_3 + \cdots + x_1x_n + x_2x_3 + \cdots + x_{n-1}x_n$$

$$s_n(x_1, x_2, \ldots, x_n) = x_1x_2 \cdots x_n$$

If it is necessary to emphasize that s_k is the kth elementary symmetric polynomial in n variables then we use the notation s_k^n but note that the superscript n is not an exponent but there only to indicate the number of variables.

Example 2.4. For $n = 3$, the elementary symmetric polynomials are

$$\begin{aligned} s_1(x_1, x_2, x_3) &= x_1 + x_2 + x_3 \\ s_2(x_1, x_2, x_3) &= x_1x_2 + x_1x_3 + x_2x_3 \\ s_3(x_1, x_2, x_3) &= x_1x_2x_3. \end{aligned} \tag{2.1}$$

and for $n = 4$ the elementary symmetric polynomials are

$$\begin{aligned} s_1(x_1, x_2, x_3, x_4) &= x_1 + x_2 + x_3 + x_4 \\ s_2(x_1, x_2, x_3, x_4) &= x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4 \\ s_3(x_1, x_2, x_3, x_4) &= x_1x_2x_3 + x_1x_2x_4 + x_2x_3x_4 \\ s_4(x_1, x_2, x_3, x_4) &= x_1x_2x_3x_4. \end{aligned} \tag{2.2}$$

For $n = 7$, there are $\binom{7}{5} = 21$ five-element subsets of $\{1, 2, \ldots, 7\}$, and thus

$s_5(x_1, x_2, \ldots, x_7)$ is the sum of 21 monomials:

$$\begin{aligned} s_5(x_1, x_2, \ldots, x_7) = {} & x_1x_2x_3x_4x_5 + x_1x_2x_3x_4x_6 + x_1x_2x_3x_4x_7 + x_1x_2x_3x_5x_6 \\ & + x_1x_2x_3x_5x_7 + x_1x_2x_3x_6x_7 + x_1x_2x_4x_5x_6 + x_1x_2x_4x_5x_7 \\ & + x_1x_2x_4x_6x_7 + x_1x_2x_5x_6x_7 + x_1x_3x_4x_5x_6 + x_1x_3x_4x_5x_7 \\ & + x_1x_3x_4x_6x_7 + x_1x_3x_5x_6x_7 + x_1x_4x_5x_6x_7 + x_2x_3x_4x_5x_6 \\ & + x_2x_3x_4x_5x_7 + x_2x_3x_4x_6x_7 + x_2x_3x_5x_6x_7 + x_2x_4x_5x_6x_7 \\ & + x_3x_4x_5x_6x_7. \end{aligned}$$

We now describe a natural way in which the elementary symmetric polynomials arise. Introduce a new variable t and consider the polynomial

$$g(t) = (t - \lambda_1)(t - \lambda_2) \cdots (t - \lambda_n).$$

Hence, $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the roots of the polynomial $g(t)$ since $g(\lambda_i) = 0$ for all $i = 1, 2, \ldots, n$. Expanding the right hand side, we now show by induction that

$$g(t) = t^n - s_1t^{n-1} + s_2t^{n-2} + \cdots + (-1)^k s_k t^{n-k} + \cdots + (-1)^{n-1} s_{n-1} t + (-1)^n s_n. \tag{2.3}$$

where the s_k appearing in the coefficients of $g(t)$ is the kth elementary symmetric polynomial evaluated at $(\lambda_1, \ldots, \lambda_n)$. We first begin with the following lemma.

Lemma 2.2.2: Recurrence Relation for s_k

Let s_k^n denote the kth elementary symmetric polynomial in the n variables $x_1, x_2, \ldots, x_n$ and let s_k^{n+1} denote the kth elementary symmetric polynomial in the $n + 1$ variables $x_1, x_2, \ldots, x_{n+1}$. Then

$$s_k^{n+1} = s_k^n + x_{n+1}s_{k-1}^n$$

Proof. By definition,

$$s_k^{n+1} = \sum_{\{i_1, i_2 \ldots, i_k\} \in I_{n+1}(k)} x_{i_1}x_{i_2} \cdots x_{i_k}$$

A k-element subset of $I_{n+1} = \{1, 2, \ldots, n, n+1\}$ that does not contain $n+1$ is an element of $I_n(k)$ and a k-element subset of I_{n+1} that does contain $n+1$ is the union of $\{n+1\}$ and a $(k-1)$-element subset of I_n. Therefore,

$$\begin{aligned} s_k^{n+1} &= \sum_{\{i_1,i_2\ldots,i_k\}\in I_n(k)} x_{i_1}x_{i_2}\cdots x_{i_k} + x_{n+1}\left[\sum_{\{i_1,i_2\ldots,i_{k-1}\}\in I_n(k-1)} x_{i_1}x_{i_2}\cdots x_{i_{k-1}}\right] \\ &= s_k^n + x_{n+1}s_{k-1}^n \end{aligned}$$

as claimed. $\square$

Theorem 2.2.3: Vieta's Formula

If $g(t) = (t-\lambda_1)(t-\lambda_2)\cdots(t-\lambda_n)$ then

$$g(t) = t^n - s_1t^{n-1} + s_2t^{n-2} + \cdots + (-1)^k s_k t^{n-k} + \cdots + (-1)^{n-1}s_{n-1}t + (-1)^n s_n.$$

where $s_k = s_k(\lambda_1, \lambda_2, \ldots, \lambda_n)$ for $k = 1, 2, \ldots, n$.

Proof. The proof is by induction on the order n of the polynomial $g(t)$. The case $n = 1$ is trivial. Assume that the claim is true for all polynomials of order n and let $g(t) = (t-\lambda_1)(t-\lambda_2)\cdots(t-\lambda_n)(t-\lambda_{n+1})$. Then $g(t) = h(t)(t-\lambda_{n+1})$ where $h(t) = (t-\lambda_1)(t-\lambda_2)\cdots(t-\lambda_n)$. Applying the induction hypothesis to $h(t)$, we have that

$$g(t) = \left(t^n - s_1^n t^{n-1} + s_2^n t^{n-2} + \cdots + (-1)^{n-1}s_{n-1}^n t + (-1)^n s_n^n\right)(t-\lambda_{n+1})$$

and then expanding and collecting like terms we obtain

$$\begin{aligned} g(t) = t^{n+1} &- (\lambda_{n+1} + s_1^n)t^n + (s_2^n + \lambda_{n+1}s_1^n)t^{n-1} \\ &+ \cdots + (-1)^n(s_n^n + \lambda_{n+1}s_{n-1}^n)t + (-1)^{n+1}\lambda_{n+1}s_n^n \end{aligned}$$

We can now apply Lemma 2.2.2 to the coefficients of $g(t)$ and obtain

$$g(t) = t^{n+1} - s_1^{n+1}t^n + s_2^{n+1}t^{n-1} + \cdots + (-1)^n s_n^{n+1} t + (-1)^{n+1}s_{n+1}^{n+1}$$

as claimed. $\square$

Example 2.5. Consider the polynomial $g(t) = t(t-3)(t+1)(t-2)$. Hence, the roots of g are $\lambda_1 = 0$, $\lambda_2 = 3$, and $\lambda_3 = -1$, and $\lambda_4 = 2$. Expanding g we obtain

$$g(t) = t^4 - 4t^3 + t^2 + 6t.$$

On the other hand, using the expressions for s_1, s_2, s_3, s_4 from (2.2), we have:

$$\begin{aligned}
s_1(0,3,-1,2) &= 0 + 3 - 1 + 2 = 4 \\
s_2(0,3,-1,2) &= (3)(-1) + (3)(2) + (-1)(2) = 1 \\
s_3(0,3,-1,2) &= (3)(-1)(2) = -6 \\
s_4(0,3,-1,2) &= (0)(3)(-1)(2) = 0.
\end{aligned}$$

Let us record the following for future reference.

Proposition 2.2.4

Consider the polynomial

$$g(t) = t^n + c_1 t^{n-1} + c_2 t^{n-2} + \cdots + c_{n-1} t + c_n.$$

Then $-c_1$ is the sum of the roots of g and $(-1)^n c_n$ is the product of the roots of g.

There is another important set of multivariate polynomials that we will encounter in the next section called the **power sums** polynomials and that are closely related with the elementary symmetric polynomials. The **power sums** polynomials in the variables $x_1, x_2, \ldots, x_n$ are the n polynomials p_1, p_2, …, p_n given by

$$p_k(x_1, x_2, \ldots, x_n) = x_1^k + x_2^k + \cdots + x_n^k.$$

The relationship between the elementary symmetric and the power sums polynomials is the following. First of all, it is clear that $s_1 = p_1$. Now,

$$\begin{aligned}
p_1^2 - p_2 &= (x_1 + x_2 + \cdots + x_n)^2 - (x_1^2 + x_2^2 + \cdots + x_n^2) \\
&= \sum_{i=1}^n x_i^2 + \sum_{1 \le i < j \le n} 2x_i x_j - (x_1^2 + x_2^2 + \cdots + x_n^2) \\
&= 2 \sum_{i<j} x_i x_j \\
&= 2s_2
\end{aligned}$$

and therefore

$$s_2 = \frac{1}{2}(p_1^2 - p_2).$$

A similar computation yields that

$$s_3 = \frac{1}{6}(p_1^3 - 3p_1p_2 + 2p_3).$$

The general relationship between the symmetric elementary and power sums polynomials is known as **Newton's identities**:

$$p_k - s_1 p_{k-1} + s_2 p_{k-2} + \cdots + (-1)^{k-1} s_{k-1} p_1 + (-1)^k k s_k = 0, \quad 1 \le k \le n \quad (2.4)$$

From Newton's identities we obtain that

$$s_k = \tfrac{1}{k}(-1)^{k-1}(p_k - s_1 p_{k-1} + \cdots + (-1)^{k-1} s_{k-1} p_1).$$

Now since $s_1 = p_1$, it is straightforward to show by induction that each elementary symmetric polynomial can be written only in terms of the power sums polynomial. To summarize, we obtain the following.

Proposition 2.2.5

Consider the polynomial $g(t) = (t - \lambda_1)(t - \lambda_2) \cdots (t - \lambda_n)$ written in expanded form

$$g(t) = t^n + c_1 t^{n-1} + c_2 t^{n-2} + \cdots c_{n-1} t + c_n.$$

The coefficients $c_1, c_2, \ldots, c_n$ can be expressed in terms of the power sums polynomials $p_1, p_2, \ldots,\ p_n$ evaluated at the roots $\lambda_1, \lambda_2, \ldots, \lambda_n$, that is, there are polynomial functions $f_1, f_2, \ldots, f_n$ such that

$$c_i = f_i(p_1, p_2, \ldots, p_n)$$

where the $p_1, p_2, \ldots, p_n$ are evaluated at $\lambda_1, \lambda_2, \ldots, \lambda_n$.

2.2.1 Exercises

Exercise 2.9. Expand the polynomial $g(x) = (t - \lambda_1)(t - \lambda_2)(t - \lambda_3)(t - \lambda_4)$ and use the expressions for s_1, s_2, s_3, s_4 in (2.2) to verify equation (2.3) for $n = 4$.

Exercise 2.10. Use Newton's identities to express s_4 in terms of p_1, p_2, p_3, p_4.

Exercise 2.11. The polynomial $g(t) = t^3 + c_1 t^2 + 2t + 8$ has $\lambda_1 = 2$ as a root. Find the other roots of g and then find c_1.

2.3 The characteristic polynomial and spectrum of a graph

In this section, we introduce 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 $\mathbf{M}$ if there exists a vector $\mathbf{x}$ such that

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

In this case, $\mathbf{x}$ is called an **eigenvector** of $\mathbf{M}$ corresponding to the eigenvalue λ. To find the eigenvalues of $\mathbf{M}$, we find the zeros of the **characteristic polynomial** of $\mathbf{M}$:

$$p(t) = \det(t\mathbf{I} - \mathbf{M}).$$

If $\mathbf{M}$ is an $n \times n$ matrix, then the characteristic polynomial $p(t)$ is an nth order polynomial and $p(\lambda) = 0$ if and only if λ is an eigenvalue of $\mathbf{M}$. From the Fundamental Theorem of Algebra, $p(t)$ has n eigenvalues, possibly repeated and complex. However, if $\mathbf{M}$ is a symmetric matrix, then an important result in linear algebra is that the eigenvalues of $\mathbf{M}$ 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 $\mathbf{M}$ is symmetric and $\mathbf{x}$ and $\mathbf{y}$ are eigenvectors of $\mathbf{M}$ corresponding to distinct eigenvalues then $\mathbf{x}$ and $\mathbf{y}$ are orthogonal, that is,

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

Moreover, if $\mathbf{M}$ is symmetric, there exists an orthonormal basis $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ of $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{M}$. Recall that $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ is an orthonormal basis of $\mathbb{R}^n$ 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 are unit vectors and are mutually orthogonal.

Definition 2.3.1: 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 $\operatorname{spec}(G)$, is the list of the eigenvalues of $\mathbf{A}$ in increasing order $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$:

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

Example 2.6. 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 2.7. 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 $\operatorname{spec}(E_n) = (0, 0, \ldots, 0)$.

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

$$\mathbf{A}\mathbf{x}_1 = (-1, 1, 0, 0) = -\mathbf{x}_1$$

and therefore $\lambda_1 = -1$ is an eigenvalue of $\mathbf{A}$. Similarly, a direct computation yields that $\mathbf{A}\mathbf{x}_2 = -\mathbf{x}_2$ and $\mathbf{A}\mathbf{x}_3 = -\mathbf{x}_3$. Hence, $\lambda_2 = \lambda_3 = -1$. Finally, we have that $\mathbf{A}\mathbf{e} = (3, 3, 3, 3) = 3\mathbf{e}$, and therefore $\lambda_4 = 3$ is an eigenvalue of $\mathbf{A}$. Therefore, the spectrum of K_n is

$$\operatorname{spec}(K_4) = (-1, -1, -1, 3)$$

and therefore the characteristic polynomial of K_4 is $p(t) = (t-3)(t+1)^3$. In general, one can show that

$$\text{spec}(K_n) = (-1, -1, \ldots, -1, n-1)$$

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 2.3.2

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

Proof. Suppose that λ is an eigenvalue of G with eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$. Suppose that the jth entry of $\mathbf{x}$ has maximum absolute value, that is, $|x_i| \leq |x_j|$ for all $i = 1, 2, \ldots, n$. Since $\mathbf{Ax} = \lambda\mathbf{x}$ it follows that

$$\lambda x_j = \sum_{i=1}^{n} \mathbf{A}(j,i) x_i$$

and therefore using the triangle inequality we obtain

$$\begin{aligned} |\lambda||x_j| = \left|\sum_{i=1}^{n} \mathbf{A}(j,i) x_i\right| &\leq \sum_{i=1}^{n} |\mathbf{A}(j,i)||x_i| \\ &= |x_j| \sum_{i=1}^{n} |\mathbf{A}(j,i)| \\ &= |x_j| \deg(v_j) \\ &\leq |x_j| \Delta(G). \end{aligned}$$

Therefore $|\lambda||x_j| \leq |x_j|\Delta(G)$, and the claim follows by dividing both sides of the inequality by $|x_j| \neq 0$. □

Proposition 2.3.3

Let $\mathrm{spec}(G) = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ and let $d_{\text{avg}} = \frac{2|E(G)|}{n}$ denote the average degree of G. Then

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

Proof. Let $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ be an orthonormal basis of $\mathbf{A} = \mathbf{A}(G)$ with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then there exists numbers $\alpha_1, \alpha_2, \ldots, \alpha_n \in \mathbb{R}$ such that $\mathbf{e} = \sum_{i=1}^n \alpha_i \mathbf{x}_i$. Let

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

denote the degree vector of G. Now

$$\mathbf{e}^T\mathbf{Ae} = \mathbf{e}^T\mathbf{d} = \sum_{i=1}^n \deg(v_i)$$

while on the other hand, since β is an orthonormal basis, we have

$$\mathbf{e}^T\mathbf{Ae} = \sum_{i=1}^n \alpha_i^2 \lambda_i.$$

Therefore,

$$\sum_{i=1}^n \deg(v_i) = \sum_{i=1}^n \alpha_i^2 \lambda_i \leq \lambda_n \sum_{i=1}^n \alpha_i^2 = \lambda_n \cdot n$$

where we have used the fact that $n = \mathbf{e}^T\mathbf{e} = \sum_{i=1}^n \alpha_i^2$ and $\lambda_i \leq \lambda_n$ for all $i = 1, 2, \ldots, n$. Therefore,

$$\frac{1}{n}\sum_{i=1}^n \deg(v_i) \leq \lambda_n$$

and this proves the first inequality. The second inequality follows from Proposition 2.3.2. $\square$

Proposition 2.3.4

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

Proof. Recall that

$$\mathbf{A}\mathbf{e} = (\deg(v_1), \deg(v_2), \ldots, \deg(v_n)).$$

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

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

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

$$\mathbf{A}\mathbf{e} = k\mathbf{e} = (k, k, \ldots, k)$$

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

Proposition 2.3.5

Let G be a k-regular graph with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n = k$. Then the complement graph $\overline{G}$ has eigenvalues $n - 1 - k, -1 - \lambda_1, -1 - \lambda_2, \ldots, -1 - \lambda_{n-1}$.

Proof. Let $\beta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ be an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{A}$ with corresponding eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n = k$. By Proposition 2.3.4, k is an eigenvalue of G with corresponding eigenvector $\mathbf{e}$, and moreover by Exercise 2.16, $\lambda_n = k$ is the maximum eigenvalue of G. We may therefore take $\mathbf{x}_n = \frac{1}{\sqrt{n}}\mathbf{e}$. Let $\mathbf{A} = \mathbf{A}(G)$ and let $\overline{\mathbf{A}} = \mathbf{A}(\overline{G})$. From Lemma 2.1.5 we have that

$$\overline{\mathbf{A}} = \mathbf{J} - \mathbf{I} - \mathbf{A}.$$

Now since $\mathbf{x}_i$ is orthogonal to $\mathbf{x}_n$ for $1 \leq i < n$ we have $\mathbf{J}\mathbf{x}_i = \mathbf{0}$ for $1 \leq i < n$. Therefore, for $1 \leq i < n$ we have

$$\overline{\mathbf{A}}\mathbf{x}_i = \mathbf{J}\mathbf{x}_i - \mathbf{I}\mathbf{x}_i - \mathbf{A}\mathbf{x}_i = -\mathbf{x}_i - \lambda_i\mathbf{x}_i = (-1 - \lambda_i)\mathbf{x}_i.$$

Since $\overline{G}$ is a regular graph with degree $(n-1-k)$, by Proposition 2.3.4 $(n-1-k)$ is an eigenvalue of $\overline{G}$ with corresponding eigenvector $\mathbf{x}_n$, and this ends the proof. □

We now consider bipartite graphs.

Theorem 2.3.6

Suppose that G is a bipartite graph. Then if λ is an eigenvalue of G then $-\lambda$ is an eigenvalue of G. Consequently, if $\pm\lambda_1, \pm\lambda_2, \ldots, \pm\lambda_q$ are the non-zero eigenvalues of G then the characteristic polynomial of G takes the form

$$p(t) = t^k(t^2 - \lambda_1^2)(t^2 - \lambda_2^2)\cdots(t^2 - \lambda_q^2).$$

where $k \geq 0$. In particular, if $n = |V(G)|$ is odd then $k \geq 1$, that is, $\lambda = 0$ is an eigenvalue of G with multiplicity k.

Proof. Since G is bipartite, there is a partition $\{X, Y\}$ of the vertex set $V(G)$ such that each edge of G has one vertex in X and the other in Y. Let $r = |X|$ and $s = |Y|$. By a relabelling of the vertices of G, we may assume that $X = \{v_1, v_2, \ldots, v_r\}$ and $Y = \{v_{r+1}, v_{r+2}, \ldots, v_{r+s}\}$. Therefore, the adjacency matrix of G takes the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{0} \end{bmatrix}.$$

Suppose that $\mathbf{z} = \left[\begin{smallmatrix} \mathbf{x} \\ \mathbf{y} \end{smallmatrix}\right]$ is an eigenvector of $\mathbf{A}$ with eigenvalue λ. Thus,

$$\mathbf{A}\mathbf{z} = \begin{bmatrix} \mathbf{B}\mathbf{y} \\ \mathbf{B}^T\mathbf{x} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}.$$

Then

$$\mathbf{A}\begin{bmatrix}\mathbf{x}\\ -\mathbf{y}\end{bmatrix} = \begin{bmatrix}-\mathbf{B}\mathbf{y}\\ \mathbf{B}^T\mathbf{x}\end{bmatrix} = -\lambda\begin{bmatrix}\mathbf{x}\\ -\mathbf{y}\end{bmatrix}.$$

Therefore, $\left[\begin{smallmatrix}\mathbf{x}\\ -\mathbf{y}\end{smallmatrix}\right]$ is an eigenvector of $\mathbf{A}$ with eigenvalue $-\lambda$. Hence, $(t^2 - \lambda^2)$ is a factor in $p(t)$. If q denotes the number of non-zero eigenvalue pairs $\pm\lambda_i$ then $k = n - 2q$ is the multiplicity of the eigenvalue $\lambda = 0$, and if n is odd then $k \geq 1$. $\square$

Example 2.9. The eigenvalues of the cycle C_n are

$$2\cos\left(\tfrac{2\pi j}{n}\right)$$

for $j = 0, 1, \ldots, n-1$.

Example 2.10. Under what condition will a k-regular graph G have $\lambda = \pm k$ as eigenvalues?

Example 2.11. Consider the complete bipartite graph $K_{r,s}$ where $r, s, \geq 1$. Show that $\lambda = 0$ is an eigenvalue of $K_{r,s}$ of multiplicity $r + s - 2$. In Exercise 2.18 you will show that $\pm\sqrt{rs}$ are the other two eigenvalues of $K_{r,s}$.

Here is a generalization of the previous example.

Example 2.12. Suppose that G_1 is a k_1-regular graph with n_1 vertices and G_2 is a k_2-regular graph with n_2 vertices. Let $\mathrm{spec}(G_1) = (\lambda_1, \lambda_2, \ldots, \lambda_{n_1})$, where $\lambda_{n_1} = k_1$, and let $\mathrm{spec}(G_2) = (\mu_1, \mu_2, \ldots, \mu_{n_2})$, where $\mu_{n_2} = k_2$. Let $G = G_1 \vee G_2$.

(a) Let $V(G_1) = \{v_1, v_2, \ldots, v_{n_1}\}$ and $V(G_2) = \{w_1, w_2, \ldots, w_{n_2}\}$. Write down the adjacency matrix of $\mathbf{A} = \mathbf{A}(G)$ if we order the vertices of G as $(v_1, v_2, \ldots, v_{n_1}, w_1, w_2, \ldots, w_{n_2})$.

(b) If $\mathbf{x}_i \neq \mathbf{e}$ is an eigenvector of G_1 with eigenvalue λ_i, with $i < n_1$, then show that $\left[\begin{smallmatrix}\mathbf{x}_i\\ \mathbf{0}\end{smallmatrix}\right]$ is an eigenvector of G with eigenvalue λ_i.

(c) If $\mathbf{y}_j \neq \mathbf{e}$ is an eigenvector of G_2 with eigenvalue μ_j, with $j < n_2$, then show that $\left[\begin{smallmatrix}\mathbf{0}\\ \mathbf{y}_j\end{smallmatrix}\right]$ is an eigenvector of G with eigenvalue μ_j.

(d) Parts (b) and (c) determine n_1+n_2-2 eigenvalues of G. Here we find the remaining two eigenvalues. Consider the vector $\mathbf{z} = \left[\begin{smallmatrix}\alpha\mathbf{e}\\ \mathbf{e}\end{smallmatrix}\right]$ where $\alpha \neq 0$ and is to be determined. Apply the eigenvector-eigenvalue condition $\mathbf{A}\mathbf{z} = \lambda\mathbf{z}$ and show that the remaining two eigenvalues of G are

$$\lambda = \frac{(k_1+k_2) \pm \sqrt{(k_2-k_1)^2 + 4n_1n_2}}{2}$$

and that

$$\alpha = \frac{-(k_2-k_1) \pm \sqrt{(k_2-k_1)^2 + 4n_1n_2}}{2n_1}$$

(e) Conclude that if $p_1(t)$ and $p_2(t)$ are the characteristic polynomials of G_1 and G_2, respectively, then the characteristic polynomial of G is

$$p(t) = \frac{p_1(t)p_2(t)}{(t-k_1)(t-k_2)}((t-k_1)(t-k_2) - n_1n_2)$$

Example 2.13. Let $d(G) = (d_1, d_2, \ldots, d_n)$ be the degree sequence of G and let λ_n be the largest eigenvalue of G. Prove that

$$\sqrt{\frac{d_1^2 + d_2^2 + \cdots + d_n^2}{n}} \leq \lambda_n$$

Hint: Use Rayleigh quotients and Perron-Frobenius. [3]

2.3.1 Exercises

Exercise 2.12. Let $\mathbf{M}$ be an $n \times n$ matrix and let $p(t)$ be the characteristic polynomial of $\mathbf{M}$. Find $p(0)$ in two ways:

(a) Using the expansion

$$p(t) = t^n - s_1t^{n-1} + s_2t^{n-2} + \cdots + (-1)^{n-1}s_{n-1}t + (-1)^n s_n$$

where as usual $s_1, s_2, \ldots, s_n$ are the elementary symmetric polynomials evaluated at the roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $p(t)$.

(b) Using the definition of $p(t)$, namely, $p(t) = \det(t\mathbf{I} - \mathbf{M})$. Hint: Recall that $\det(\alpha\mathbf{M}) = \alpha^n \det(\mathbf{M})$ for any $\alpha \in \mathbb{R}$.

Conclude that $\det(\mathbf{M}) = \lambda_1\lambda_2\cdots\lambda_n$, that is, that $\det(\mathbf{M})$ is the product of the eigenvalues of $\mathbf{M}$.

Exercise 2.13. By direct hand computation, find the characteristic polynomial and spectrum of the graph $G = C_3 \vee K_1$.

Exercise 2.14. Let $G_1 = C_4 \oplus K_1$ and let $G_2 = E_4 \vee K_1$.
(a) Draw the graphs G_1 and G_2. Explain why G_1 and G_2 are not isomorphic.
(b) Find the characteristic polynomials and eigenvalues of G_1 and G_2.
(c) What can you conclude based on parts (a) and (b)?

Exercise 2.15. Prove that if G has at least one edge then G has at least one negative and one positive eigenvalue. (Hint: Use Proposition 2.3.3 and the fact that $0 = \operatorname{tr}(\mathbf{A}) = \lambda_1 + \lambda_2 + \cdots + \lambda_n$ where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $\mathbf{A}$.)

Exercise 2.16. Let G be a k-regular graph. Prove that $|\lambda_i| \leq k$ for all eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of G.

Exercise 2.17. Recall that u, v are twin vertices if $N(u)\backslash\{v\} = N(v)\backslash\{u\}$, that is, u and v have the same neighbors (other than themselves). Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Prove that if v_1 and v_2 are twin vertices then $\mathbf{x} = \mathbf{e}_1 - \mathbf{e}_2$ is an eigenvector of G with eigenvalue
(a) $\lambda = 0$ if v_1 and v_2 are not adjacent, and
(b) $\lambda = -1$ if v_1 and v_2 are adjacent.

Exercise 2.18. Consider the complete bipartite graph $K_{r,s}$ where $r, s \geq 1$.
(a) Show that the vector

$$\mathbf{z} = (\underbrace{\sqrt{s}, \sqrt{s}, \ldots, \sqrt{s}}_{r \text{ times}}, \underbrace{\sqrt{r}, \sqrt{r}, \ldots, \sqrt{r}}_{s \text{ times}})$$

is an eigenvector of $K_{r,s}$ with eigenvalue $\sqrt{rs}$.

(b) Find an eigenvector for $-\sqrt{rs}$.

Exercise 2.19. Let G_1 and G_2 be graphs with characteristic polynomials $p_1(t)$ and $p_2(t)$, respectively. What is the characteristic polynomial of $G_1 \oplus G_2$? Show all your work. Hint: See Exercise 2.6 and use the fact that

$$\det \begin{bmatrix} \mathbf{X} & \mathbf{0} \\ \mathbf{0} & \mathbf{Y} \end{bmatrix} = \det(\mathbf{X}) \det(\mathbf{Y}).$$

Exercise 2.20. Prove that if $\lambda = \frac{p}{q}$ is a rational eigenvalue of a graph G then in fact λ is an integer, that is, $q = 1$. (Hint: Rational root theorem)

2.4 Cospectral graphs

In this section, we consider the question of whether it is possible to uniquely determine a graph from its spectrum. To that end, we say that two graphs G_1 and G_2 are **cospectral** if they have the same (adjacency) eigenvalues. Our first task is to show that isomorphic graphs are cospectral. It turns out, however, that there are non-isomorphic graphs with the same eigenvalues and we will supply some examples. We will then use our results from Section 2.2 to identify structural properties shared by cospectral graphs.

To show that two isomorphic graphs are cospectral, we use the fact that isomorphic graphs have **similar** adjacency matrices. Recall that two matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ are **similar** if there exists an invertible matrix $\mathbf{P}$ such that

$$\mathbf{A}_2 = \mathbf{P}^{-1}\mathbf{A}_1\mathbf{P}.$$

Similar matrices share many properties. For example:

Proposition 2.4.1

If $\mathbf{A}_1$ and $\mathbf{A}_2$ are similar then the eigenvalues of $\mathbf{A}_1$ and $\mathbf{A}_2$ are equal.

Proof. By definition, there exists an invertible matrix $\mathbf{P}$ such that $\mathbf{A}_2 = \mathbf{P}^{-1}\mathbf{A}_1\mathbf{P}$. Let $p_1(t) = \det(t\mathbf{I} - \mathbf{A}_1)$ and let $p_2(t) = \det(t\mathbf{I} - \mathbf{A}_2)$, that is, $p_i(t)$ is the characteristic polynomial of $\mathbf{A}_i$, for $i = 1, 2$. Then

$$\begin{aligned}
p_2(t) &= \det(t\mathbf{I} - \mathbf{A}_2) \\
&= \det(t\mathbf{P}^{-1}\mathbf{P} - \mathbf{P}^{-1}\mathbf{A}_1\mathbf{P}) \\
&= \det(\mathbf{P}^{-1}(t\mathbf{I} - \mathbf{A}_1)\mathbf{P}) \\
&= \det(\mathbf{P}^{-1})\det(t\mathbf{I} - \mathbf{A}_1)\det(\mathbf{P}) \\
&= \det(t\mathbf{I} - \mathbf{A}_1) \\
&= p_1(t)
\end{aligned}$$

where we used the fact that $\det(\mathbf{P}^{-1})\det(\mathbf{P}) = 1$. Hence, $p_1(t) = p_2(t)$, and therefore $\mathbf{A}_1$ and $\mathbf{A}_2$ have the same eigenvalues. $\square$

Hence, if we can show that the adjacency matrices of isomorphic graphs G_1 and G_2 are similar then G_1 and G_2 are cospectral. To do this, we study how permutations $\sigma \in S_n$ can be represented by matrices. For the permutation $\sigma \in S_n$ define the $n \times n$ matrix $\mathbf{P}$ as follows. Let $\mathbf{e}_1, \ldots, \mathbf{e}_n$ denote the standard basis vectors in $\mathbb{R}^n$ thought of as column vectors. Define the matrix $\mathbf{P}$ as

$$\mathbf{P} = \begin{bmatrix} \mathbf{e}_{\sigma(1)}^T \\ \mathbf{e}_{\sigma(2)}^T \\ \mathbf{e}_{\sigma(3)}^T \\ \vdots \\ \mathbf{e}_{\sigma(n)}^T \end{bmatrix}.$$

For example, for the permutation $\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 6 & 5 & 2 & 1 & 4 \end{pmatrix}$ the matrix $\mathbf{P}$ is

$$\mathbf{P} = \begin{bmatrix} \mathbf{e}_{\sigma(1)}^T \\ \mathbf{e}_{\sigma(2)}^T \\ \mathbf{e}_{\sigma(3)}^T \\ \mathbf{e}_{\sigma(4)}^T \\ \mathbf{e}_{\sigma(5)}^T \\ \mathbf{e}_{\sigma(6)}^T \end{bmatrix} = \begin{bmatrix} \mathbf{e}_3^T \\ \mathbf{e}_6^T \\ \mathbf{e}_5^T \\ \mathbf{e}_2^T \\ \mathbf{e}_1^T \\ \mathbf{e}_4^T \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}. \tag{2.5}$$

Notice that $\mathbf{P}$ can also be obtained by starting with the identity matrix $\mathbf{I}$ and sending column i of $\mathbf{I}$ to column $\sigma(i)$. Therefore, written out in column form we have

$$\mathbf{P} = \begin{bmatrix} \mathbf{e}_{\sigma^{-1}(1)} & \mathbf{e}_{\sigma^{-1}(2)} & \mathbf{e}_{\sigma^{-1}(3)} & \cdots & \mathbf{e}_{\sigma^{-1}(n)} \end{bmatrix}.$$

The matrix $\mathbf{P}$ is called the **permutation matrix** associated to σ. The columns of any permutation matrix $\mathbf{P}$ form an orthonormal basis of $\mathbb{R}^n$ since the columns of $\mathbf{P}$ are just the standard basis vectors of $\mathbb{R}^n$ (of course in a rearranged order). Hence, permutations matrices are **orthogonal matrices**, in other words $\mathbf{P}^T\mathbf{P} = \mathbf{P}\mathbf{P}^T = \mathbf{I}$. Hence, $\mathbf{P}^{-1} = \mathbf{P}^T$, and this implies that $\det(\mathbf{P}) = \pm 1$ for any permutation matrix $\mathbf{P}$.

We now present the linear-algebraic version of the notion of isomorphic graphs. In the following proof, we use the fact that for any $n \times n$ matrix $\mathbf{M}$, the (i,j) entry of $\mathbf{M}$ can be determined by the computation

$$\mathbf{M}_{i,j} = \mathbf{e}_i^T \mathbf{M} \mathbf{e}_j.$$

Theorem 2.4.2

Let G be a graph with adjacency matrix $\mathbf{A}$. If $\mathbf{P}$ is a permutation matrix then $\mathbf{P}^T\mathbf{A}\mathbf{P}$ is the adjacency matrix of some graph that is isomorphic to G. Conversely, for any graph H that is isomorphic to G there exists a permutation matrix $\mathbf{P}$ such that $\mathbf{P}^T\mathbf{A}\mathbf{P}$ is the adjacency matrix of H.

Proof. Let $\sigma : V \to V$ be a permutation with permutation matrix $\mathbf{P}$. Recall that we can write

$$\mathbf{P} = \begin{bmatrix} \mathbf{e}_{\sigma^{-1}(1)} & \mathbf{e}_{\sigma^{-1}(2)} & \mathbf{e}_{\sigma^{-1}(3)} & \cdots & \mathbf{e}_{\sigma^{-1}(n)} \end{bmatrix}$$

and then $\mathbf{P}\mathbf{e}_j = \mathbf{e}_{\sigma^{-1}(j)}$ for any standard basis vector $\mathbf{e}_j$. Put $\mathbf{B} = \mathbf{P}^T\mathbf{A}\mathbf{P}$ and note that $\mathbf{B}$ is symmetric because $\mathbf{B}^T = (\mathbf{P}^T\mathbf{A}\mathbf{P})^T = \mathbf{P}^T\mathbf{A}^T(\mathbf{P}^T)^T = \mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{B}$. Let $i, j \in \{1, 2, \ldots, n\}$ and let $k = \sigma(i)$ and let $\ell = \sigma(j)$. Consider the entry $\mathbf{B}_{k,\ell}$:

$$\begin{aligned} \mathbf{B}_{k,\ell} &= \mathbf{e}_k^T \mathbf{B} \mathbf{e}_\ell \\ &= \mathbf{e}_k^T \mathbf{P}^T \mathbf{A} \mathbf{P} \mathbf{e}_\ell \\ &= (\mathbf{P}\mathbf{e}_k)^T \mathbf{A} (\mathbf{P}\mathbf{e}_\ell) \\ &= \mathbf{e}_{\sigma^{-1}(k)} \mathbf{A} \mathbf{e}_{\sigma^{-1}(\ell)} \\ &= \mathbf{e}_i \mathbf{A} \mathbf{e}_j \\ &= \mathbf{A}_{i,j}. \end{aligned}$$

We have proved that $\mathbf{B}_{\sigma(i),\sigma(j)} = \mathbf{A}_{i,j}$ for all $i, j \in \{1, 2, \ldots, n\}$. This proves that all the entries of $\mathbf{B}$ are either 0 or 1 and the diagonal entries of $\mathbf{B}$ are zero since they are zero for $\mathbf{A}$. Hence, $\mathbf{B}$ is the adjacency matrix of a graph, say H. Now, since $\mathbf{B}_{\sigma(i),\sigma(j)} = \mathbf{A}_{i,j}$ then $\{i,j\}$ is an edge in G if and only if $\{\sigma(i),\sigma(j)\}$ is an edge in H. Hence, $G \cong H$ with isomorphism σ.

Conversely, let H be a graph isomorphic to G. Then there exists a permutation $\sigma : V \to V$ such that $\{i,j\}$ is an edge in G if and only if $\{\sigma(i),\sigma(j)\}$ is an edge in H. Let $\mathbf{P}$ be the permutation matrix of σ. Our computation above shows that $(\mathbf{P}^T\mathbf{A}\mathbf{P})_{\sigma(i),\sigma(j)} = \mathbf{A}_{i,j}$. Hence, the $0-1$ matrix $\mathbf{P}^T\mathbf{A}\mathbf{P}$ has a non-zero entry at $(\sigma(i),\sigma(j))$ if and only if $\mathbf{A}$ has a non-zero entry at (i,j). Hence, $\mathbf{P}^T\mathbf{A}\mathbf{P}$ is the adjacency matrix of H and the proof is complete. $\square$

Here is a rephrasing of the previous theorem.

Corollary 2.4.3

Let $\mathbf{A}_1$ and $\mathbf{A}_2$ be the adjacency matrices of two graphs G_1 and G_2 on the vertex set $V = \{1,2,\ldots,n\}$, respectively. Then G_1 and G_2 are isomorphic if and only if there exists a permutation matrix $\mathbf{P}$ such that $\mathbf{A}_2 = \mathbf{P}^T\mathbf{A}_1\mathbf{P}$.

Using Theorem 2.4.2 and the definition of an automorphism, the following is immediate.

Proposition 2.4.4

Let $G = (V,E)$ be a graph and let $\sigma : V \to V$ be a permutation with matrix representation $\mathbf{P}$. Then σ is an automorphism of G if and only if $\mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{A}$, or equivalently, $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{A}$.

Combining Corollary 2.4.3 and Proposition 2.4.1 we obtain the following.

Corollary 2.4.5: 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. For example, one can verify that the graphs $G_1 = C_4 \oplus K_1$ and $G_2 = E_4 \vee K_1$ have the same eigenvalues but are not isomorphic since G_1 is disconnected and G_2 is connected. These two graphs are the smallest non-isomorphic cospectral graphs. The smallest connected non-isomorphic cospectral graphs are shown in Figure 2.1.

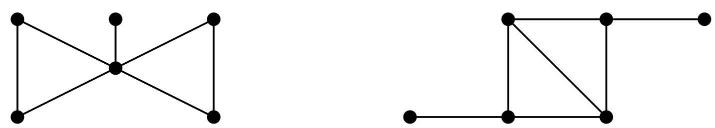


Figure 2.1: Smallest connected non-isomorphic cospectral graphs

We now investigate what graph properties can be deduced from the eigenvalues of a graph, and in particular, we will focus on the coefficients of the characteristic polynomial of a graph and some of the properties they reveal about the graph. Recall from Section 2.2 that for any polynomial $p(t)$ with roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ it holds that

$$p(t) = t^n - s_1 t^{n-1} + s_2 t^{n-2} + \cdots + (-1)^{n-1} s_{n-1} t + (-1)^n s_n \tag{2.6}$$

where $s_1, \ldots, s_n$ are the elementary symmetric polynomials evaluated $\lambda_1, \lambda_2, \ldots, \lambda_n$. From Section 2.2, the elementary symmetric polynomials $s_1, s_2, \ldots, s_n$ can be written in terms of the power sums $p_1, p_2, \ldots, p_k$, and it turns out that if $p(t)$ is the characteristic polynomial of a matrix $\mathbf{M}$ then there is a very simple relationship between the power sums $p_1, p_2, \ldots, p_n$ and the entries of $\mathbf{M}$. Consider first $p_1 = s_1$ via a 3×3 matrix:

$$\begin{aligned} p(t) = \det(t\mathbf{I} - \mathbf{M}) &= \det \begin{bmatrix} t - m_{11} & m_{12} & m_{13} \\ m_{21} & t - m_{22} & m_{23} \\ m_{31} & m_{32} & t - m_{33} \end{bmatrix} \\ &= (t - m_{11})(t - m_{22})(t - m_{33}) + g(t) \end{aligned}$$

where g is a polynomial whose degree is at most one. Expanding we obtain

$$p(t) = t^3 - (m_{11} + m_{22} + m_{33})t^2 + h(t)$$

where $h(t)$ is a polynomial whose degree is at most one. This shows that

$$p_1 = m_{11} + m_{22} + m_{33} = \operatorname{tr}(\mathbf{M}).$$

In the general $n \times n$ case, a similar argument shows that the coefficient of t^{n-1} in $p(t) = \det(t\mathbf{I} - \mathbf{M})$ is $-(m_{11} + m_{22} + \cdots + m_{nn}) = -\operatorname{tr}(\mathbf{M})$. On the other hand, if the roots of $p(t)$ are $\lambda_1, \lambda_2, \ldots, \lambda_n$ then $p_1 = s_1 = \lambda_1 + \lambda_2 + \cdots + \lambda_n$. To summarize:

Proposition 2.4.6

Suppose that the $n \times n$ matrix $\mathbf{M}$ has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then

$$\operatorname{tr}(\mathbf{M}) = \lambda_1 + \lambda_2 + \cdots + \lambda_n.$$

In other words, the trace of $\mathbf{M}$ is the sum of the eigenvalues of $\mathbf{A}$.

Alternatively, we have shown that

$$p_1 = \operatorname{tr}(\mathbf{M}).$$

We now want to relate the power sums $p_2, \ldots, p_n$ with the entries of $\mathbf{M}$ but first we need the following.

Lemma 2.4.7

If λ is an eigenvalue of $\mathbf{M}$ then λ^k is an eigenvalue of $\mathbf{M}^k$.

Proof. If $\mathbf{M}\mathbf{x} = \lambda\mathbf{x}$ then

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

By induction,

$$\mathbf{M}^{k+1}\mathbf{x} = \mathbf{M}^k(\mathbf{M}\mathbf{x}) = \mathbf{M}^k(\lambda\mathbf{x}) = \lambda\mathbf{M}^k\mathbf{x} = \lambda \cdot \lambda^k\mathbf{x} = \lambda^{k+1}\mathbf{x}.$$

Therefore, if $\mathbf{M}$ has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ then $\mathbf{M}^k$ has eigenvalues λ_1^k, λ_2^k, $\ldots, \lambda_n^k$. □

As a consequence we obtain the following.

Proposition 2.4.8

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $\mathbf{M}$ then

$$\operatorname{tr}(\mathbf{M}^k) = p_k(\lambda_1, \lambda_2, \ldots, \lambda_n) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k.$$

Proof. By Lemma 2.4.7, the eigenvalues of $\mathbf{M}^k$ are $\lambda_1^k, \lambda_2^k, \ldots, \lambda_n^k$. By Proposition 2.4.6 applied to $\mathbf{M^k}$, it holds that

$$\operatorname{tr}(\mathbf{M}^k) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k = p_k(\lambda_1, \lambda_2, \ldots, \lambda_k).$$

□

Proposition 2.4.8 is important because it relates the power sums $p_1, p_2, \ldots, p_k$ evaluated at the eigenvalues with the entries of $\mathbf{M}$ via the numbers $\operatorname{tr}(\mathbf{A}^k)$. From this we can for example prove the following.

Theorem 2.4.9

Let $\mathbf{M}$ and $\mathbf{N}$ be $n \times n$ matrices. Then $\mathbf{M}$ and $\mathbf{N}$ have the same eigenvalues if and only if $\operatorname{tr}(\mathbf{M}^k) = \operatorname{tr}(\mathbf{N}^k)$ for $1 \leq k \leq n$.

Proof. Suppose that $\mathbf{M}$ and $\mathbf{N}$ have the same eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then by Proposition 2.4.8 we have

$$\operatorname{tr}(\mathbf{M}^k) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k$$

and

$$\operatorname{tr}(\mathbf{N}^k) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k$$

and therefore $\operatorname{tr}(\mathbf{M}^k) = \operatorname{tr}(\mathbf{N}^k)$ for all $k \geq 1$. Conversely, if $\operatorname{tr}(\mathbf{M}^k) = \operatorname{tr}(\mathbf{N}^k)$ for $1 \leq k \leq n$ then by Proposition 2.2.5 the coefficients of the characteristic polynomials of $\mathbf{M}$ and $\mathbf{N}$ are equal since the coefficients of the characteristic polymials can be written in terms of $p_k = \operatorname{tr}(\mathbf{M}^k) = \operatorname{tr}(\mathbf{N}^k)$. Hence, $\mathbf{M}$ and $\mathbf{N}$ have the same characteristic polynomial and therefore the same eigenvalues. $\square$

For our purposes, Proposition 2.4.8 is the main tool to relate the spectrum of a graph with its structural properties. For example, we obtain the following.

Theorem 2.4.10: Walks and Cospectrality

Let G_1 and G_2 be graphs each with n vertices. Then G_1 and G_2 are cospectral if and only if for each $k \in \{1, 2, \ldots n\}$, the total number of closed walks in G_1 of length k equals the total number of walks in G_2 of length k.

Proof. By Theorem 2.4.9, if G_1 and G_2 have the same eigenvalues then $\operatorname{tr}(\mathbf{A}_1^k) = \operatorname{tr}(\mathbf{A}_2^k)$ for all $1 \leq k \leq n$. By Theorem 2.1.1, the number $\operatorname{tr}(\mathbf{A}_1^k)$ is the total number of closed walks of length k and the claim follows. $\square$

Example 2.14. Let $\operatorname{spec}(G) = (\lambda_1, \lambda_2, \ldots, \lambda_n)$. Suppose that $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 56$. Find the number of edges of G.

In the next theorem, we relate the first few coefficients of the characteristic polynomial of a graph with some of the structural properties of a graph. The main tool being used here is Proposition 2.4.8.

Theorem 2.4.11

Let G be a graph with characteristic polynomial

$$p(t) = t^n + c_1 t^{n-1} + c_2 t^{n-2} + \cdots + c_{n-1} t + c_n.$$

If G has m edges, t triangles, and q cycles of length four then

$$\begin{aligned} c_1 &= 0 \\ c_2 &= -m \\ c_3 &= -2t \\ c_4 &= -2q + \frac{1}{2}m(m+1) - \frac{1}{2}\sum_{i=1}^{n} \deg(v_i)^2. \end{aligned}$$

Proof. Since $\mathbf{A}$ has zeros on the diagonal then

$$c_1 = -s_1 = -\operatorname{tr}(\mathbf{A}) = 0.$$

From the Newton identities (2.4), and using $p_1 = s_1 = 0$, we have

$$c_2 = s_2 = -\frac{1}{2}(p_2 - p_1^2) = -\frac{1}{2}p_2.$$

Now $p_2 = \operatorname{tr}(\mathbf{A}^2)$ and since $\operatorname{tr}(\mathbf{A}^2) = 2m$ (Corollary 2.1.2) we conclude that

$$p_2 = \operatorname{tr}(\mathbf{A}^2) = 2m.$$

Therefore,

$$c_2 = -\frac{1}{2}p_2 = -m.$$

Now consider $c_3 = -s_3$. We have from the Newton identities that

$$s_3 = \frac{1}{6}(p_1^3 - 3p_1p_2 + 2p_3) = \frac{1}{3}p_3 = \frac{1}{3}\operatorname{tr}(\mathbf{A}^3).$$

From Corollary 2.1.2, we have $\operatorname{tr}(\mathbf{A}^3) = 6t$ and therefore $c_3 = -s_3 = -2t$ as claimed. Finally, from Newton's identities we have

$$c_4 = s_4 = -\frac{1}{4}(p_4 - s_1p_3 + s_2p_2 - s_3p_1) = -\frac{1}{4}(p_4 + s_2p_2).$$

Now from Corollary 2.1.2, we have $p_4 = 8q - 2m + 2\sum_{i=1}^{n} \deg(v_i)^2$, $p_2 = 2m$, and therefore

$$\begin{aligned}
c_4 &= -\frac{1}{4}(p_4 + s_2 p_2) \\
&= -\frac{1}{4}\left(8q - 2m + 2\sum_{i=1}^{n} \deg(v_i)^2 - 2m^2\right) \\
&= -2q + \frac{1}{2}m(m+1) - \frac{1}{2}\sum_{i=1}^{n} \deg(v_i)^2
\end{aligned}$$

as claimed. □

From Theorem 2.4.11 we now obtain a few graph characteristics that are shared by cospectral graphs. For example, if G_1 and G_2 are cospectral then they have the same characteristic polynomial. Theorem 2.4.11 then implies that G_1 and G_2 have the same number of edges and the same number of triangles.

Corollary 2.4.12

If G_1 and G_2 are cospectral then they have the same number of edges and the same number of triangles.

A natural question to ask is if the degree sequence is a property that must be shared by cospectral graphs. The answer in general is no. For example, in Figure 2.2 we display two non-isomoprhic cospectral trees with distinct degree sequences. For trees, however, the following example shows that the sum of the squares of the degrees is equal for cospectral trees.

Example 2.15. Suppose that G_1 and G_2 are graphs with at least $n \geq 5$ vertices and suppose that they have the same number of 4-cycles. Let $d(G_1) = (d_1, d_2, \ldots, d_n)$ and let $d(G_2) = (\delta_1, \delta_2, \ldots, \delta_n)$ be their respective degree sequences. If G_1 and G_2 are cospectral show that

$$\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} \delta_i^2.$$

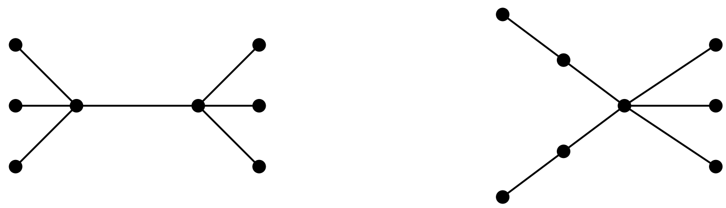


Figure 2.2: Two non-isomorphic cospectral trees with distinct degree sequences; there are many others.

Solution: If G_1 and G_2 are cospectral then their characteristic polynomials are equal, and in particular the coefficient c_4 of t^{n-4} in their characteristic polynomials are equal. Also, they must have the same number of edges. Since G_1 and G_2 have the same number of C_4's, Theorem 2.4.11 implies that $\sum_{i=1}^n d_i^2 = \sum_{i=1}^n \delta_i^2$. This example is applicable to trees since trees have no cycles.

Example 2.16. Suppose that G is a bipartite graph with spectrum $\mathrm{spec}(G) = (\lambda_1, \lambda_2, \ldots, \lambda_n)$. Prove that if k is odd then

$$p_k(\lambda_1, \lambda_2, \ldots, \lambda_n) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k = 0.$$

Solution: Let $\{X, Y\}$ be a bipartition of G. Suppose that $(w_0, w_1, \ldots, w_k)$ is a closed walk in G and without loss of generality suppose that $w_0 \in X$. Then $w_i \in Y$ for i odd and $w_j \in X$ for j even. Since $w_k = w_0 \in X$ it follows that k is necessarily even. Hence, all closed walks in G have even length. By Proposition 2.4.8, $\mathrm{tr}(\mathbf{A}^k) = p_k(\lambda_1, \ldots, \lambda_n)$ for all $k \geq 1$, and $\mathrm{tr}(\mathbf{A}^k)$ is the total number of closed walks of length k. Hence, $\mathrm{tr}(\mathbf{A}^k) = 0$ for k odd and the claim is proved.

Example 2.17. The graph G has spectrum $\mathrm{spec}(G) = (-2, 1-\sqrt{5}, 0, 0, 1+\sqrt{5})$ and degree sequence $d(G) = (4, 3, 3, 3, 3)$. Find the number of edges, triangles, and 4-cycles in G.

Example 2.18. Use Theorem 2.4.11 to find the characteristic polynomial of P_5. (Hint: P_5 is bipartite.)

2.4.1 Exercises

Exercise 2.21. Prove that if G is a k-regular graph with n vertices and $\operatorname{spec}(G) = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ then

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

Exercise 2.22. A 3-regular graph G with $n = 8$ vertices has characteristic polynomial

$$p(t) = t^8 - 12t^6 - 8t^5 + 38t^4 + 48t^3 - 12t^2 - 40t - 15.$$

Find the number of edges m, number of triangles t, and number of 4-cycles q of G.

Exercise 2.23. Two trees G_1 and G_2 have degree sequence $d(G_1) = (5, 3, 2, 2, 1, 1, 1, 1, 1, 1)$ and $d(G_2) = (3, 3, 2, 2, 2, 2, 1, 1, 1, 1)$. Could G_1 and G_2 be cospectral? Explain.

Exercise 2.24. A graph G has spectrum $\operatorname{spec}(G) = (-2, -1, 0, 0, 1, 2)$. How many closed walks of length 4 are in G? What about closed walks of length 5?

Exercise 2.25. A tree G has degree sequence $d(G) = (1, 1, 1, 2, 3)$. Find the characteristic polynomial of G. (HINT: Recall that a tree is bipartite, and recall Theorem 2.3.6.)

2.5 Bipartite Graphs

The following is a spectral characterization of bipartite graphs.

Theorem 2.5.1

Let G be a graph on n vertices. The following are equivalent.

(i) G is bipartite

(ii) λ is a non-zero eigenvalue of $\mathbf{A}$ if and only if $-\lambda$ is an eigenvalue of $\mathbf{A}$

(iii) $\sum_{i=1}^{n} \lambda_i^k = 0$ for k odd.

(iv) $\mathrm{tr}(\mathbf{A}^k) = 0$ for k odd.

Proof. Suppose that G is bipartite and let $V = V(G)$. The vertex set V can be partitioned into two disjoint parts X and Y such that any edge $e \in E(G)$ has one vertex in X and one in Y. Therefore, by an appropriate labelling of the vertices, the adjacency matrix of G takes the form

$$\mathbf{A} = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$$

where B is a $|X| \times |Y|$ matrix. Suppose that $\xi = \left[\begin{smallmatrix} \xi_1 \\ \xi_2 \end{smallmatrix}\right]$ is an eigenvector of $\mathbf{A}$ with eigenvalue $\lambda \neq 0$, where $\xi \in \mathbb{R}^{|X|}$ and $\xi_2 \in \mathbb{R}^{|Y|}$. Then $\mathbf{A}\xi = \lambda\xi$ implies that

$$\mathbf{A}\xi = \begin{bmatrix} B\xi_2 \\ B^T\xi_1 \end{bmatrix} = \lambda \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix}.$$

Consider the vector $\tilde{\xi} = \left[\begin{smallmatrix} -\xi_1 \\ \xi_2 \end{smallmatrix}\right]$. Then

$$\mathbf{A}\tilde{\xi} = \begin{bmatrix} B\xi_2 \\ -B^T\xi_1 \end{bmatrix} = \begin{bmatrix} \lambda\xi_1 \\ -\lambda\xi_2 \end{bmatrix} = -\lambda \begin{bmatrix} -\xi_1 \\ \xi_2 \end{bmatrix} = -\lambda\tilde{\xi}.$$

Hence, $\tilde{\xi}$ is an eigenvector of $\mathbf{A}$ with eigenvalue $-\lambda$. This proves (i) $\Longrightarrow$ (ii). Now assume that (ii) holds. Then there are an even number of non-zero eigenvalues, say $\pm\lambda_1, \pm\lambda_2, \ldots, \pm\lambda_r$, where $n = 2r + q$, and q is the number of zero eigenvalues. If k is odd then $\sum_{i=1}^{n} \lambda_i^k = 0$. This proves (ii) $\Longrightarrow$ (iii). Now assume that (iii) holds. Since $\mathrm{tr}(\mathbf{A}^k) = \sum_{i=1}^{n} \lambda_i^k$ it follows that $\mathrm{tr}(\mathbf{A}^k) = 0$ for k odd. This proves (iii) $\Longrightarrow$ (iv). Now assume (iv) holds. It is known that the (i, i) entry of $\mathbf{A}^k$ are the number of walks starting and ending at vertex i. Hence, the total number of cycles of length k in G is bounded by $\operatorname{tr}(\mathbf{A}^k)$. By assumption, if k is odd then $\operatorname{tr}(\mathbf{A}^k) = 0$ and thus there are no cycles of odd length in G. This implies that G is bipartite and proves (iv) $\Longrightarrow$ (i). This ends the proof. $\square$

From the previous theorem, it follows that if $\pm\lambda_1, \pm\lambda_2, \ldots, \pm\lambda_r$ are the non-zero eigenvalues of $\mathbf{A}$ and $\mathbf{A}$ has the zero eigenvalue of multiplicity $p \geq 0$ then the characteristic poly of $\mathbf{A}$ is

$$p(t) = t^p(t^2 - \lambda_1^2)(t^2 - \lambda_2^2) \cdots (t^2 - \lambda_r^2)$$

From this it follows that at least half of the coefficients $s_1, s_2, \ldots, s_n$ in the expansion of $p(t)$ are zero, namely all the odd coefficients. For example, if say $r = 3$ and $p = 1$ then

$$\begin{aligned} p(t) &= t(t^2 - \lambda_1^2)(t^2 - \lambda_2^2)(t^2 - \lambda_3^2) \\ &= t(t^6 - s_2t^4 + s_3t^2 - s_2) \\ &= t^7 - s_2t^5 + s_4t^3 - s_6t \end{aligned}$$

so that $s_1 = s_3 = s_5 = s_7 = 0$. Another way to see this is using the Newton identities.

Corollary 2.5.2

Let G be a bipartite graph on n vertices and let $p(t)$ be the characteristic polynomial of G:

$$p(t) = t^n - s_1t^{n-1} + s_2t^{n-2} + \cdots + (-1)^{n-1}s_{n-1}t + (-1)^n s_n.$$

Then $s_k = 0$ for k odd.

Proof. Using the Newton identities, we have

$$s_k = \tfrac{1}{k}(-1)^{k-1} \sum_{j=0}^{k-1} p_{k-j}s_j$$

for $1 \leq k \leq n$. If G is bipartite then $p_\ell = \mathrm{tr}(\mathbf{A}^\ell) = 0$ for all $\ell \geq 1$ odd. Let k be odd and assume by induction that $s_1, s_3, \ldots, s_{k-1}$ are all zero. Then the only terms $p_{k-j}s_j$ that survive in the expression for s_k are those where j is even. If j is even then necessarily $k-j$ is odd, and thus $p_{k-j} = 0$. Hence $s_k = 0$ as claimed. $\square$

As a consequence of Corollary 2.5.2, if G is a bipartite graph on n vertices and n is odd then then $s_n = 0$ and thus $\lambda = 0$ is an eigenvalue of $\mathbf{A}$.

Chapter 3

Graph Colorings

A university is organizing a conference on undergraduate research that will contain n student presentations. Prior to the conference, the participants selected which presentations they plan to attend and the conference organizers would like to schedule the presentations (each of the same time length) so that participants can attend all the presentations they selected and the presentation they will deliver. The university has many rooms to use for the conference and can therefore schedule presentations in parallel. The organizers would like to minimize the time for all presentations to complete. This scheduling problem can be described using a graph as follows. Let $v_1, v_2, \ldots, v_n$ be the presentations. The presentations v_i and v_j are adjacent if there is a participant who will attend both v_i and v_j. Let $\{1, 2, \ldots, k\}$ be the number of time slots during which parallel presentations will be held. The scheduling problem is then to assign to each presentation a time slot $s \in \{1, 2, \ldots, k\}$ so that adjacent presentations receive a distinct time slot.

3.1 The basics

We begin with the definition of a graph coloring.

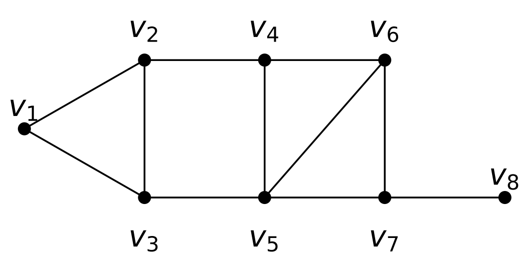
Definition 3.1.1: Colorings

Let $G = (V, E)$ be a graph and let k be a positive integer. A **k-coloring** of the graph G is a function $f : V \to \{1, 2, \ldots, k\}$ such that if v_i and v_j are adjacent then $f(v_i) \neq f(v_j)$. If G has a k-coloring then we say that G is **k-colorable**. The set of numbers $\{1, 2, \ldots, k\}$ are called the **colors** of the coloring f.

Example 3.1. For each graph, find a coloring.
(a) $G = C_4 \vee K_1$
(b) $G = P_5$
(c) G is two K_3's connected by a bridge
(d) $G = E_4$
(e) $G = K_4$

Suppose that $f : V(G) \to \{1, \ldots, k\}$ is a k-coloring of G. Let $C_i = \{v \in V \mid f(v) = i\}$ and assume $C_i \neq \emptyset$ for each $i = 1, 2, \ldots, k$. By definition, C_i consists of vertices that are colored with the same color i and we call C_i a **color class** induced by f. By definition of a coloring, any two vertices in C_i are not adjacent. In general, a non-empty subset $C \subset V(G)$ is called an **independent set** if no two vertices in C are adjacent. Hence, if $C_1, C_2, \ldots, C_k$ are the color classes induced by f then each non-empty color class C_i is an independent set. Moreover, since each vertex receives a color, $\{C_1, C_2, \ldots, C_k\}$ is a partition of the vertex set $V(G)$.

Example 3.2. Obtain a coloring of the given graph and list the color classes.



If G is k-colorable then it is also k'-colorable for any $k' \geq k$ (prove this!). Given a graph G, it is natural then to ask for the smallest integer $k \geq 1$ such that G is k-colorable. This number is given a special name.

Definition 3.1.2: Chromatic Number

The **chromatic number** of G, denoted by $\chi(G)$, is the smallest integer k such that G is k-colorable.

It is clear that if G has at least one edge then $\chi(G) \geq 2$.

Example 3.3. Prove that

$$\chi(C_n) = \begin{cases} 2, & \text{if } n \text{ is even,} \\ 3, & \text{if } n \text{ is odd.} \end{cases}$$

Solution: Label the vertices of C_n so that $E(C_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_nv_1\}$ and recall that we must have $n \geq 3$. Suppose that $n \geq 3$ is odd. Define $f : V \to \{1, 2, 3\}$ as follows: let $f(v_i) = 1$ if $i < n$ is odd, let $f(v_j) = 2$ if j is even, and let $f(v_n) = 3$. Then $f : V(C_n) \to \{1, 2, 3\}$ is a coloring. Suppose by contradiction that $\tilde{f} : V \to \{1, 2\}$ is a coloring of C_n. We can assume without loss of generality that $\tilde{f}(v_1) = 1$. Then $\tilde{f}(v_j) = 2$ if j is even. Since $v_n \sim v_{n-1}$, and $n - 1$ is even, we must have $\tilde{f}(v_n) = 1$. However, $v_n \sim v_1$ and thus $\tilde{f}$ is not a coloring. Hence, $\chi(C_n) = 3$ if n is odd.

Now suppose that $n \geq 3$ is even. Then $f : V \to \{1, 2\}$ define by $f(v_i) = 1$ if i is odd and $f(v_j) = 2$ if j is even is a coloring. Hence, $\chi(C_n) \leq 2$ and thus $\chi(G) = 2$ since C_n is not the empty graph.

Example 3.4. Compute the chromatic numbers of the wheels $W_5 = C_5 \vee K_1$ and $W_6 = C_6 \vee K_1$. What about $W_n = C_n \vee K_1$ for any $n \geq 3$?

Example 3.5. Prove that $\chi(G_1 \oplus G_2 \oplus \cdots \oplus G_r) = \max\{\chi(G_1), \chi(G_2), \ldots, \chi(G_r)\}$.

Example 3.6. Prove that if $\chi(G) = n$ then $G = K_n$.

3.2 Bounds on the chromatic number

Given a graph G with n vertices, we may color each vertex with a distinct color and obtain a n-coloring. This shows that $\chi(G) \leq n$. It is clear that a coloring of K_n must have at least n colors and thus $\chi(K_n) = n$. On the other hand, the empty graph E_n can be colored (properly) with only one color and thus $\chi(E_n) = 1$. However, if G has at least one edge then $2 \leq \chi(G)$. We therefore have the following.

Proposition 3.2.1

For any graph G not equal to K_n or E_n, we have that $2 \leq \chi(G) \leq n - 1$.

A lower bound on $\chi(G)$ is obtained through the notion of a clique and clique number of a graph.

Definition 3.2.2: Cliques

A subset $W \subset V(G)$ is called a **clique** if all vertices in W are mutually adjacent. In other words, W is a clique if and only if $G[W]$ is a complete graph. The **clique number** of a graph G is the cardinality of a largest clique in G, and is denoted by $\omega(G)$.

Example 3.7. What is the clique number of a cycle? More generally, of a bipartite graph?

If W is a clique in G then any coloring of G must assign distinct colors to vertices in W, and thus any coloring of G must contain at least $\omega(G)$ colors. We therefore obtain the following.

Theorem 3.2.3

For any graph G we have $\omega(G) \leq \chi(G)$.

Example 3.8. As an example of a graph for which $\omega(G) < \chi(G)$, take a cycle C_n of odd length. In Example 3.3 we showed that $\chi(C_n) = 3$ if n is odd; on the other hand $\omega(C_n) = 2$ for all $n \geq 3$.

Recall that $C \subset V(G)$ is an independent set if no two vertices in C are adjacent. The **independence number** of G, denoted by $\alpha(G)$, is the cardinality of a largest independent set in G.

Example 3.9. Prove that $\omega(\overline{G}) = \alpha(G)$.

Solution: Let C be an independent set with cardinality $\alpha(G)$. Then C is a clique in $\overline{G}$ and therefore $\alpha(G) \leq \omega(\overline{G})$. Conversely, suppose that W is a largest clique in $\overline{G}$. Then W is an independent in G. Therefore, $\omega(\overline{G}) \leq \alpha(G)$. This proves the claim. □

Suppose that $\{C_1, C_2, \ldots, C_k\}$ are the color classes of a k-coloring in G. Then $|C_i| \leq \alpha(G)$ for all $i = 1, 2, \ldots, k$. It follows that

$$n = \sum_{i=1}^{k} |C_i| \leq \sum_{i=1}^{k} \alpha(G) = k\alpha(G).$$

We may take $k = \chi(G)$ and therefore

$$n \leq \chi(G)\alpha(G).$$

Suppose now that C is a largest independent set in $V(G)$, and thus $|C| = \alpha(G)$. Color all vertices in C with color 1. The remaining $n - \alpha(G)$ vertices may be colored with distinct colors, say $\{2, \ldots, n - \alpha(G)\}$. This produces a $k = n - \alpha(G) + 1$ coloring of G. Therefore,

$$\chi(G) \leq n - \alpha(G) + 1.$$

To summarize:

Theorem 3.2.4

For every graph G it holds that

$$\frac{n}{\alpha(G)} \leq \chi(G) \leq n - \alpha(G) + 1$$

We now describe a greedy algorithm that always produces a coloring. Let $v_1, v_2, \ldots, v_n$ be an ordering of the vertices of G. For each vertex v_i, let $n_i \geq 0$ be the number of vertices adjacent to v_i that are lower in the order, that is, $\nu_i = |\{v_j \,|\, j < i,\ v_i v_j \in E(G)\}|$. It is clear that $\mu_i \leq \Delta(G)$ and thus $\mu = \max_{1 \leq i \leq n} \mu_i \leq \Delta(G)$. Hence, for each vertex v_i, the number of neighbors of v_i that are lower in the order is at most $\mu \geq 0$.

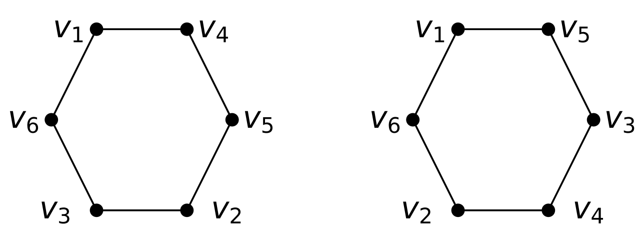
Theorem 3.2.5: Greedy Colorings

With the notation above, it holds that $\chi(G) \leq \mu + 1$. In particular, $\chi(G) \leq \Delta(G) + 1$.

Proof. Consider the set of colors $\{1, \ldots, \mu + 1\}$. Color v_1 with the color 1. Suppose that $v_1, \ldots, v_i$ have been colored so that no adjacent vertices received the same color. Now consider v_{i+1}. The number of vertices adjacent to v_{i+1} that have already been colored is at most μ. Hence, we can color v_{i+1} with $\mu + 1$ or with a lower color and thereby produce a proper coloring of the vertices $v_1, \ldots, v_{i+1}$. By induction, this proves that G can be colored with at most $\mu + 1$ colors. □

The following example shows that the number of colors needed in the greedy algorithm depends on the chosen ordering of the vertices.

Example 3.10. Consider the cycle C_6 with vertices labelled in two different ways as shown below. Apply the greedy coloring algorithm in each case.



Example 3.11. Verify that if G is a complete graph or a cycle with an odd number vertices then the inequality in Theorem 3.2.5 is an equality when $\mu = \Delta(G)$.

I turns out that complete graphs and cycles of odd length are the only graphs for which equality holds in Theorem 3.2.5. This is known as Brook's theorem.

Theorem 3.2.6: Brook's Theorem

If G is a connected graph that is neither a complete graph or an odd cycle then $\chi(G) \leq \Delta(G)$.

Example 3.12 (Greedy algorithm producing chromatic coloring)**.** In this exercise, we are going to prove that there is a labelling of the vertices of G so that the greedy algorithm uses exactly $k = \chi(G)$ colors. Suppose that $C_1, C_2, \ldots, C_k$ are the color classes of **some** chromatic coloring of G and let $m_i = |C_i|$ for $i = 1, 2 \ldots, k$. Label the vertices of G so that the first m_1 vertices are in C_1, the next m_2 vertices are in C_2, and repeatedly until the last m_k vertices are in C_k. Explicitly, $C_1 = \{v_1, v_2, \ldots, v_{m_1}\}$, $C_2 = \{v_{m_1+1}, v_{m_1+2}, \ldots, v_{m_1+m_2}\}$, until finally $C_k = \{v_{n-m_k+1}, v_{n-m_k+2}, \ldots, v_n\}$. Since C_1 is an independent set, we can color all vertices in C_1 with color 1. Now consider the vertices in C_2. If $v \in C_2$ is adjacent to a vertex in C_1 then we must color v with color 2, otherwise we can color v with color 1. Since C_2 is an independent set, after this re-coloring the vertices in C_2 receiving the same color are not adjacent. Now consider the vertices in C_3. For $v \in C_3$, we can choose one of the colors $\{1, 2, 3\}$ to color v; for example, if v is not adjacent to any vertex in C_1 then color v with color 1, if v is not adjacent to any vertex in C_2 then color v with color 2; otherwise we need to color v with 3. Since C_3 is an independent set, the vertices in C_3 receiving the same color are not adjacent. By induction, suppose that we have colored all vertices up to and including C_{j-1}. Any vertex in $v \in C_j$ is adjacent to at most $j-1$ colored vertices, all of which have been colored with one of $1, 2, \ldots, j-1$. Hence, to color $v \in C_j$ we can choose the smallest available color from $\{1, 2, \ldots, j\}$. This proves that the greedy algorithm uses at most k colors. Since $k = \chi(G)$, the greedy algorithm uses exactly k colors. We note that, in general, the new coloring will produce distinct color classes.

As an example, consider the chromatic 4-coloring of the graph G in Figure 3.1. The coloring is indeed chromatic since $\chi(G) = \omega(G) = 4$. The

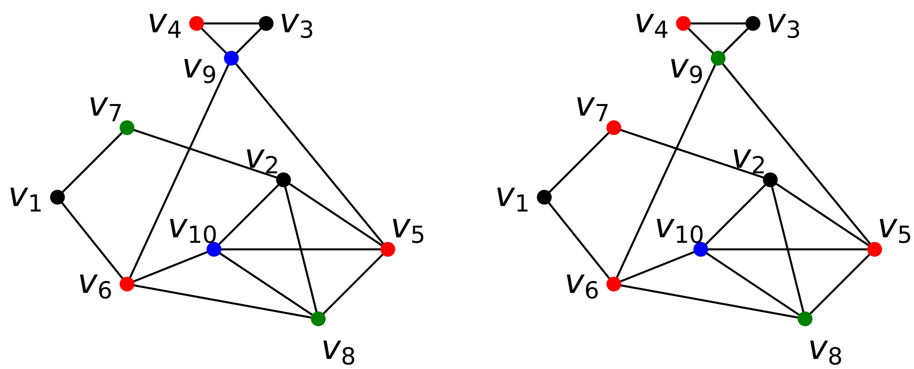


Figure 3.1: A labelling of G from a chromatic coloring for which the greedy algorithm produces a (new) chromatic coloring

color classes are $C_1 = \{v_1, v_2, v_3\}$, $C_2 = \{v_4, v_5, v_6\}$, $C_3 = \{v_7, v_8\}$, and $C_4 = \{v_9, v_{10}\}$. Starting with the labelling shown in Figure 3.1, and performing the greedy algorithm, we obtain a new coloring with color classes $\widetilde{C}_1 = \{v_1, v_2, v_3\}$, $\widetilde{C}_2 = \{v_4, v_5, v_6, v_7\}$, $\widetilde{C}_3 = \{v_8, v_9\}$, and $\widetilde{C}_4 = \{v_{10}\}$. Note that this produces a distinct chromatic coloring of G.

Example 3.13. Let G be a k-chromatic graph, that is, $k = \chi(G)$. Show that in every k-coloring of G, there exists at least one vertex in each color class that is adjacent to at least one vertex in each of the other color classes. Deduce that G has at least k vertices with degree at least $k - 1$.

Solution: Let $C_1, C_2, \ldots, C_k$ be the color classes of a k-chromatic coloring of G. Suppose by contradiction that some color class C_i contains no vertex that is adjacent to at least one vertex in each of the other classes. We can assume without loss of generality that this color class is C_k. We will re-color the vertices in C_k to produce a $(k-1)$ coloring as follows. Since each $v \in C_k$ is non-adjacent to at least one of the other color classes, there is a color available in $\{1, 2, \ldots, k-1\}$ to re-color $v \in C_k$. Hence, this re-coloring of G produces a $(k-1)$ coloring which is a contradiction since $k = \chi(G)$. Thus, every color class has at least one vertex adjacent to the other color classes. This clearly implies the existence of k vertices with degree at least $k - 1$. $\square$

The following theorem gives in many cases a better upper bound than Brook's theorem [4].

Theorem 3.2.7

Let G be a graph and let $\lambda_{\max}$ denote the largest eigenvalue of the adjacency matrix of G. Then $\chi(G) \leq 1 + \lambda_{\max}$. Moreover, equality holds if and only if G is a complete graph or an odd cycle.

If G has a large clique then $\chi(G)$ is also large since $\omega(G) \leq \chi(G)$. In every non-trivial clique (i.e., a clique containing at least 3 vertices), there is a triangle. Hence, if G has no triangles then $\omega(G) = 2$, and thus it is reasonable to investigate whether graphs with no triangles have small $\chi(G)$. Surprisingly, this is not the case.

Theorem 3.2.8: Mycielski 1955

For any $k \geq 1$, there exists a k-chromatic graph with no triangles.

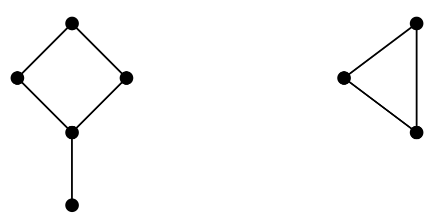
Proof. The proof is by induction on $k \geq 1$. If $k = 1$ then K_1 is a triangle-free k-chromatic graph and when $k = 2$ then K_2 is a triangle-free k-chromatic graph. Assume that G_k is a triangle-free k chromatic graph and let $v_1, v_2, \ldots, v_n$ be the vertices of G_k. Add new vertices $u_1, u_2, \ldots, u_n$ and v, and connect u_i to v and also to the neighbors of v_i, for $i = 1, 2, \ldots, n$. Denote the resulting graph by G_{k+1}. Any k-coloring of G_k can be extended to a $(k+1)$-coloring of G_{k+1} by coloring u_i with the same color as v_i, for $i = 1, 2, \ldots, n$, and coloring v with $k+1$. Hence, $\chi(G_{k+1}) \leq k+1$. Assume that G_{k+1} is k-colorable and suppose without loss of generality that v is colored with k. Then no vertex u_i is colored with k. If v_j is colored with k then recolor it with the same color as u_j. Since no vertex u_i is colored with k, this produces a $(k-1)$-coloring of G_k, which is a contradiction. Hence, $\chi(G_{k+1}) = k+1$. We now prove G_{k+1} is triangle-free. Since $\{u_1, u_2, \ldots, u_n\}$ is an independent set in G_{k+1} and no vertex v_i is adjacent to v, any triangle in G_{k+1} (if any) must consist of two vertices v_i and v_j and one vertex u_k. But if v_i, v_j, u_k are the vertices of a triangle in G_{k+1} then $v_i \sim u_k$ and $v_j \sim u_k$ implies that $v_i \sim v_k$ and $v_j \sim v_k$ and thus v_i, v_j, v_k are the vertices of a triangle in G_k, which is a contradiction. Hence, G_{k+1} is triangle-free and the proof is complete. $\square$

The punchline of Theorem 3.2.8 is that the chromatic number can get arbitrarily high even if we limit in the strongest way the size of the largest clique.

3.3 The Chromatic Polynomial

For each non-negative integer $k \geq 0$ let $P_G(k)$ be the number of distinct k-colorings of G. The function P_G was introduced by **George Birkhoff** (1912) in his quest to prove the Four Color Theorem for planar graphs. Let us clarify what we mean by "distinct colorings". Recall that a k-coloring of G is a function $f : V(G) \to \{1, \ldots, k\}$. Hence, f_1 and f_2 are two distinct k-colorings if $f_1(v) \neq f_2(v)$ for at least one vertex $v \in V(G)$, that is, at least one vertex of G is colored differently in the colorings f_1 and f_2. Before we proceed we note that if G has at least one vertex then $P_G(0) = 0$ since there is no way to color the vertices of a graph with $k = 0$ colors.

Example 3.14. For each graph shown below, produce two distinct colorings using $k = 2$ and $k = 3$ colorings, respectively.



Let us prove that P_G is an invariant.

Theorem 3.3.1

If G_1 and G_2 are isomorphic graphs then $P_{G_1}(k) = P_{G_2}(k)$ for every integer $k \geq 0$.

Proof. This is left as an important exercise. □

Consider the empty graph $G = E_n$ and let $k \geq 1$. We can color vertex v_1 with any of the colors $\{1, 2, \ldots, k\}$, we can color v_2 with any of the colors $\{1, 2, \ldots, k\}$, etc. Any such k-coloring is and thus the number of k-colorings of $G = E_n$ is $P_G(k) = k^n$.

Now consider the other extreme, i.e., consider $G = K_n$. If $k < n$ then there are no k-colorings of G, and thus $P_G(k) = 0$ for $k < n$. Suppose then that $k \geq n$. We start by coloring v_1 by choosing any of the k colors. Then we have $(k-1)$ color choices to color v_2, then $(k-2)$ color choices to color v_3, and inductively we have $(k-(n-1))$ color choices for v_n. Hence, the number of k-colorings of K_n is

$$P_{K_n}(k) = k(k-1)(k-2)\ldots(k-(n-1)).$$

Notice that our formula for $P_{K_n}(k)$ is a polynomial function in k, as was for $P_{E_n}(k) = k^n$. Now, the polynomial expression we obtained for $P_{K_n}(k)$ has the property that $P_{k_n}(x) = 0$ if $x \in \{0, 1, \ldots, n-1\}$ which is exactly the statement that there are no colorings of K_n using less than n colors. If for example $k = n$ then we obtain

$$P_{K_n}(n) = n(n-1)(n-2)\ldots 1 = n!$$

Proposition 3.3.2

For any graph G it holds that

$$\chi(G) = \min\{k \in \{0, 1, \ldots, n\} \mid P_G(k) > 0\}.$$

Equivalently, $P_G(k) > 0$ if and only if $k \geq \chi(G)$.

Proof. If $P_G(k) > 0$ then there is a k-coloring of G and thus by definition of $\chi(G)$ we have $\chi(G) \leq k$. If on the other hand $k \geq \chi(G)$ then since we can color G with $\chi(G)$ colors then we can certainly color G with k colors and thus $P_G(k) > 0$. By definition of $\chi(G)$, if $k < \chi(G)$ then there are no k-colorings of G and thus $P_G(k) = 0$. □

Directly finding $P_G(k)$ for anything other than $G = K_n$ or $G = E_n$ as we did above quickly becomes a non-trivial exercise. There is, as we describe below, a recursive reductive approach to compute $P_G(k)$. Before we state the relevant theorem, we need some notation. If e is an edge recall that $G - e$ is the graph obtained by deleting the edge e. We define the graph G/e as the graph obtained by removing the edge e, identifying the end-vertices of e, and eliminating any multiple edges.

Example 3.15. Draw any graph G, pick an edge e, and draw G/e.

Theorem 3.3.3: Chromatic Reduction

For any graph G and $e \in E(G)$ it holds that

$$P_G(k) = P_{G-e}(k) - P_{G/e}(k).$$

Proof. We consider the number of colorings of $G - e$. We partition the of colorings of $G - e$ into two types. The first are the colorings in which the end-vertices of e are colored differently. Each such coloring is clearly a coloring of G. Hence, there are $P_G(k)$ such colorings. The second are the colorings in which the end-vertices of e are colored the same. Each such coloring is clearly a coloring of G/e. The number of such colorings is $P_{G/e}(k)$. Hence, the total number of colorings of $G - e$ is

$$P_{G-e}(k) = P_G(k) + P_{G/e}(k)$$

and the claim follows. □

The upshot of the reduction formula

$$P_G(k) = P_{G-e}(k) - P_{G/e}(k)$$

is that $P_{G/e}$ has one less vertex and edge than G and $G-e$ has one less edge and might have more components than G. Regarding the latter case, the following will be useful.

Proposition 3.3.4: Colorings of Unions

If $G = G_1 \oplus G_2$ then

$$P_G(k) = P_{G_1}(k)P_{G_2}(k).$$

Proof. By definition, $V(G_1 \oplus G_2) = V(G_1) \cup V(G_2)$. The number of ways to properly color the vertices in $V(G_1)$ is $P_{G_1}(k)$ and the number of ways to properly color the vertices in $V(G_2)$ is $P_{G_2}(k)$. Since both colorings can be done independently, the result follows. □

Example 3.16. Find the chromatic polynomials of the graphs shown in Figure 3.2.

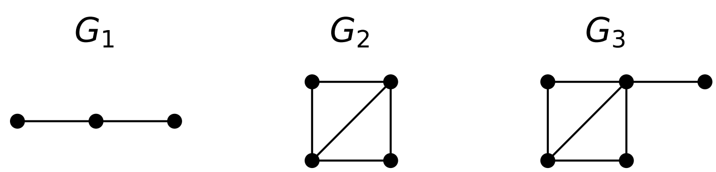


Figure 3.2: Graphs for Example 3.16

We now prove some basic properties of the function $P_G(k)$.

Theorem 3.3.5: Chromatic Polynomial

Let G be a graph of order n. The function $P_G(k)$ is a monic polynomial of degree n with integer coefficients.

Proof. We induct over the number of edges. If G has no edges then $G = E_n$ and we showed above that $P_G(k) = k^n$. This proves the base case. Now suppose the claim holds for all graphs with no more than $m \geq 0$ edges and let G be a graph with $m+1$ edges and n vertices. Pick any edge $e \in E(G)$. By the chromatic reduction theorem, $P_G(k) = P_{G-e}(k) - P_{G/e}(k)$. The graph $G - e$ contains m edges and n vertices, and G/e has $n-1$ vertices and no more than m edges. By induction, $P_{G-e}(k)$ is a monic polynomial of degree n with integer coefficients and $P_{G/e}(k)$ is a monic polynomial of degree $n-1$ with integer coefficients. Hence, $P_G(k)$ is a monic polynomial of degree n with integer coefficients. □

Based on the result of Theorem 3.3.5, we call $P_G(k)$ the **chromatic polynomial** of the graph G.

Lemma 3.3.6: Alternating Coefficients

For any graph G, the chromatic polynomial $P_G(k)$ can be written in the form

$$P_G(k) = k^n - a_1k^{n-1} + a_2k^{n-2} - a_3k^{n-3} + \cdots + (-1)^{n-1}a_{n-1}k$$

where $a_j \geq 0$.

Proof. We induct over the number of edges. If G is the empty graph then $P_G(k) = k^n$ clearly satisfies the claim. Suppose the claim is true for all graphs with no more than $m \geq 0$ edges and let G be a graph with $m+1$ edges and n vertices. By induction, we may write that

$$P_{G-e}(k) = k^n + \sum_{j=1}^{n-1}(-1)^j a_j k^{n-j}$$

where $a_j \geq 0$ and

$$P_{G/e}(k) = k^{n-1} + \sum_{j=2}^{n-1}(-1)^{j+1} b_j k^{n-j}$$

where $b_j \geq 0$. Then

$$\begin{aligned}
P_G(k) &= P_{G-e}(k) - P_{G/e}(k) \\
&= k^n + \sum_{j=1}^{n-1}(-1)^j a_j k^{n-j} - k^{n-1} + \sum_{j=2}^{n-1}(-1)^j b_j x^{n-j} \\
&= k^n - (a_1+1)k^{n-1} + \sum_{j=2}^{n-1}(-1)^j (a_j + b_j) k^{n-j}
\end{aligned}$$

and this proves the claim. □

We now prove an important property about the coefficients of $P_G(k)$ when G is connected but first we need the following lemma.

Lemma 3.3.7

Suppose that G contains $n \geq 2$ vertices. If G is connected then G/e is connected for any $e \in E(G)$.

Proof. The proof is left as an exercise. □

Theorem 3.3.8

If G is connected then the coefficients of $k, k^2, \ldots, k^n$ in $P_G(k)$ are all non-zero.

Proof. The proof is by induction on the number of edges. If $m = 1$ then $G = P_2$ and it is not hard to see that $P_G(k) = k(k-1) = k^2 - k$. Hence, the claim holds for $m = 1$. Assume that the claim holds for all connected graphs with at most $m \geq 1$ edges and let G be a graph with $m+1$ edges and n vertices. If $e \in E(G)$ then G/e has at most m edges and thus by induction the coefficients of $k, k^2, \ldots, k^{n-2}$ in $P_{G/e}(k)$ are non-zero. Using the notation in the proof of

Lemma 3.3.6, we may write that $P_{G/e}(k) = k^{n-1} + \sum_{j=2}^{n-1}(-1)^{j+1}b_j k^{n-j}$ where $b_j > 0$. Again, using the notation in the proof of Lemma 3.3.6 we may write

$$P_G(k) = k^n - (a_1 + 1)k^{n-1} + \sum_{j=2}^{n-1}(-1)^j(a_j + b_j)k^{n-j}$$

where $a_j \geq 0$. This proves that the coefficients of $k, k^2 \ldots, k^{n-1}$ in $P_G(k)$ are all non-zero. $\square$

We now consider the case of disconnected graphs.

Theorem 3.3.9

If $G = G_1 \oplus G_2 \oplus \cdots \oplus G_r$ and G has n vertices then

$$P_G(k) = k^n - a_1 k^{n-1} + a_2 k^{n-2} - \cdots + (-1)^{n-r}a_{n-r}k^r.$$

Moreover, $a_j > 0$ for all $j = 1, \ldots, n - r$.

Proof. By Proposition 3.3.4 we have

$$P_G(k) = P_{G_1}(k)P_{G_2}(k)\cdots P_{G_r}(k)$$

Since each $P_{G_i}(k)$ has no constant term, the smallest possible non-zero term in $P_G(k)$ is k^r. By Theorem 3.3.8, the coefficient of k in each of $P_{G_i}(k)$ is non-zero. The coefficient of k^r in $P_G(k)$ is the product of the coefficients of k in $P_{G_i}(k)$ for $i = 1, 2, \ldots, r$. Hence, the coefficient of k^r in $P_G(k)$ is non-zero.

We now prove that each $a_j > 0$ for $j = 1, 2, \ldots, n - r$. The proof is by induction on the number of vertices. The case $n = 1$ is trivial. Assume that the claim holds for all graphs with at most $n \geq 1$ vertices and let G be a graph with $n + 1$ vertices and r components $G_1, G_2, \ldots, G_r$. Then G/e is a graph with n vertices and r components and $G - e$ is a graph with $n + 1$ vertices and at least r components. We may therefore write that $P_{G-e}(k) = k^{n+1} + \sum_{j=1}^{n+1-r}(-1)^j a_j k^{n+1-j}$ where $a_j \geq 0$ and by induction

$P_{G/e}(k) = k^n + \sum_{j=1}^{n-r}(-1)^j b_j k^{n-j}$ where $b_j > 0$. Therefore,

$$P_G(k) = k^{n+1} - (a_1+1)k^n + \sum_{j=1}^{n-r}(-1)^j(a_{j+1}+b_j)k^{n-j}$$

and since $a_1 + 1 > 0$ and $a_{j+1} + b_j > 0$ for $j = 1, \ldots, n-r$ this proves the claim. □

We now discuss some of the properties of the roots of a chromatic polynomial. Let $\chi = \chi(G)$ and suppose that k is a non-negative inter. If $0 \leq k < \chi$ then there are no colorings k-colorings and therefore $P_G(k) = 0$. Thus, there exists integers $m_j \geq 1$, for $j = 0, 1, \ldots, \chi - 1$, and a polynomial $f(z)$ not having $0, 1, \ldots, \chi - 1$ as roots such that

$$P_G(z) = z^{m_0}(z-1)^{m_1}\cdots(z-(\chi-1))^{m_{\chi-1}}f(z).$$

If $k \geq \chi$ then $P_G(k) > 0$ and therefore $f(k) > 0$. Thus, f has no non-negative integer roots. Any negative integer roots of P_G would therefore be supplied entirely by f. However, the following shows that will not happen.

Theorem 3.3.10: Non-Negative Roots

The chromatic polynomial of any graph does not contain any roots in $(-\infty, 0)$.

Proof. By Proposition 3.3.4, we can sssume that G is connected. Thus

$$P_G(x) = x^n + \sum_{j=1}^{n-1}(-1)^j a_j x^{n-j}$$

where $a_j > 0$ (by Theorem 3.3.8). Suppose that $-\lambda \in (-\infty, 0)$ and thus

$\lambda > 0$. Then

$$P_G(-\lambda) = (-1)^n\lambda^n + \sum_{j=1}^{n-1}(-1)^j a_j(-1)^{n-j}\lambda^{n-j}$$

$$= (-1)^n\left(\lambda^n + \sum_{j=1}^{n-1} a_j\lambda^{n-j}\right).$$

Since $\lambda > 0$ and $a_j > 0$ for all $j = 1, \ldots, n-1$, it follows that $P_G(-\lambda) \neq 0$. □

Many graphs, however, have chromatic polynomials with complex roots.

Example 3.17. The chromatic polynomial of the graph in Figure 3.3 is $P_G(x) = x(x-1)(x-2)(x^2-4x+5)$ which has complex roots $2 \pm i$.

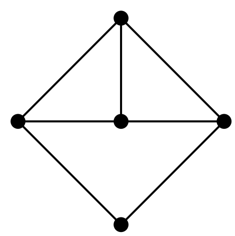


Figure 3.3: Graph with complex chromatic roots

Proposition 3.3.11

For any graph G of order n and m edges, the coefficient of k^{n-1} in $P_G(k)$ is $-m$.

Proof. The proof is by induction on the number of edges. If G has $m = 1$ edges and n vertices then G is the union of P_2 and E_{n-2}. Therefore,

$$P_G(k) = P_{P_2}(k)P_{E_{n-2}}(k) = k(k-1)k^{n-2} = k^{n-1}(k-1) = k^n - k^{n-1}$$

and the claim follows. Assume that the claim holds for all graphs with at most $m \geq 1$ edges and suppose that G has $(m+1)$ edges and n vertices. By the proof of Lemma 3.3.6, we have

$$P_G(k) = k^n - (a_1+1)k^{n-1} + \sum_{j=2}^{n-1} (-1)^j k^{n-j}.$$

where $P_{G-e}(k) = k^n - a_1 k^{n-1} + \cdots + (-1)^{n-1} a_{n-1} k$. By induction $a_1 = m$ and the claim holds. □

Theorem 3.3.12: Chromatic Polynomial of a Tree

A graph G with n vertices is a tree if and only if

$$P_G(k) = k(k-1)^{n-1}.$$

Proof. We first prove that if G is a tree on n vertices then $P_G(k) = k(k-1)^{n-1}$. The proof is by induction on $n \geq 2$. If $G = P_2$ then $P_G(k) = k(k-1)$ and the claim follows. Assume by induction that the claim holds for all trees with at most $n \geq 2$ vertices and let G be a tree with $n+1$ vertices. Since G is a tree, it has a leaf u whose neighbor is say v. Let $e = \{u, v\}$. By the chromatic reduction theorem, $P_G(k) = P_{G-e}(k) - P_{G/e}(k)$. The graph G/e is a tree with n vertices and thus $P_{G/e}(k) = k(k-1)^{n-1}$. On the other hand, $G - e$ is the union of a tree on n vertices and K_1. Thus, by induction we have $P_{G-e} = k(k-1)^{n-1}k = k^2(k-1)^{n-1}$. Therefore,

$$P_G(k) = k^2(k-1)^{n-1} - k(k-1)^{n-1} = k(k-1)^{n-1}(k-1) = k(k-1)^n$$

and the claim follows.

Now suppose that G has n vertices and $P_G(k) = k(k-1)^{n-1}$. Expanding we obtain

$$P_G(k) = k(k^{n-1} - (n-1)k^{n-2} + \cdots + (-1)^{n-1}) = k^n - (n-1)k^{n-1} + \cdots + (-1)^{n-1}k$$

and thus by Propositon 3.3.11 we have $|E(G)| = n - 1$. Since the coefficient of k in $P_G(k)$ is non-zero, by Theorem 3.3.9 it follows that G is connected. Hence, G is a tree. □

Example 3.18 (**Chromatic polynomial of cycle graph**). Use the chromatic reduction theorem to prove that the chromatic polynomial of a cycle $G = C_n$ is

$$P_G(k) = (k-1)^n + (-1)^n(k-1)$$

Solution: For $n = 3$ we have

$$\begin{aligned}
P_G(k) &= k(k-1)(k-2) \\
&= (k-1+1)(k-1)(k-1-1) \\
&= (k-1+1)(k-1)^2 - (k-1+1)(k-1) \\
&= (k-1)^3 + (k-1)^2 - (k-1)^2 - (k-1)
\end{aligned}$$

and thus $P_G(k) = (k-1)^3 + (-1)^3(k-1)$ as claimed. Assume that the claim holds for n and consider $G = C_{n+1}$. For any $e \in E(C_{n+1})$ we have that $C_{n+1} - e$ is P_{n+1} and C_{n+1}/e is C_n. Using the chromatic reduction theorem, the induction hypothesis, and the fact that P_{n+1} is a tree we obtain

$$\begin{aligned}
P_G(k) &= k(k-1)^n - [(k-1)^n + (-1)^n(k-1)] \\
&= k(k-1)^n - (k-1)^n + (-1)^{n+1}(k-1) \\
&= (k-1)^{n+1} + (-1)^{n+1}(k-1)
\end{aligned}$$

and this completes the proof.

Example 3.19. Show that $P_{G\vee K_1}(k) = kP_G(k-1)$. Use this to find the chromatic polynomial of the wheel graph $W_n = C_n \vee K_1$.

3.3.1 Exercises

Exercise 3.1. In this question you are going to prove that the chromatic polynomial is an isomorphism invariant.

(a) Suppose that G_1 and G_2 are isomorphic and $\sigma : V(G_1) \to V(G_2)$ is an isomorphism. Suppose that $f : V(G_1) \to \{1, \ldots, k\}$ is a coloring of G_1. Define the function $f_\sigma : V(G_2) \to \{1, \ldots, k\}$ by $f_\sigma(u) = f(\sigma^{-1}(u))$. Prove that f_σ is a coloring of G_2.

(b) Deduce from part (a) that $P_{G_1}(k) \leq P_{G_2}(k)$.

(c) Now explain why $P_{G_2}(k) \leq P_{G_1}(k)$.

(d) Conclude.

Exercise 3.2. Let $C_1, C_2, \ldots, C_k$ be the color classes of a coloring of G. We will say that C_i is adjacent to C_j if there exists $v_i \in C_i$ and $v_j \in C_j$ such that $v_i \sim v_j$.

(a) Give an example of a connected graph and a coloring of that graph that produces color classes $C_1, C_2, \ldots, C_k$ for which there exists some C_i and C_j (distinct) that are not adjacent.

(b) Prove that if $C_1, C_2, \ldots, C_k$ are the color classes of a **chromatic** coloring of a graph G (that is, $k = \chi(G)$) then C_i is adjacent C_j for every distinct color classes C_i and C_j.

(c) Deduce from part (b) that the number of edges in a graph G is at least $\binom{\chi(G)}{2}$.

Exercise 3.3. Provide a proof of Lemma 3.3.7, that is, prove that if G is connected then G/e is connected for any $e \in E(G)$.

Exercise 3.4. Find $P_G(x)$ if $G = P_2 \vee E_3$. (Hint: G is planar so draw it that way.)

Exercise 3.5. Explain why $P(x) = x^6 - 12x^5 + 53x^4 - 106x^3 + 96x^2 - 32x$ is not the chromatic polynomial of any graph G. (Hint: WolframAlpha)

Exercise 3.6. For any graph G, let $t(G)$ be the number of triangles in G. If $P_G(k) = k^n + \sum_{j=1}^{n-1}(-1)^j a_j k^{n-j}$ prove that

$$a_2 = \binom{m}{2} - t(G)$$

where $m = |E(G)|$. (Hint: Induct over the number of edges $m \geq 2$ and use the Chromatic Reduction theorem. You will also need Proposition 3.3.11.)

Chapter 4

Laplacian Matrices

4.1 The Laplacian and Signless Laplacian Matrices

We first define the incidence matrix of a graph.

Definition 4.1.1: Incidence Matrix

Let $G = (V, E)$ be a graph where $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. The **incidence matrix** of G is the $n \times m$ matrix $\mathbf{M}$ such that

$$\mathbf{M}(i,j) = \begin{cases} 1, & \text{if } v_i \in e_j \\ 0, & \text{otherwise.} \end{cases}$$

Hence, the rows of $\mathbf{M}$ are indexed by the vertices of G and the columns of $\mathbf{M}$ are indexed by the edges of G. The only non-zero entries of column $\mathbf{M}(:,j)$ (there are only two non-zero entries) correspond to the indices of the vertices incident with edge e_j. Similarly, the non-zero entries of the row $\mathbf{M}(i,:)$ correspond to all the edges incident to vertex v_i. Hence, $\sum_{j=1}^{m} \mathbf{M}(i,j) = \deg(v_i)$.

Example 4.1. Find the incidence matrix of the graphs given below.

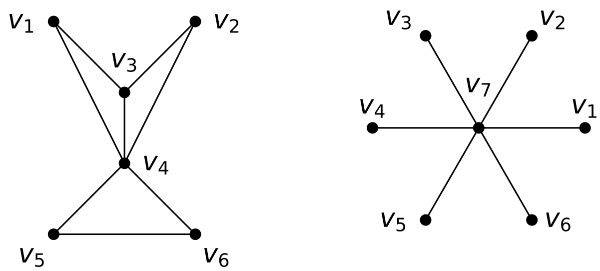


Figure 4.1: Two graphs

The **signless Laplacian** matrix of G is the $n \times n$ matrix defined as

$$\mathbf{Q}(G) := \mathbf{M}\mathbf{M}^T$$

When no confusion arises we write $\mathbf{Q}$ instead of $\mathbf{Q}(G)$. Notice that

$$\mathbf{Q}^T = (\mathbf{M}\mathbf{M}^T)^T = (\mathbf{M}^T)^T\mathbf{M}^T = \mathbf{M}\mathbf{M}^T$$

and thus $\mathbf{Q}$ is a symmetric matrix. We now find an alternative expression for $\mathbf{Q}$. Let $\mathbf{D}$ be the $n \times n$ diagonal matrix whose ith diagonal entry is $\mathbf{D}(i,i) = \deg(v_i)$. The matrix $\mathbf{D}$ is called the **degree** matrix of G.

Proposition 4.1.2

For any graph G it holds that $\mathbf{Q} = \mathbf{D} + \mathbf{A}$.

Proof. We have that

$$\mathbf{Q}(i,j) = \mathbf{M}(i,:)\mathbf{M}^T(:,j) = \sum_{k=1}^{m} \mathbf{M}(i,k)\mathbf{M}^T(k,j) = \sum_{k=1}^{m} \mathbf{M}(i,k)\mathbf{M}(j,k)$$

If $i = j$ then

$$\mathbf{Q}(i,i) = \sum_{k=1}^{m} \mathbf{M}(i,k)\mathbf{M}(i,k) = \sum_{k=1}^{m} \mathbf{M}(i,k) = \deg(v_i).$$

On the other hand, if $i \neq j$ then $\mathbf{Q}(i,j)$ is the product of the ith row and the jth row of $\mathbf{M}$, and the only possibly non-zero product is when $\mathbf{M}(i,:)$ and $\mathbf{M}(j,:)$ have a non-zero entry in the same column, which corresponds to v_i and v_j incident with the same edge. $\square$

Before we can define the Laplacian matrix of a graph we need the notion of an orientation on a graph. An **orientation** of G is an assignment of a direction to each edge $e \in E$ by declaring one vertex incident with e as the **head** and the other vertex as the **tail**. Formally, an orientation of G is a function $g : E(G) \to V(G) \times V(G)$ such that $g(\{u, v\})$ is equal to one of (u, v) or (v, u). If $g(\{u, v\}) = (u, v)$ then we say that u is the **tail** and v is the **head** of the edge $e = \{u, v\}$.

Definition 4.1.3: Oriented Incidence Matrix

Let $G = (V, E)$ be a graph where $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$, and let $g : E \to V \times V$ be an orientation of G. The **oriented incidence matrix N** of G is the $n \times m$ matrix defined by

$$\mathbf{N}(i, j) = \begin{cases} 1, & \text{if } v_i \text{ the head of } e_j \\ -1, & \text{if } v_i \text{ the tail of } e_j \\ 0, & \text{if } v_i \notin e_j \end{cases}$$

The **Laplacian matrix** of G relative to the orientation g is the $n \times n$ matrix

$$\mathbf{L}(G) := \mathbf{N}\mathbf{N}^T.$$

As with the signless Laplacian matrix, the Laplacian matrix is a symmetric matrix. When no confusion arises, we write $\mathbf{L}$ instead of $\mathbf{L}(G)$.

Example 4.2. Assign an orientation to the left graph in Figure 4.1 and compute the associated oriented incidence matrix $\mathbf{N}$. Then compute $\mathbf{L} = \mathbf{N}\mathbf{N}^T$.

Proposition 4.1.4

For any graph G it holds that $\mathbf{L}(G) = \mathbf{D} - \mathbf{A}$. Consequently, $\mathbf{L}$ is independent of the orientation chosen.

Proof. The proof is similar to the that of the signless Laplacian matrix. That $\mathbf{L}$ is independent of the orientation follows since $\mathbf{D}$ and $\mathbf{A}$ are independent of any orientation. ☐

Let $\mathbf{e} = (1, 1, \ldots, 1)$ be the all ones vector. Then

$$\mathbf{Le} = \mathbf{De} - \mathbf{Ae} = \begin{bmatrix} \deg(v_1) \\ \deg(v_2) \\ \vdots \\ \deg(v_n) \end{bmatrix} - \begin{bmatrix} \deg(v_1) \\ \deg(v_2) \\ \vdots \\ \deg(v_n) \end{bmatrix} = \mathbf{0}$$

Therefore $\lambda = 0$ is an eigenvalue of $\mathbf{L}$ with corresponding eigenvector $\mathbf{e}$. We now show that $\mathbf{Q}$ and $\mathbf{L}$ have non-negative eigenvalues. To that end, we say that a symmetric matrix $\mathbf{Z}$ is **positive semi-definite** if $\mathbf{x}^T\mathbf{Z}\mathbf{x} \geq 0$ for all non-zero $\mathbf{x}$ and is **positive definite** if $\mathbf{x}^T\mathbf{Z}\mathbf{x} > 0$ for all non-zero $\mathbf{x}$.

Proposition 4.1.5: Positive Definite Matrices

A symmetric matrix $\mathbf{Z}$ is positive definite if and only if every eigenvalue of $\mathbf{Z}$ is positive. Similarly, $\mathbf{Z}$ is positive semi-definite if and only if every eigenvalue of $\mathbf{Z}$ is non-negative.

Proof. Since $\mathbf{Z}$ is symmetric, there exists an orthonormal basis $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ of $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{Z}$. Thus, $\mathbf{x}_i^T\mathbf{x}_j = 0$ if $i \neq j$ and $\mathbf{x}_i^T\mathbf{x}_i^T = 1$. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the corresponding eigenvalues, that is, $\mathbf{Z}\mathbf{x}_i = \lambda_i\mathbf{x}_i$. Suppose that $\mathbf{Z}$ is positive definite (the proof for positive semi-definiteness is identical). Then $\mathbf{x}^T\mathbf{Z}\mathbf{x} > 0$ for all non-zero $\mathbf{x}$. Now,

$$\mathbf{x}_i^T\mathbf{Z}\mathbf{x}_i = \mathbf{x}_i^T(\lambda_i\mathbf{x}_i) = \lambda_i\mathbf{x}_i^T\mathbf{x}_i = \lambda_i$$

Therefore, $\lambda_i = \mathbf{x}_i^T\mathbf{Z}\mathbf{x}_i > 0$ is positive. This shows that if $\mathbf{Z}$ is positive definite then all eigenvalues of $\mathbf{Z}$ are positive. Conversely, suppose that $\mathbf{Z}$ has all positive eigenvalues and let $\mathbf{x}$ be an arbitrary non-zero vector. Since $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ is a basis for $\mathbb{R}^n$, there are constants $c_1, \ldots, c_n$, not all zero, such that $\mathbf{x} = c_1\mathbf{x}_1 + c_2\mathbf{x}_2 + \cdots + c_n\mathbf{x}_n$. Then,

$$\mathbf{x}^T\mathbf{Z}\mathbf{x} = c_1^2\lambda_1 + c_2^2\lambda_2 + \cdots + c_n^2\lambda_n$$

and since at least one c_i is non-zero and all eigenvalues are positive, we conclude that $\mathbf{x}^T\mathbf{Z}\mathbf{x} > 0$. $\square$

Corollary 4.1.6

The Laplacian and signless Laplacian matrices are positive semi-definite.

Proof. Recall that $\mathbf{L}\mathbf{e} = \mathbf{0}$ and thus $\mathbf{e}^T\mathbf{L}\mathbf{e} = 0$. Now, by definition of $\mathbf{L}$, for any vector $\mathbf{x}$ we have

$$\mathbf{x}^T\mathbf{L}\mathbf{x} = \mathbf{x}^T\mathbf{N}\mathbf{N}^T\mathbf{x} = (\mathbf{N}^T\mathbf{x})^T \cdot (\mathbf{N}^T\mathbf{x}) = \|\mathbf{N}^T\mathbf{x}\|^2 \geq 0.$$

We conclude that $\mathbf{x}^T\mathbf{L}\mathbf{x} \geq 0$ for all $\mathbf{x}$, and therefore $\mathbf{L}$ is positive semi-definite. The proof for $\mathbf{Q}$ is identical. $\square$

Since $\mathbf{L}$ is a symmetric matrix, and as we have just shown is positive semi-definite, the eigenvalues of $\mathbf{L}$ can be ordered as

$$0 = \mu_1 \leq \mu_2 \leq \mu_3 \leq \cdots \leq \mu_n$$

The Laplacian matrix reveals many useful connectivity properties of a graph.

Theorem 4.1.7

A graph G is connected if and only if $\mu_1 = 0$ is a simple eigenvalue of $\mathbf{L}$. Moreover, the algebraic multiplicity of μ_1 is the number of components of G.

Proof. We first recall that $\mathbf{e}$ is an eigenvector of $\mathbf{L}$ with eigenvalue $\mu_1 = 0$. Suppose that $G = G_1 \oplus G_2 \oplus \cdots \oplus G_k$. For any vector $\mathbf{x}$ we have

$$\mathbf{x}^T\mathbf{L}\mathbf{x} = \mathbf{x}^T\mathbf{N}\mathbf{N}^T\mathbf{x} = \|\mathbf{N}^T\mathbf{x}\|^2 = \sum_{v_iv_j \in E} (x_i - x_j)^2.$$

Since $E(G) = E(G_1) \sqcup E(G_2) \sqcup \cdots \sqcup E(G_k)$ (where $\sqcup$ denotes disjoint union) we can write

$$\mathbf{x}\mathbf{L}^T\mathbf{x} = \sum_{v_iv_j \in E(G_1)} (x_i - x_j)^2 + \sum_{v_iv_j \in E(G_2)} (x_i - x_j)^2 + \cdots + \sum_{v_iv_j \in E(G_k)} (x_i - x_j)^2$$

Suppose now that $\mathbf{L}\mathbf{x} = \mathbf{0}$, that is, $\mathbf{x}$ is an eigenvector of $\mathbf{L}$ with eigenvalue μ_1. Then $\mathbf{x}^T\mathbf{L}\mathbf{x} = 0$ and from our computation above we deduce that $\sum_{v_iv_j \in E(G_a)} (x_i - x_j)^2 = 0$ for each component G_a of G. Hence, the entries of $\mathbf{x}$ are equal on each component of G. If G is connected then $\mathbf{x}$ has all entries equal and thus $\mathbf{x}$ is a multiple of $\mathbf{e}$. This proves that the geometric multiplicity, and thus the algebraic multiplicity, of μ_1 is one and thus μ_1 is a simple eigenvalue. Conversely, assume that G is disconnected with components $G_1, G_2, \ldots, G_k$ where $k \geq 2$, and let $n = |V(G)|$. Let $\mathbf{z}_i \in \mathbb{R}^n$ be the vector with entries equal to 1 on each vertex of component G_i and zero elsewhere. Then $\mathbf{N}^T\mathbf{z}_i = \mathbf{0}$ and therefore $\mathbf{L}\mathbf{z}_i = \mathbf{N}\mathbf{N}^T\mathbf{z}_i = \mathbf{0}$. Since $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_k$ is a linearly independent set of vectors, this proves that the multiplicity of μ_1 is at least k. However, since each component G_i is by definition connected and we have proved that a connected graph has μ_1 as a simple eigenvalue, μ_1 has algebraic multiplicity exactly k. $\square$

Since $\mathbf{Q}$ is a symmetric matrix and is semi-positive definite, the eigenvalues of $\mathbf{Q}$ can be ordered as

$$0 \leq q_1 \leq q_2 \leq \cdots \leq q_n$$

Note that in general we can only say that $0 \leq q_1$.

Example 4.3. The signless Laplacian matrix of the graph on the left in Figure 4.1 is

$$\mathbf{Q} = \begin{bmatrix} 2 & 0 & 1 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 0 & 0 \\ 1 & 1 & 3 & 1 & 0 & 0 \\ 1 & 1 & 1 & 5 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 & 2 \end{bmatrix}$$

and $\det(\mathbf{Q}) = 80$. Hence, $0 < q_1$.

Theorem 4.1.8

Suppose that G is connected. The least eigenvalue of $\mathbf{Q}$ is $q_1 = 0$ if and only if G is bipartite. In this case, 0 is a simple eigenvalue.

Proof. As in the proof for the Laplacian matrix, for any $\mathbf{x} \in \mathbb{R}^n$ we have

$$\mathbf{x}^T\mathbf{Q}\mathbf{x} = \mathbf{x}^T\mathbf{M}\mathbf{M}^T\mathbf{x} = \|\mathbf{M}^T\mathbf{x}\|^2 = \sum_{v_iv_j \in E} (x_i + x_j)^2.$$

Suppose that $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is an eigenvector of $\mathbf{Q}$ with eigenvalue $q_1 = 0$. Then $\mathbf{x}^T\mathbf{Q}\mathbf{x} = 0$ and therefore $x_i = -x_j$ for every edge $v_iv_j \in E$. Let $C_1 = \{v_i \in V \mid x_i > 0\}$, $C_2 = \{v_j \in V \mid x_j < 0\}$, and $C_3 = \{v_k \in V \mid x_k = 0\}$. Since $\mathbf{x}$ is a non-zero vector, C_1 and C_2 are non-empty, and moreover $C_1 \cap C_2 = \emptyset$. Any vertex in C_3 is not adjacent to any vertex in C_1 or C_2. Indeed, if $v_k \in C_3$ and $v_k \sim v_i$ then necessarily $0 = x_k = -x_i = 0$ and thus $v_i \in C_3$. Since G is connected this implies that $C_3 = \emptyset$. This proves that C_1 and C_2 is a partition of $V(G)$. Moreover, if $v_iv_j \in E$ and $v_i \in C_1$ then necessarily $v_j \in C_2$, and vice-versa. This proves that $\{C_1, C_2\}$ is a bipartition of G, and thus G is bipartite.

Now suppose that G is bipartite and let $\{X, Y\}$ be a bipartition of G. Let $\alpha \neq 0$ and let $\mathbf{x}$ be the vector whose entries on X are α and on Y are $-\alpha$. Thus, if $\mathbf{M}$ denotes the incidence matrix of G then $\mathbf{M}^T\mathbf{x} = \mathbf{0}$. Therefore $\mathbf{Q}\mathbf{x} = \mathbf{M}\mathbf{M}^T\mathbf{x} = \mathbf{0}$ and thus $\mathbf{x}$ is an eigenvector of $\mathbf{Q}$ with eigenvalue $q_1 = 0$. Now suppose that $\mathbf{z}$ is another eigenvector of $\mathbf{M}$ with eigenvalue q_1. Then $\mathbf{M}\mathbf{z} = \mathbf{0}$ implies that $z_i = -z_j$ for $v_iv_j \in E$. Since G is connected, $\mathbf{z}$ is completely determined by its value at i since there is a path from v_i to any vertex in G. Thus $\mathbf{z}$ is a multiple of $\mathbf{x}$, and this proves that $q_1 = 0$ is a simple eigenvalue. $\square$

Corollary 4.1.9

For any graph G, the multiplicity of $q_1 = 0$ as an eigenvalue of G is the number of bipartite components of G.

Example 4.4. Prove that $\mathbf{L}(G) + \mathbf{L}(\overline{G}) = n\mathbf{I} - \mathbf{J}$ and use it to show that if $\text{spec}(\mathbf{L}) = (0, \mu_2, \mu_3, \ldots, \mu_n)$ then $\text{spec}(\overline{\mathbf{L}}) = (0, n - \mu_n, n - \mu_{n-1}, \ldots, n - \mu_2)$ where $\overline{\mathbf{L}}$ is the Laplacian of $\overline{G}$.

Example 4.5. Suppose that the adjacency matrix of G has eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. If G is a k-regular graph, find the eigenvalues of $\mathbf{L}$ and $\mathbf{Q}$.

Example 4.6. Find the Laplacian and signless Laplacian eigenvalues of the complete graph K_n.

4.1.1 Exercises

Exercise 4.1. Label the vertices of C_4 so that $v_i \sim v_{i+1}$ for $i = 1, 2, 3$. Find the Laplacian matrix of C_4. Do the same for C_5. What about for C_n for arbitrary $n \geq 4$?

Exercise 4.2. Recall that for any $n \times n$ matrix $\mathbf{Z}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, if

$$\det(t\mathbf{I} - \mathbf{Z}) = t^n - s_1 t^{n-1} + s_2 t^{n-2} + \cdots + (-1)^n s_n$$

is the characteristic polynomial of $\mathbf{Z}$ then

$$\begin{aligned} s_1 &= \text{tr}(\mathbf{Z}) = \lambda_1 + \lambda_2 + \cdots + \lambda_n \\ s_n &= \det(\mathbf{Z}) = \lambda_1 \lambda_2 \cdots \lambda_n \end{aligned}$$

Using this fact, find the coefficient of t^{n-1} of the characteristic polynomial $\det(t\mathbf{I} - \mathbf{L})$ for any Laplacian matrix $\mathbf{L}$. What about the constant term of $\det(t\mathbf{I} - \mathbf{L})$?

Exercise 4.3. Let G_1 be a graph with n_1 vertices and Laplacian eigenvalues $0 = \alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_{n_1}$, and let G_2 be a graph with n_2 vertices and Laplacian eigenvalues $0 = \beta_1 \leq \beta_2 \leq \cdots \leq \beta_{n_2}$. In this problem you are going to find the Laplacian eigenvalues of $G = G_1 \vee G_2$. Recall that G is obtained by taking the union of G_1 and G_2 and then connecting each vertex in G_1 to every vertex in G_2. Hence $|V(G)| = n_1 + n_2$ and $E(G) = E(G_1) \cup E(G_2) \cup \{\{u, v\} \mid u \in V(G_1), v \in V(G_2)\}$.

(a) Suppose that the vertices of G are labelled so that the first n_1 vertices are from G_1 and the next n_2 vertices are from G_2. Let $\mathbf{L}_1 = \mathbf{L}(G_1)$ and $\mathbf{L}_2 = \mathbf{L}(G_2)$, and we note that $\mathbf{L}_1$ is a $n_1 \times n_1$ matrix and $\mathbf{L}_2$ is a $n_2 \times n_2$ matrix. Explain why

$$\mathbf{L}(G) = \begin{bmatrix} \mathbf{L}_1 + n_2\mathbf{I} & -\mathbf{J} \\ -\mathbf{J} & \mathbf{L}_2 + n_1\mathbf{I} \end{bmatrix}.$$

where as usual $\mathbf{I}$ is the identity matrix and $\mathbf{J}$ is the all ones matrix, each of appropriate size.

(b) Consider the vector $\mathbf{z} = (n_2, n_2, \ldots, n_2, -n_1, -n_1, \ldots, -n_1)$ where n_2 appears n_1 times and n_1 appears n_2 times. Note that $\mathbf{z}$ can be written as $\mathbf{z} = (n_2\mathbf{e}, -n_1\mathbf{e})$ where $\mathbf{e}$ is the all ones vector of appropriate size. Show that $\mathbf{z}$ is an eigenvector of $\mathbf{L}(G)$ and find the corresponding eigenvalue.

(c) Suppose that $\mathbf{x} \in \mathbb{R}^{n_1}$ is an eigenvector of $\mathbf{L}_1$ with eigenvalue α_i for $i \geq 2$. Let $\mathbf{z} = (\mathbf{x}, \mathbf{0}_{n_2})$ where $\mathbf{0}_{n_2}$ is the zero vector in $\mathbb{R}^{n_2}$. Using the fact that $\mathbf{e}^T\mathbf{x} = 0$, show that $\mathbf{z}$ is an eigenvector of $\mathbf{L}$ with eigenvalue $n_2 + \alpha_i$. Hence, this shows that $n_2 + \alpha_2, \ldots, n_2 + \alpha_{n_1}$ are eigenvalues of $\mathbf{L}$.

(d) Suppose that $\mathbf{y} \in \mathbb{R}^{n_2}$ is an eigenvector of $\mathbf{L}_2$ with eigenvalue β_j for $j \geq 2$. Let $\mathbf{z} = (\mathbf{0}_{n_1}, \mathbf{y})$ where $\mathbf{0}_{n_1}$ is the zero vector in $\mathbb{R}^{n_1}$. Using the fact that $\mathbf{e}^T\mathbf{y} = 0$, show that $\mathbf{z}$ is an eigenvector of $\mathbf{L}$ with eigenvalue $n_1 + \beta_j$. Hence, this shows that $n_1 + \beta_2, \ldots, n_1 + \beta_{n_2}$ are eigenvalues of $\mathbf{L}$.

(e) Parts (a), (b), (c) produce $n_1 + n_2 - 1$ eigenvalues of $\mathbf{L}$. What is the missing eigenvalue of $\mathbf{L}$?

4.2 The Matrix Tree Theorem

Recall that H is a **subgraph** of G if $V(H) \subset V(G)$ and $E(H) \subset E(G)$. A subgraph H of G is a **spanning subgraph** of G if $V(H) = V(G)$. Hence, a spanning subgraph of G is obtained by deleting some of the edges of G but keeping all vertices. If H is a spanning subgraph of G and H is a tree then we say that H is a **spanning tree** of G. The proof of the following lemma is left as an exercise.

Lemma 4.2.1

A graph G is connected if and only if G has a spanning tree.

Example 4.7. Find all of the spanning trees of the graph G shown below.

The Matrix Tree theorem provides a way to count the number of spanning trees in a graph G using the cofactors of the Laplacian matrix $\mathbf{L}$. Recall that for any $n \times n$ matrix $\mathbf{Z}$, the (i, j)**-cofactor** of $\mathbf{Z}$ is $(-1)^{i+j} \det(\mathbf{Z}_{i,j})$ where $\mathbf{Z}_{i,j}$ is the $(n-1) \times (n-1)$ matrix obtained by deleting the ith row and the jth column of $\mathbf{Z}$. Clearly, if $\mathbf{Z}$ is an integer matrix then each cofactor is an integer. The **cofactor matrix** of $\mathbf{Z}$ is the $n \times n$ matrix $\mathrm{Cof}(\mathbf{Z})$ with entries $\mathrm{Cof}(\mathbf{Z})(i, j) = (-1)^{i+j} \det(\mathbf{Z}_{i,j})$. Using the definition of the determinant, one can show that

$$\mathbf{Z}\,\mathrm{Cof}(\mathbf{Z})^T = \det(\mathbf{Z})\mathbf{I}. \tag{4.1}$$

Moreover, if $\mathbf{Z}$ is symmetric then $\mathrm{Cof}(\mathbf{Z})$ is also symmetric.

Lemma 4.2.2

For any graph G, there exists an integer $\tau(G)$ such that $\mathrm{Cof}(\mathbf{L}) = \tau(G)\mathbf{J}$, in other words,

$$\tau(G) = (-1)^{i+j} \det(\mathbf{L}_{i,j})$$

for all i, j.

Proof. Using the fact that $\det(\mathbf{L}) = 0$ and (4.1) we obtain $\mathbf{L}\,\mathrm{Cof}(\mathbf{L})^T = \det(\mathbf{L})\mathbf{I} = \mathbf{0}$. Suppose that G is connected. Then any vector in the kernel of $\mathbf{L}$ is a multiple of $\mathbf{e}$. Now since $\mathbf{L}\,\mathrm{Cof}(\mathbf{L})^T = \mathbf{0}$, it follows that each row of $\mathrm{Cof}(\mathbf{L})$ is a multiple of the all ones vector $\mathbf{e}$, i.e., each row of $\mathrm{Cof}(\mathbf{L})$ is constant. Since $\mathrm{Cof}(\mathbf{L})$ is symmetric, this implies that $\mathrm{Cof}(\mathbf{Z})$ is a constant matrix, i.e., $\mathrm{Cof}(\mathbf{L}) = \tau(G)\mathbf{J}$ for some integer $\tau(G)$. If G is disconnected, then the kernel of $\mathbf{L}$ is at least two-dimensional and therefore $\mathrm{rank}(\mathbf{L}) \leq n-2$. This implies that every cofactor of $\mathbf{L}$ is zero. Hence, in this case $\tau(G) = 0$. □

Theorem 4.2.3: Matrix Tree Theorem

For any graph G, $\tau(G)$ is the number of spanning trees of G.

Chapter 5

Regular Graphs

5.1 Strongly Regular Graphs

A graph G is called **strongly regular** with parameters (n, k, s, t) if G is a n-vertex, k-regular graph such that any two adjacent vertices have s common neighbors and any two non-adjacent vertices have t common neighbors.

Lemma 5.1.1

If G is strongly regular with parameters (n, k, s, t) then $\overline{G}$ is strongly regular with parameters $(n, \overline{k}, \overline{s}, \overline{t})$ where

$$\begin{aligned}\overline{k} &= n - k - 1\\ \overline{s} &= n - 2 - 2k + t\\ \overline{t} &= n - 2k + s\end{aligned}$$

Proof. It is clear that $\overline{k} = n - k - 1$. Let v_i and v_j be two adjacent vertices in G, and thus v_j and v_j are non-adjacent in $\overline{G}$. In G, let Ω_i be the vertices adjacent to v_i that are not adjacent to v_j and let Ω_j be the vertices adjacent to v_j that are not adjacent to v_i, and let $\Gamma_{i,j}$ be the set of vertices not adjacent to neither v_i nor v_j. Therefore, in $\overline{G}$ the non-adjacent vertices v_i and v_j have $|\Gamma_{i,j}|$ common neighbors. Since $|\Omega_i| = |\Omega_j| = k - s - 1$ and $\Omega_i \cap \Omega_j = \emptyset$ we have

$$n = |\Gamma_{i,j}| + |\Omega_i| + |\Omega_j| + s + 2$$

from which it follows that $|\Gamma_{i,j}| = n - 2k + s$. Hence, in $\overline{G}$, any non-adjacent vertices have $\overline{t} = n - 2k + s$ common neighbors. The formula for $\overline{s}$ is left as an exercise (Exercise 5.1). □

Example 5.1. Let G be a strongly regular graph with parameters (n, k, s, t) and suppose that G is not the complete graph. Prove that G is connected if and only if $t > 0$. In this case, deduce that $\mathrm{diam}(G) = 2$.

Proposition 5.1.2

Let G be a strongly regular graph with parameters (n, k, s, t). Then

$$\mathbf{A}^2 = k\mathbf{I} + s\mathbf{A} + t(\mathbf{J} - \mathbf{I} - \mathbf{A}) \tag{5.1}$$

Proof. The (i, j) entry of $\mathbf{A}^2$ is the number of walks of length 2 from v_i to v_j. If v_i and v_j are adjacent then they have s common neighbors and each such neighbor determines a walk from v_i to v_j of length 2. On the other hand, if v_i and v_j are non-adjacent then they have t common neighbors and each such neighbor determines a walk from v_i to v_j of length 2. If $v_i = v_j$ then the number of walks from v_i to v_j is k. Hence,

$$(\mathbf{A}^2)_{i,j} = \begin{cases} s, & v_iv_j \in E(G) \\ t, & v_iv_j \notin E(G) \\ k, & i = j \end{cases}$$

This yields the desired formula for $\mathbf{A}^2$. □

Theorem 5.1.3: Eigenvalues of a SRG

The adjacency matrix of a strongly regular graph has only three eigenvalues. If G is a strongly regular graph with parameters (n, k, s, t) then the eigenvalues of $\mathbf{A}$ besides k are

$$\alpha = \frac{(s-t)+\sqrt{\Delta}}{2}$$
$$\beta = \frac{(s-t)-\sqrt{\Delta}}{2}$$

where $\Delta = (s-t)^2 + 4(k-t)$, with algebraic multiplicities

$$m_\alpha = \frac{1}{2}\left((n-1) - \frac{2k+(n-1)(s-t)}{\sqrt{\Delta}}\right)$$

$$m_\beta = \frac{1}{2}\left((n-1) + \frac{2k+(n-1)(s-t)}{\sqrt{\Delta}}\right)$$

Proof. Let $\mathbf{z}$ be an eigenvector of $\mathbf{A}$ corresponding to an eigenvalue λ not equal to k. Then $\mathbf{z}$ is orthogonal to the all ones vector and thus $\mathbf{Jz} = \mathbf{0}$. Then from (5.1) we have $\mathbf{A}^2 - (s-t)\mathbf{A} - (k-t)\mathbf{I} = t\mathbf{J}$ and therefore

$$(\lambda^2 - (s-t)\lambda - (k-t))\mathbf{z} = 0$$

and therefore $\lambda^2 - (s-t)\lambda - (k-t) = 0$. The roots of the polynomial $x^2 - (s-t)x - (k-t) = 0$ are precisely α and β. Since $\mathrm{tr}(\mathbf{A})$ is the sum of the eigenvalues of $\mathbf{A}$, $\mathrm{tr}(\mathbf{A}) = 0$, and k has multiplicity one, we have $m_\alpha + m_\beta = n-1$ and $\alpha m_\alpha + \beta m_\beta + k = 0$. Solving these equations for m_α and m_β yield $m_\alpha = -\frac{(n-1)\beta+k}{\alpha-\beta}$ and $m_\beta = \frac{(n-1)\alpha+k}{\alpha-\beta}$, and substituting the expression for α and β yield stated expressions. $\square$

5.1.1 Exercises

Exercise 5.1. Finish the proof of Lemma 5.1.1.

Chapter 6

Quotient Graphs

6.1 Linear algebra review

Let us first recall some basics from linear algebra. Let $\mathbf{Y}$ be a $n \times n$ matrix. The **kernel** of $\mathbf{Y}$ (frequently called the **nullspace** of $\mathbf{Y}$) is the set

$$\ker(\mathbf{Y}) = \{\mathbf{v} \in \mathbb{R}^n \mid \mathbf{Y}\mathbf{v} = \mathbf{0}\}.$$

In other words, the kernel of $\mathbf{Y}$ consists of vectors that get mapped to the zero vector when multiplied by $\mathbf{Y}$. Clearly, the zero vector $\mathbf{0}$ is in $\ker(\mathbf{Y})$ since $\mathbf{Y0} = \mathbf{0}$ and in fact $\ker(\mathbf{Y})$ is a **subspace** of $\mathbb{R}^n$ because it is closed under scalar multiplication and scalar addition (verify this!). We say that $\mathbf{Y}$ has a trivial kernel if $\ker(\mathbf{Y}) = \{\mathbf{0}\}$, that is, if the only vector in $\ker(\mathbf{Y})$ is the zero vector. In a first course in linear algebra you proved that $\mathbf{Y}$ has a trivial kernel if and only if $\mathbf{Y}$ is invertible (if and only if $\det(\mathbf{Y}) \neq 0$).

Now let $\mathbf{M}$ be a $n \times n$ matrix with real entries. Given a non-zero vector $\mathbf{v} \in \mathbb{R}$ if it holds that

$$\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$$

for some number $\lambda \in \mathbb{R}$ then we say that $\mathbf{v}$ is an **eigenvector** of $\mathbf{M}$ with **eigenvalue** λ. We will say that $(\mathbf{v}, \lambda)$ is an **eigenpair** of $\mathbf{M}$. Notice that we require $\mathbf{v}$ to be non-zero, and that $\mathbf{v} \in \mathbb{R}^n$ and also $\lambda \in \mathbb{R}$. We are restricting our considerations only to real eigenvectors and real eigenvalues although it is easy to construct matrices $\mathbf{M}$ with real entries that do not have real eigenvectors/eigenvalues, such as

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

However, because the matrices we will study have only real eigenvectors and eigenvalues, this lost of generality will not be too restrictive.

If $(\mathbf{v}, \lambda)$ is an eigenpair of $\mathbf{M}$, then from $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$ we can write that $\lambda\mathbf{v} - \mathbf{M}\mathbf{v} = \mathbf{0}$ or equivalently by factoring $\mathbf{v}$ on the right we have

$$(\lambda\mathbf{I} - \mathbf{M})\mathbf{v} = \mathbf{0}.$$

Hence, $\mathbf{M}$ will have an eigenvector $\mathbf{v}$ associated to λ if the matrix

$$\mathbf{Y}_\lambda = \lambda\mathbf{I} - \mathbf{M}$$

has a **non-trivial** kernel. Now, $\mathbf{Y}_\lambda$ as a non-trivial kernel if and only if $\mathbf{Y}_\lambda$ is not invertible if and only if $\det(\mathbf{Y}_\lambda) = 0$. Hence, the only way that λ is an eigenvalue of $\mathbf{M}$ is if

$$\det(\lambda\mathbf{I} - \mathbf{M}) = 0.$$

If we replace λ by a variable x then to find the eigenvalues of $\mathbf{M}$ we must therefore find the roots of the polynomial

$$p(x) = \det(x\mathbf{I} - \mathbf{M})$$

that is, we must find numbers λ such that $p(\lambda) = 0$. The polynomial $p(x)$ is called the **characteristic polynomial** of $\mathbf{M}$ and we have just showed that the roots of $p(x)$ are exactly the eigenvalues of $\mathbf{M}$. Notice that to compute the polynomial $p(x)$ we do not need any information about the eigenvectors of $\mathbf{M}$ and $p(x)$ is only used to find the eigenvalues. However, if λ is known to be a root of $p(x)$ then any vector in $\ker(\lambda\mathbf{I} - \mathbf{M})$ is an eigenvector of $\mathbf{M}$ with corresponding eigenvalue λ. Now since $\ker(\lambda\mathbf{I} - \mathbf{M})$ is a subspace of $\mathbb{R}^n$ it has a basis, say $\beta_\lambda = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k\}$, consisting of eigenvectors of $\mathbf{M}$ with eigenvalue λ. The dimension of the subspace $\ker(\lambda\mathbf{I} - \mathbf{M})$ is called the **geometric multiplicity** of λ and $\ker(\lambda\mathbf{I} - \mathbf{M})$ is sometimes called the **eigenspace** associated to λ because it is where all the eigenvectors associated to λ live.

If λ is an eigenvalue of $\mathbf{M}$, the **algebraic multiplicity** of λ is the number of times that λ appears as a root of the characteristic polynomial $p(x)$. An eigenvalue is said to be **simple** if its algebraic multiplicity is one and said to be **repeated** otherwise. The geometric multiplicity is always less than or equal to the algebraic multiplicity.

Example 6.1. Suppose that $\mathbf{M}$ is a 6×6 matrix with characteristic polynomial

$$p(x) = \det(x\mathbf{I} - \mathbf{M}) = x^6 - 4x^5 - 12x^4.$$

By inspection we can factor $p(x)$:

$$p(x) = x^4(x^2 - 4x - 12) = x^4(x - 6)(x + 2).$$

Therefore, the eigenvalues of $\mathbf{M}$ are $\lambda_1 = 0$, $\lambda_2 = 6$ and $\lambda_3 = -2$, and thus $\mathbf{M}$ has only three **distinct** eigenvalues (even though it is a 6×6 matrix). The algebraic multiplicity of λ_1 is 4 and it is thus repeated, while λ_2 and λ_3 are both simple eigenvalues. Thus, as a set, the eigenvalues of $\mathbf{M}$ are $\{0, 6, -2\}$, whereas if we want to list all the eigenvalues of $\mathbf{M}$ in say increasing order we obtain

$$(-2, 0, 0, 0, 0, 6).$$

The latter is sometimes called the "set of eigenvalues listed with multiplicities" or the "list of eigenvalues with multiplicities".

Example 6.2 (This is an important example)**.** If $\mathbf{M}$ is a $n \times n$ matrix and has n simple eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ (i.e., all have algebraic multiplicity 1) then each eigenspace $\ker(\lambda_i\mathbf{I} - \mathbf{M})$ is one-dimensional (i.e., it is a line in $\mathbb{R}^n$ through the origin). Therefore, if $\mathbf{v}$ and $\mathbf{w}$ are two eigenvectors associated to the same eigenvalue λ_i then $\mathbf{v}$ and $\mathbf{w}$ are scalar multiplies of each other, that is, $\mathbf{v} = \alpha\mathbf{w}$ for some non-zero $\alpha \in \mathbb{R}$.

Let us now focus on the case that $\mathbf{M}$ is a **symmetric** matrix, that is, $\mathbf{M}^T = \mathbf{M}$. One of the most important results in linear algebra is that the eigenvalues of $\mathbf{M}$ are all real numbers and moreover there exists an **orthonormal basis** of $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{M}$. Hence, if $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of $\mathbf{M}$ (some of which may be repeated) then we are guaranteed the existence of an orthonormal basis $\beta = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ of $\mathbb{R}^n$ such that $\mathbf{M}\mathbf{v}_i = \lambda_i \mathbf{v}_i$ for all $i = 1, 2, \ldots, n$. If we set $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ to be the diagonal matrix with ith diagonal entry equal to λ_i and set $\mathbf{X} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_n \end{bmatrix}$ then the condition $\mathbf{M}\mathbf{v}_i = \lambda_i \mathbf{v}_i$ for all $i = 1, 2, \ldots, n$ can be written as the matrix equation

$$\mathbf{M}\mathbf{X} = \mathbf{X}\mathbf{\Lambda}$$

and therefore

$$\mathbf{M} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}.$$

However, since $\mathbf{X}^{-1} = \mathbf{X}^T$ (because $\mathbf{X}$ is an orthogonal matrix) we have that

$$\mathbf{M} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^T.$$

Example 6.3. In Python, one can compute the eigenvalues and eigenvectors of a symmetric matrix by using the function `eigh` which is contained in the module `numpy.linalg` or `scipy.linalg`. The function `eigh` returns a 2-tuple where the first element is an array of the eigenvalues and the second element is an orthogonal matrix consisting of the eigenvectors. For example, a typical call to `eigh` is

```
E, X = numpy.linalg.eigh(M)
```

and `E` is a $1 \times n$ array that stores the eigenvalues and `X` is a $n \times n$ numpy array whose columns consist of orthonormal eigenvectors of $\mathbf{M}$. For example, to confirm that the 3rd column of `X` is an eigenvector whose eigenvalue is the 3rd entry of `E` we type

```
M @ X[:, 2] - E[2] * X[:, 2]
```

and the returned value should be the zero vector of length n. To verify that `X` is an orthogonal matrix (i.e., that $\mathbf{X}^T\mathbf{X} = \mathbf{I}$) type:

```
X.T @ X
```

6.2 Automorphisms and eigenpairs

Recall that if $\mathbf{P}$ is the permutation matrix of the permutation $\sigma \in S_n$ then $\sigma \in \text{Aut}(G)$ if and only if $\mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{A}$ or equivalently $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{A}$. Our first result describes how eigenvectors behave under the action of an automorphism of G.

Proposition 6.2.1

Let G be a graph with adjacency matrix $\mathbf{A}$ and suppose that $\mathbf{P}$ is the permutation matrix representation of an automorphism $\sigma \in \text{Aut}(G)$. If $(\mathbf{v}, \lambda)$ is an eigenpair of $\mathbf{A}$ then so is $(\mathbf{P}\mathbf{v}, \lambda)$.

Proof. Let $\mathbf{v}$ be an eigenvector of $\mathbf{A}$ with eigenvalue λ, that is, $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$. Since $\mathbf{P}$ is an automorphism of G we have that $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{A}$ and therefore

$$\mathbf{A}\mathbf{P}\mathbf{v} = \mathbf{P}\mathbf{A}\mathbf{v} = \mathbf{P}\lambda\mathbf{v} = \lambda\mathbf{P}\mathbf{v}.$$

Thus, $\mathbf{P}\mathbf{v}$ is an eigenvector of $\mathbf{A}$ with the same eigenvalue λ as $\mathbf{v}$. ☐

Example 6.4. Consider the graph G shown in Figure 6.1 with adjacency matrix

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

The spectrum $\text{spec}(G) = (\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6)$ of G and corresponding eigenvectors written as the columns of the matrix $\mathbf{X} = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 & \mathbf{v}_4 & \mathbf{v}_5 & \mathbf{v}_6\end{bmatrix}$

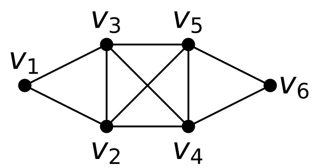


Figure 6.1: Graph for Example 6.4

are

$$\operatorname{spec}(G) = \left(-2, -1, -1, \frac{3-\sqrt{17}}{2}, 1, \frac{3+\sqrt{17}}{2}\right)$$

$$\mathbf{X} = \begin{bmatrix} -1 & 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & -1 & -0.28 & -1 & 1.78 \\ 1 & 0 & 1 & -0.28 & -1 & 1.78 \\ -1 & -1 & 0 & -0.28 & 1 & 1.78 \\ -1 & 1 & 0 & -0.28 & 1 & 1.78 \\ 1 & 0 & 0 & 1 & 2 & 1 \end{bmatrix}$$

One can verify that for instance $\sigma = (1\ 6)(2\ 5)(3\ 4)$ is an automorphism of G. If $\mathbf{P}$ denotes the permutation matrix of σ, one can verify that $\mathbf{P}\mathbf{v}_1 = -\mathbf{v}_1$ which is an eigenvector of $\mathbf{A}$ with same eigenvalue as $\mathbf{v}_1$. As another example, one can verify that $\mathbf{P}\mathbf{v}_4 = \mathbf{v}_4$ and that $\mathbf{P}\mathbf{v}_2 = \mathbf{v}_3$. Hence, in some cases $\mathbf{P}\mathbf{v}_i$ is a scalar multiple of $\mathbf{v}_i$ and in some cases $\mathbf{P}\mathbf{v}_i$ is a non-scalar multiple of $\mathbf{v}_i$; the latter case can occur if the eigenvalue associated to $\mathbf{v}_i$ is repeated as it occurs with $\mathbf{v}_2$ and $\mathbf{v}_3$ (in this case $\lambda_2 = \lambda_3 = -1$).

Our next result relates the algebraic multiplicities of the eigenvalues of $\mathbf{A}$ with the order of the automorphisms of G.

Proposition 6.2.2

Let G be a graph with adjacency matrix $\mathbf{A}$. If $\mathbf{A}$ has simple eigenvalues then every non-identity automorphism of G has order $k = 2$. In particular, the automorphism group $\operatorname{Aut}(G)$ is an abelian group.

Proof. Since $\mathbf{A}$ has simple eigenvalues then $\ker(\lambda\mathbf{I} - \mathbf{A})$ is one-dimensional, and therefore $\mathbf{P}\mathbf{v} = \alpha\mathbf{v}$ for some scalar $\alpha \neq 0$ (see Example 6.2). Therefore, multiplying the equation $\mathbf{Pv} = \alpha\mathbf{v}$ by $\mathbf{P}$ on the left we obtain

$$\mathbf{P}^2\mathbf{v} = \mathbf{P}\alpha\mathbf{v} = \alpha\mathbf{P}\mathbf{v} = \alpha^2\mathbf{v}.$$

Now since $\mathbf{P}$ is an orthogonal matrix, $\|\mathbf{Pv}\| = \|\mathbf{v}\|$, and thus $\alpha = \pm 1$ which implies that $\alpha^2 = 1$. Therefore,

$$\mathbf{P}^2\mathbf{v} = \mathbf{v}.$$

Hence, the matrix $\mathbf{P}^2$ has $\mathbf{v}$ as an eigenvector with eigenvalue 1. Since $\mathbf{v}$ was an arbitrary eigenvector of $\mathbf{A}$, if $\beta = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ is a basis of $\mathbb{R}^n$ consisting of orthonormal eigenvectors of $\mathbf{A}$ then β consists of eigenvectors of $\mathbf{P}^2$ all of which have eigenvalue 1. Therefore, if $\mathbf{X} = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_n\end{bmatrix}$ then

$$\mathbf{P}^2\mathbf{X} = \mathbf{X}$$

and therefore since $\mathbf{X}$ is invertible we have

$$\mathbf{P}^2 = \mathbf{I}.$$

Thus σ^2 is the identity permutation and consequently σ has order $k = 2$. That $\mathrm{Aut}(G)$ is abelian then follows from Example 1.28. □

Remark 6.1. Proposition 6.2.2 does not say that $\mathrm{Aut}(G)$ will necessarily contain non-trivial automorphisms (of order 2). In fact, most graphs will have distinct eigenvalues and a trivial automorphism group, that is, $\mathrm{Aut}(G) = \{\mathrm{id}\}$. What Proposition 6.2.2 does say is that **if** there is any non-trivial automorphism $\sigma \in \mathrm{Aut}(G)$ then σ has order $k = 2$ whenever $\mathbf{A}$ has distinct eigenvalues.

Before we move on, we need to recall the notion of a partition of a set V. A **partition** of V is a collection $\pi = \{C_1, C_2, \ldots, C_k\}$ of subsets $C_i \subset V$ such that $V = \bigcup_{i=1}^k C_i$ and $C_i \cap C_j = \emptyset$ for all $i \neq j$. The subsets C_i are called the **cells** of the partition π. If π has k-cells then it is called a k**-partition**. For example, if $V = \{1, 2, 3, \ldots, 10\}$ then $\pi =$

$\{\{6,9,5,10\},\{1,4\},\{2,3,7\},\{8\}\}$ is a partition of V and it has $k=4$ cells. The **unit partition** of $V=\{1,2,\ldots,n\}$ is the partition that contains only one cell, namely, $\{\{1,2,\ldots,n\}\}$ and the **discrete partition** of V is the partition that contains n cells, namely, $\{\{1\},\{2\},\ldots,\{n\}\}$. We will refer to these partitions as the **trivial partitions** of V.

Remark 6.2. Given a set $V=\{1,2,\ldots,n\}$, how many partitions of V are there? The total number of partitions of an n-element set is the **Bell number** B_n. The first several Bell numbers are $B_0=1$, $B_1=1$, $B_2=2$, $B_3=5$, $B_4=15$, $B_5=52$, and $B_6=203$. The Bell numbers satisfy the recursion

$$B_{n+1}=\sum_{k=0}^{n}\binom{n}{k}B_k.$$

See the Wiki page on Bell numbers for more interesting facts.

Every permutation $\sigma\in S_n$ induces a partition of V as follows. Suppose that σ has r cycles in its cycle decomposition:

$$\sigma=\underbrace{(i_1\ i_2\ \cdots\ i_{m_1})}_{\sigma_1}\underbrace{(i_{m_1+1}\ i_{m_1+2}\ \cdots\ i_{m_2})}_{\sigma_2}\cdots\underbrace{(i_{m_{r-1}+1}\ i_{m_{r-1}+2}\ \cdots\ i_{m_r})}_{\sigma_r}.$$

The r sets formed from the integers within each cycle of σ and the singleton sets formed from the remaining integers fixed by σ forms a **partition** of the vertex set $V=\{1,2,\ldots,n\}$. In other words, if $j_1,j_2,\ldots,j_m$ are the integers fixed by σ, and we set $k=r+m$, then if we set

$$\begin{aligned}
C_1 &= \{i_1,i_2,\cdots,i_{m_1}\}\\
C_2 &= \{i_{m_1+1},i_{m_1+2},\cdots,i_{m_2}\}\\
&\vdots\\
C_r &= \{i_{m_{r-1}+1},i_{m_{r-1}+2},\cdots,i_{m_r}\}\\
C_{r+1} &= \{j_1\}\\
&\vdots\\
C_k &= \{j_m\}
\end{aligned}$$

then $\pi = \{C_1, C_2, \ldots, C_k\}$ is a partition of $V = \{1, 2, \ldots, n\}$. The notation is messy but an example will make the above clear.

Example 6.5. As an example, consider $\sigma \in S_{12}$ given by

$$\sigma = (1\ 5)(2\ 3)(7\ 8\ 4\ 11)(9\ 12\ 6)(10)$$

Hence, σ fixes the integer 10. Thus, if we set $C_1 = \{1, 5\}$, $C_2 = \{2, 3\}$, $C_3 = \{7, 8, 4, 11\}$, $C_4 = \{9, 12, 6\}$, $C_5 = \{10\}$, then $\pi = \{C_1, C_2, C_3, C_4, C_5\}$ is a partition of the vertex set $V = \{1, 2, \ldots, 12\}$. We say that the partition π is **induced** by the permutation σ.

Suppose now that $\sigma \in \mathrm{Aut}(G)$ and let $\pi = \{C_1, C_2, \ldots, C_k\}$ be the partition of V induced by the cycle decomposition of σ. Pick a cell C_i and pick a vertex $u \in C_i$ and suppose that u has d neighbors in cell C_j, say that they are $\{v_1, \ldots, v_d\}$. Since σ sends a vertex in one cell to a vertex in the same cell (recall that each cell consists of the integers in a cycle) then necessarily $\sigma(u) \in C_i$ and $\sigma(v_\ell) \in C_j$ for $\ell = 1, \ldots, d$. Now since $\sigma \in \mathrm{Aut}(G)$, it follows that $\{\sigma(u), \sigma(v_\ell)\} \in E(G)$ and therefore the neighbors of $\sigma(u)$ in C_j are $\{\sigma(v_1), \sigma(v_2), \ldots, \sigma(v_d)\}$. Hence, the **number** of vertices in C_j adjacent to $\sigma(u)$ is equal to the number of vertices in C_j adjacent to u, in this case d. Since σ cycles through all the vertices in C_i, it follows that **all the vertices in C_i have the same number of neighbors in C_j**. Surprisingly, this observation turns out to be an important one.

We introduce some notation to capture what we have just discussed. Given a partition $\pi = \{C_1, C_2, \ldots, C_k\}$ of V, define for any vertex $v \in V$ the **degree of v in C_j** by

$$\deg(v, C_j) = \text{the number of vertices in } C_j \text{ adjacent to } v.$$

Formally, if $N(v)$ denotes all the vertices adjacent to v then

$$\deg(v, C_j) = |N(v) \cap C_j|.$$

Using this notation, what we showed above is that for any two cells C_i and C_j contained in a partition induced by an automorphism of G, the number

$$\deg(u, C_j)$$

is the same for all $u \in C_i$. Now, $\deg(u, C_j)$ could be zero and it is certainly less than $|C_j|$. We can reverse the role of the cells C_i and C_j and conclude that $\deg(v, C_i)$ is the same for all $v \in C_j$. However, it is not necessarily the case that $\deg(v, C_i)$ will equal $\deg(u, C_j)$. Lastly, we could also consider the case that $C_i = C_j$ and thus for $u \in C_i$ the number $\deg(u, C_i)$ is the number of vertices in C_i adjacent to u. We summarize our discussion with the following lemma.

Lemma 6.2.3

Suppose that $\sigma \in \mathrm{Aut}(G)$ and let $\pi = \{C_1, C_2, \ldots, C_k\}$ be the partition induced by the cycle decomposition of σ. Then for any pair of cells C_i and C_j it holds that

$$\deg(u, C_j) = \deg(v, C_j)$$

for all $u, v \in C_i$.

Example 6.6. Consider the graph G shown in Figure 6.2, which is called the Petersen graph. One can verify that $\sigma = (1\ 10)(2\ 8\ 5\ 7)(3\ 6\ 4\ 9)$ is an

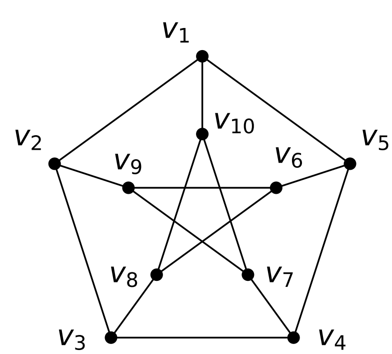


Figure 6.2: The Petersen graph

automorphism of G. Consider the induced partition $\pi = \{\{1, 10\}, \{2, 8, 5, 7\},$

$\{3, 6, 4, 9\}\}$, and let C_1, C_2, C_3 be the cells of π. For any vertex $v \in C_1$, one can verify that $\deg(v, C_1) = 1$, $\deg(v, C_2) = 2$, and $\deg(v, C_3) = 0$. For any vertex $w \in C_2$, one can verify that $\deg(w, C_1) = 1$, $\deg(w, C_2) = 0$, and $\deg(w, C_3) = 2$. Lastly, for any vertex $u \in C_3$, one can verify that $\deg(u, C_1) = 0$, $\deg(u, C_2) = 2$, and $\deg(u, C_3) = 1$. We summarize our results using a matrix which we denote by

$$\mathbf{A}_\pi = \begin{bmatrix} \deg(v, C_1) & \deg(v, C_2) & \deg(v, C_3) \\ \deg(w, C_1) & \deg(w, C_2) & \deg(w, C_3) \\ \deg(u, C_1) & \deg(u, C_2) & \deg(u, C_3) \end{bmatrix} = \begin{bmatrix} 1 & 2 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}.$$

As another example, $\sigma = (1\ 3\ 9)(4\ 6\ 10)(5\ 8\ 7)$ is an automorphism of G and the induced partition is $\pi = \{\{1, 3, 9\}, \{4, 6, 10\}, \{5, 8, 7\}, \{2\}\}$. One can verify that for any $v \in C_1$ it holds that $\deg(v, C_1) = 0$, $\deg(v, C_2) = 1$, $\deg(v, C_3) = 1$, and $\deg(v, C_4) = 1$. Also, for any $w \in C_2$ it holds that $\deg(w, C_1) = 1$, $\deg(w, C_2) = 0$, $\deg(w, C_3) = 2$, and $\deg(v, C_4) = 0$. Similar verifications can be made for vertices in C_3 and C_4, and in this case

$$\mathbf{A}_\pi = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 2 & 0 \\ 1 & 2 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{bmatrix}.$$

In the next section, we will see how the degree conditions that exist for a partition induced by an automorphism exist for more general partitions not necessarily arising from an automorphism.

6.3 Equitable partitions of graphs

In this section, we will introduce the notion of an equitable partition of a graph and how we can use such partitions to define a notion of a quotient graph. We begin with two examples.

Example 6.7. Consider again the Petersen graph in Figure 6.2. One can verify that $\pi = \{\{1,2,3,4,7,10\},\{5,8,9\},\{6\}\}$ is not the partition induced by any automorphism of G. However, one can verify that **for any** $v \in C_1$ it holds that $\deg(v, C_1) = 2$, $\deg(v, C_2) = 1$, and $\deg(v, C_3) = 0$, that **for any** $u \in C_2$ it holds that $\deg(u, C_1) = 2$, $\deg(u, C_2) = 0$, and $\deg(u, C_3) = 1$; and finally that **for any** $w \in C_3$ it holds that $\deg(w, C_1) = 0$, $\deg(w, C_2) = 3$, and $\deg(w, C_3) = 0$. Hence, even though π is not induced by any automorphism, it still satisfies the degree conditions that are satisfied by a partition induced by an automorphism. In this case,

$$\mathbf{A}_\pi = \begin{bmatrix} 2 & 1 & 0 \\ 2 & 0 & 1 \\ 0 & 3 & 0 \end{bmatrix}.$$

Example 6.8. Consider the graph G shown in Figure 6.3, which is called the Frucht graph. This graph has a trivial automorphism group, i.e., $\mathrm{Aut}(G) = \{\mathrm{id}\}$. However, it contains the type of partitions that satisfy the degree conditions of the partitions induced by an automorphism. For example, for $\pi = \{\{1,5,7,12\},\{3,6,9,11\},\{2,4,8,10\}\}$, one can verify that **for any** $u \in C_1$ it holds that $\deg(u, C_1) = 1$, $\deg(u, C_2) = 1$, and $\deg(u, C_3) = 1$; **for any** $v \in C_2$ it holds that $\deg(v, C_1) = 1$, $\deg(v, C_2) = 0$, and $\deg(v, C_3) = 2$; and finally **for any** $w \in C_3$ it holds that $\deg(w, C_1) = 1$, $\deg(w, C_2) = 2$, and $\deg(w, C_3) = 0$. Hence, in this case

$$\mathbf{A}_\pi = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{bmatrix}.$$

Let us now define the vertex partitions that will be of interest to us and that generalize the partitions induced by automorphisms of a graph.

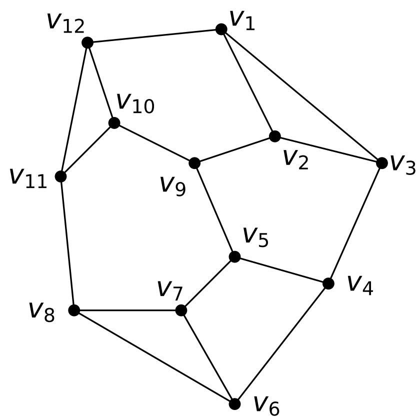


Figure 6.3: A graph with trivial automorphism group but with non-trivial equitable partitions

Definition 6.3.1: Equitable Partitions

Let $G = (V, E)$ be graph and let $\pi = \{C_1, C_2, \ldots, C_k\}$ be a partition of V. If for each pair of cells (C_i, C_j) (not necessarily distinct) it holds that $\deg(u, C_j) = \deg(v, C_j)$ for every $u, v \in C_i$ then we say that π is an **equitable partition** of V.

By Lemma 6.2.3, every partition induced by an automorphism is an equitable partition, however, Examples 6.7-6.8 show that the converse does not hold, that is, **not every equitable partition is induced by an automorphism**. In fact, numerical evidence indicates that the proportion of equitable partitions induced by an automorphism tends to zero as $n \to \infty$.

There is an elegant linear-algebraic way to characterize an equitable partition that is very useful and which gives insight into the structure of the eigenvectors of a graph. We first need to introduce some notation and review more linear algebra.

Let $\pi = \{C_1, C_2, \ldots, C_k\}$ be a partition of $V = \{1, 2, \ldots, n\}$. For any cell C_i let $\mathbf{c}_i \in \mathbb{R}^n$ denote the vector whose entries are equal to 1 on the integer indices in C_i and zero elsewhere. For example, if $C_i = \{2, 4, 7\}$ and $n = 9$ then $\mathbf{c}_i = (0, 1, 0, 1, 0, 0, 1, 0, 0)$, i.e., $\mathbf{c}_i$ has a 1 in positions $\{2, 4, 7\}$ and zero elsewhere. The vector $\mathbf{c}_i$ is called the **characteristic vector** (or indicator vector) of the cell C_i. We define the **characteristic matrix** of π as the $n \times k$ matrix whose columns are the characteristic vectors of the cells of π:

$$\mathbf{C} = \begin{bmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_k \end{bmatrix}.$$

Notice that if π has k cells then $\mathbf{C}$ is a $n \times k$ matrix. Also, and more importantly, since π is a partition of V, the columns of $\mathbf{C}$ are orthogonal, and thus $\operatorname{rank}(\mathbf{C}) = k$.

Example 6.9. If $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$ then $\pi = \{\{1, 4, 6\}, \{2, 5\}, \{7, 8\}, \{3\}\}$ is a partition of V with cells $C_1 = \{1, 4, 6\}$, $C_2 = \{2, 5\}$, $C_3 = \{7, 8\}$, $C_4 = \{3\}$, and π is a 4-partition. The characteristic matrix of π is

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

Now, since $\mathbf{C}$ has orthogonal columns then we have

$$\mathbf{C}^T\mathbf{C} = \begin{bmatrix} \mathbf{c}_1^T\mathbf{c}_1 & 0 & 0 & 0 \\ 0 & \mathbf{c}_2^T\mathbf{c}_2 & 0 & 0 \\ 0 & 0 & \mathbf{c}_3^T\mathbf{c}_3 & 0 \\ 0 & 0 & 0 & \mathbf{c}_4^T\mathbf{c}_4 \end{bmatrix} = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Notice that the diagonals are just the cardinalities of the cells, i.e., $\mathbf{c}_i^T\mathbf{c}_i = |C_i|$.

For any $n \times k$ matrix $\mathbf{C}$ recall that the **image** of $\mathbf{C}$ (frequently called the **range** of $\mathbf{C}$) is

$$\operatorname{img}(\mathbf{C}) = \{\mathbf{C}\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^k\}.$$

The image of $\mathbf{C}$ is a subspace and more concretely, it is the subspace spanned by the columns of $\mathbf{C}$ (frequently called the **column space** of $\mathbf{C}$). To see this, if $\mathbf{C} = \begin{bmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_k \end{bmatrix}$ then for $\mathbf{x} = (x_1, x_2, \ldots, x_k)$ we have

$$\mathbf{C}\mathbf{x} = x_1\mathbf{c}_1 + x_2\mathbf{c}_2 + \cdots + x_k\mathbf{c}_k$$

and thus $\mathbf{C}\mathbf{x}$ is a linear combination of the columns of $\mathbf{C}$, i.e., $\mathbf{C}\mathbf{x} \in \operatorname{span}\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_k\}$. We now introduce the following important notion.

Definition 6.3.2: Invariant Subspace

Let $\mathbf{A}$ be a $n \times n$ matrix and let $\mathsf{W} \subseteq \mathbb{R}^n$ be a subspace. If for every $\mathbf{x} \in \mathsf{W}$ it holds that $\mathbf{A}\mathbf{x} \in \mathsf{W}$ then we say that W is **A-invariant**.

Hence, a subspace W is $\mathbf{A}$-invariant if $\mathbf{A}$ maps any element in W back to an element in W. There is no reason to expect that this will be true for an arbitrary subspace and so that is why such subspaces are singled out. Suppose that W is $\mathbf{A}$-invariant and let $\beta = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ be a basis for W and consider the matrix $\mathbf{W} = \begin{bmatrix} \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_k \end{bmatrix}$. Now, since W is $\mathbf{A}$-invariant then $\mathbf{A}\mathbf{y}_i \in \mathsf{W}$ and therefore $\mathbf{A}\mathbf{y}_i$ can be written as a linear combination of the basis vectors β. Therefore, there is some vector $\mathbf{b}_i \in \mathbb{R}^k$ such that

$$\mathbf{A}\mathbf{y}_i = \mathbf{W}\mathbf{b}_i.$$

This holds for each $i = 1, 2, \ldots, k$ and therefore if we set $\mathbf{B} = \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_k \end{bmatrix}$ then

$$\mathbf{A}\mathbf{W} = \mathbf{W}\mathbf{B}.$$

Example 6.10. Suppose that $\mathbf{A}$ has eigenvalue λ and let $\beta = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$ be a set of linearly independent eigenvectors of $\mathbf{A}$ with eigenvalue λ (m is necessarily $\leq$ the geometric multiplicity of λ). Consider the subspace $\mathsf{W} = \operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$. Let $\mathbf{x} \in \mathsf{W}$ so that there exists constants $\alpha_1, \alpha_2, \ldots, \alpha_m$ such that $\mathbf{x} = \alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \cdots + \alpha_m\mathbf{v}_m$. Then,

$$\begin{aligned}
\mathbf{A}\mathbf{x} &= \mathbf{A}(\alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \cdots + \alpha_m\mathbf{v}_m) \\
&= \mathbf{A}(\alpha_1\mathbf{v}_1) + \mathbf{A}(\alpha_2\mathbf{v}_2) + \cdots + \mathbf{A}(\alpha_m\mathbf{v}_m) \\
&= \alpha_1\mathbf{A}\mathbf{v}_1 + \alpha_2\mathbf{A}\mathbf{v}_2 + \cdots + \alpha_m\mathbf{A}\mathbf{v}_m \\
&= \alpha_1\lambda\mathbf{v}_1 + \alpha_2\lambda\mathbf{v}_2 + \cdots + \alpha_m\lambda\mathbf{v}_m
\end{aligned}$$

from which we see that $\mathbf{Ax} \in \operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$, that is, $\mathbf{Ax} \in \mathsf{W}$. Hence, W is $\mathbf{A}$-invariant.

Although not true for a general matrix $\mathbf{A}$, if $\mathbf{A}$ is **symmetric** then every $\mathbf{A}$-invariant subspace W has a basis of eigenvectors of $\mathbf{A}$. This fact is so important that we state it as a theorem.

Theorem 6.3.3

If $\mathbf{A}$ is a symmetric $n \times n$ matrix and W is $\mathbf{A}$-invariant then there exists a basis of W consisting of eigenvectors of $\mathbf{A}$.

Proof. Suppose that W is k-dimensional and let $\beta = \{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_k\}$ be an orthonormal basis of W. Since W is $\mathbf{A}$-invariant then for each $i \in \{1, 2, \ldots, k\}$ there exists constants $b_{1,i}, b_{2,i}, \ldots, b_{k,i}$ such that

$$\mathbf{Aw}_i = b_{1,i}\mathbf{w}_1 + b_{2,i}\mathbf{w}_2 + \cdots + b_{k,i}\mathbf{w}_k.$$

If we let $\mathbf{B}$ be the $k \times k$ matrix with entries $\mathbf{B}_{j,i} = b_{j,i}$ and we put $\mathbf{W} = \begin{bmatrix}\mathbf{w}_1 & \mathbf{w}_2 & \cdots & \mathbf{w}_k\end{bmatrix}$ then

$$\mathbf{AW} = \mathbf{WB}. \tag{6.1}$$

Now since β is an orthonormal basis we have that $\mathbf{W}^T\mathbf{W} = \mathbf{I}_{k\times k}$ and therefore multiplying (6.1) by $\mathbf{W}^T$ on the left we obtain that

$$\mathbf{B} = \mathbf{W}^T\mathbf{AW}.$$

Now since $\mathbf{A}$ is symmetric it follows that $\mathbf{B}$ is symmetric and thus $\mathbf{B}$ has k linearly independent eigenvectors, say $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$, with associated eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$. We claim that $\mathbf{x}_i = \mathbf{Wv}_i$ is an eigenvector of $\mathbf{A}$ with eigenvalue λ_i. We compute

$$\begin{aligned}\mathbf{A}\mathbf{x}_i &= \mathbf{A}\mathbf{W}\mathbf{v}_i \\ &= \mathbf{W}\mathbf{B}\mathbf{v}_i \\ &= \mathbf{W}\lambda_i\mathbf{v}_i \\ &= \lambda_i\mathbf{W}\mathbf{v}_i \\ &= \lambda_i\mathbf{x}_i.\end{aligned}$$

The eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ are clearly contained in W and they are linearly independent since $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$ are linearly independent and the matrix $\mathbf{W}$ has rank k. □

We are now finally ready to characterize an equitable partition in terms of the invariant subspaces of the adjaceny matrix.

Theorem 6.3.4: Equitable Partitions and Invariant Subspaces

Let $G = (V, E)$ be a graph with adjacency matrix $\mathbf{A}$. Let π be a k-partition of V with characteristic matrix $\mathbf{C}$. Then π is an equitable partition of G if and only if $\text{img}(\mathbf{C})$ is $\mathbf{A}$-invariant. Equivalently, π is equitable if and only if there exists a matrix $\mathbf{B} \in \mathbb{R}^{k\times k}$ such that $\mathbf{AC} = \mathbf{CB}$. In this case, $\mathbf{B} = (\mathbf{C}^T\mathbf{C})^{-1}\mathbf{C}^T\mathbf{AC}$.

Proof. Let $\pi = \{C_1, C_2, \ldots, C_k\}$ and let $\mathbf{C} = \begin{bmatrix}\mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_k\end{bmatrix}$, where $\mathbf{c}_i$ is the characteristic vector of cell C_i. Let $\mathbf{C}_i = \text{diag}(\mathbf{c}_i)$, in other words, $\mathbf{C}_i$ is the diagonal matrix containing a 1 in diagonal entry (j, j) if $j \in C_i$ and zero other wise. Hence, $\mathbf{I} = \mathbf{C}_1 + \mathbf{C}_2 + \cdots + \mathbf{C}_k$. For any cell C_j let

$$\mathbf{d}_j = \begin{bmatrix}\deg(v_1, C_j) \\ \deg(v_2, C_j) \\ \deg(v_2, C_j) \\ \vdots \\ \deg(v_n, C_j)\end{bmatrix}$$

Then it is not hard to see that $\mathbf{A}\mathbf{c}_j = \mathbf{d}_j$, and therefore we can write

$$\mathbf{A}\mathbf{c}_j = \mathbf{C}_1\mathbf{d}_j + \mathbf{C}_2\mathbf{d}_j + \cdots + \mathbf{C}_k\mathbf{d}_j.$$

For each $i \in \{1, 2, \ldots, k\}$ we have

$$(\mathbf{C}_i\mathbf{d}_j)(u) = \begin{cases} \deg(u, C_j), & \text{if } u \in C_i \\ 0, & \text{otherwise} \end{cases}$$

Therefore, if $\deg(u, C_j) = \deg(v, C_j)$ for all $u, v \in C_i$ then $\mathbf{C}_i\mathbf{d}_j = \deg(u, C_j)\mathbf{c}_i$ for any $u \in C_i$. Hence, if π is equitable then

$$\mathbf{A}\mathbf{c}_j = \deg(u_1, C_j)\mathbf{c}_1 + \deg(u_2, C_j)\mathbf{c}_2 + \cdots + \deg(u_k, C_j)\mathbf{c}_k$$

where $u_i \in C_i$, and thus $\mathbf{A}\mathbf{c}_j \in \operatorname{img}(\mathbf{C})$. Conversely, if $\mathbf{A}\mathbf{c}_j \in \operatorname{img}(\mathbf{C})$ then our computations above show that necessarily $\deg(u, C_j) = \deg(v, C_j)$ for all $u, v \in C_i$, and thus π is equitable. $\square$

The matrix $\mathbf{B}$ in Theorem 6.3.4 is actually $\mathbf{B} = \mathbf{A}_\pi$ that appeared in Examples 6.7-6.8. To be precise, if $\pi = \{C_1, C_2, \ldots, C_k\}$ is an equitable partition then $\deg(u, C_j)$ is the same for all $u \in C_i$. We can therefore unambiguously define

$$\deg(C_i, C_j) = \deg(u, C_j)$$

for some $u \in C_i$. Then one can show that

$$\mathbf{A}_\pi = \begin{bmatrix} \deg(C_1, C_1) & \deg(C_1, C_2) & \cdots & \deg(C_1, C_k) \\ \deg(C_2, C_1) & \deg(C_2, C_2) & \cdots & \deg(C_2, C_k) \\ \vdots & \vdots & \cdots & \vdots \\ \deg(C_k, C_1) & \deg(C_k, C_2) & \cdots & \deg(C_k, C_k) \end{bmatrix}$$

and as discussed before in general $\deg(C_i, C_j) \neq \deg(C_j, C_i)$, i.e., $\mathbf{A}_\pi$ is not necessarily symmetric. The proof of Theorem 6.3.4 shows that

$$\mathbf{A}\mathbf{C} = \mathbf{C}\mathbf{A}_\pi$$

that is, $\mathbf{A}_\pi = (\mathbf{C}^T\mathbf{C})^{-1}\mathbf{C}^T\mathbf{A}\mathbf{C}$.

Let us now discuss how the existence of an equitable partition imposes constraints on the eigenvectors of $\mathbf{A}$. Suppose that π is a partition of V and $\mathbf{C}$ is its characteristic matrix. Then $\mathrm{img}(\mathbf{C})$ consists of vectors that have the same numerical value on the entries of each cell. For instance, if

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

then if $\mathbf{x} = (\alpha, \beta, \gamma, \rho)$ then

$$\mathbf{y} = \mathbf{C}\mathbf{x} = \alpha \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \gamma \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} + \rho \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \\ \rho \\ \alpha \\ \beta \\ \alpha \\ \gamma \\ \gamma \end{bmatrix}.$$

Hence, a vector $\mathbf{y} \in \mathrm{img}(\mathbf{C})$ has the same values on the entries $C_1 = \{1, 4, 6\}$, the same values on entries $C_2 = \{2, 5\}$, the same values on entries $C_3 = \{7, 8\}$, and the same values on entries $C_4 = \{3\}$ (this is trivial because C_4 is a singleton cell). Now, **if** π is an equitable partition then $\mathsf{W} = \mathrm{img}(\mathbf{C})$ is $\mathbf{A}$-invariant and therefore by Theorem 6.3.3 since $\mathbf{A}$ is symmetric there is a basis of $\mathrm{img}(\mathbf{C})$ consisting of eigenvectors of $\mathbf{A}$. These eigenvectors therefore have entries that are equal on each of the cells of π and there will be k of these eigenvectors (linearly independent) if π is a k-partition.

We consider a specific example. Consider again the Frucht graph G which we reproduce in Figure 6.4. The Frucht graph has three non-trivial equitable partitions, one of which is

$$\pi = \{\{1, 5, 7, 12\}, \{3, 6, 9, 11\}, \{2, 4, 8, 10\}\}.$$

Hence, since π is a $k = 3$ partition then there exists $k = 3$ linearly independent eigenvectors of $\mathbf{A}$ whose entries on the cells of π are equal. The eigenvectors

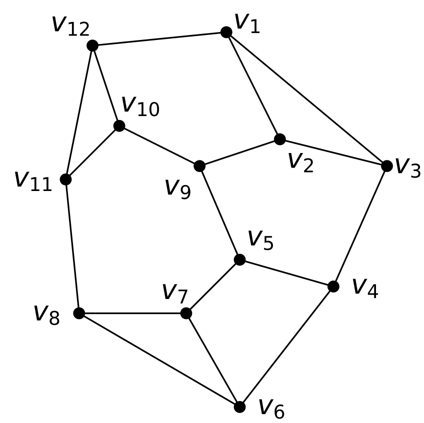


Figure 6.4: The Frucht graph

(rounded to two decimal places) of $\mathbf{A}$ are (as columns):

$$\mathbf{X} = \begin{bmatrix}
0.17 & 0.00 & -0.48 & 0.40 & -0.17 & 0.12 & 0.41 & 0.11 & 0.33 & 0.18 & 0.36 & -0.29 \\
-0.14 & 0.35 & -0.00 & -0.56 & -0.17 & 0.00 & -0.20 & 0.44 & 0.00 & 0.31 & 0.32 & -0.29 \\
-0.20 & -0.35 & 0.27 & 0.14 & 0.50 & -0.27 & -0.20 & -0.14 & 0.27 & 0.40 & 0.22 & -0.29 \\
0.44 & 0.35 & 0.00 & -0.04 & -0.17 & -0.00 & -0.20 & -0.63 & 0.00 & 0.31 & -0.18 & -0.29 \\
-0.51 & -0.00 & -0.12 & 0.03 & -0.17 & -0.33 & 0.41 & -0.16 & -0.48 & 0.18 & -0.21 & -0.29 \\
-0.31 & -0.35 & -0.15 & -0.10 & -0.17 & 0.60 & -0.20 & -0.02 & 0.21 & 0.04 & -0.43 & -0.29 \\
0.39 & 0.00 & 0.00 & -0.27 & 0.50 & 0.00 & 0.41 & 0.29 & -0.00 & -0.00 & -0.43 & -0.29 \\
-0.10 & 0.35 & 0.27 & 0.46 & -0.17 & -0.27 & -0.20 & 0.33 & 0.27 & -0.22 & -0.35 & -0.29 \\
0.36 & -0.35 & 0.21 & 0.27 & -0.17 & 0.15 & -0.20 & 0.26 & -0.60 & 0.04 & 0.14 & -0.29 \\
-0.20 & 0.35 & -0.27 & 0.14 & 0.50 & 0.27 & -0.20 & -0.14 & -0.27 & -0.40 & 0.22 & -0.29 \\
0.15 & -0.35 & -0.33 & -0.30 & -0.17 & -0.48 & -0.20 & -0.09 & 0.12 & -0.49 & 0.07 & -0.29 \\
-0.05 & -0.00 & 0.60 & -0.16 & -0.17 & 0.21 & 0.41 & -0.24 & 0.15 & -0.36 & 0.28 & -0.29
\end{bmatrix}$$

Observe that the eigenvectors in columns 2, 7, 12 all have entries that are constant on the cells of π. What can we say about the eigenvectors of $\mathbf{A}$ not contained in $\operatorname{img}(\mathbf{C})$? It turns out that because $\mathbf{A}$ is symmetric then the **orthogonal complement** of the subspace $\mathsf{W} = \operatorname{img}(\mathbf{C})$ is also $\mathbf{A}$-invariant, where the orthogonal complement of W is the set of vectors orthogonal to vectors in W. The orthogonal complement of a subspace W is denoted by

$\mathsf{W}^\perp$ and thus

$$\mathsf{W}^\perp = \{\mathbf{z} \in \mathbb{R}^n \mid \langle \mathbf{z}, \mathbf{w} \rangle = 0 \text{ for all } \mathbf{w} \in \mathsf{W}\}.$$

Since $\mathsf{W}^\perp$ is $\mathbf{A}$-invariant, by Theorem 6.3.3, there is a basis of $\mathsf{W}^\perp$ consisting of eigenvectors $\mathbf{A}$. One can show that for $\mathsf{W} = \operatorname{img}(\mathbf{C})$ it holds that

$$\mathsf{W}^\perp = \ker(\mathbf{C}^T).$$

It is not hard to see that $\mathbf{z} \in \ker(\mathbf{C}^T)$ if and only if the sum of the entries of $\mathbf{z}$ on each cell sum to zero. Hence, the remaining eigenvectors of $\mathbf{A}$ not contained in $\operatorname{img}(\mathbf{C})$ have the property that the sum of their entries on each cell sum to zero. We summarize with the following.

Proposition 6.3.5

Suppose that $\pi = \{C_1, C_2, \ldots, C_k\}$ is an equitable partition of G. Then the eigenvectors of $\mathbf{A}$ can be split into two groups, namely, those that are constant on the cells of π (i.e., contained in $\operatorname{img}(\mathbf{C})$) and those that sum to zero on the cells of π (i.e., contained in $\ker(\mathbf{C}^T)$).

Example 6.11. Another partition of the Frucht graph is

$$\pi = \{\{3, 7, 10\}, \{1, 2, 4, 5, 6, 8, 9, 11, 12\}\}$$

so that π is a $k = 2$ partition. One can verify that $\mathbf{A}$ has $k = 2$ linearly independent eigenvectors that are constant on the cells of π, namely, the 5th eigenvector and the last. The remaining $n - k = 12 - 2 = 10$ eigenvectors sum to zero on the cells of π. For example, for the first eigenvector $\mathbf{v}_1 = (0.17, -0.14, -0.20, 0.44, -0.51, -0.31, 0.39, -0.10, 0.36, -0.20, 0.15, -0.05)$ the sum of the entries on cell $C_1 = \{3, 7, 10\}$ is $-0.20 + 0.39 - 0.20 \approx 0$ (due to rounding errors) and the sum of the entires on cell $C_2 = \{1, 2, 4, 5, 6, 8, 9, 11, 12\}$ is $0.17 - 0.14 + 0.44 - 0.51 - 0.31 - 0.10 + 0.36 + 0.15 - 0.05 \approx 0$ (again due to rounding errors).

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