Eigenspace Structure of Certain Graph Classes

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Dedicated to my family for their loving support.

"The pure and simple Truth is rarely pure, and never simple."
Oscar Wilde

In one way or the other, countless people have contributed to the success of this work. Most of them may simply not be aware of their role because their mere presence sufficed to help create the friendly and motivating environment in which I was allowed to live and work.

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Contents

1 Introduction

The topics treated in this thesis stem from the area of algebraic graph theory which uses algebraic methods to derive structural results on graphs. Our focus is the study of eigenvalues and eigenspaces of finite, simple, loopless and usually undirected graphs.

The crucial construct we will deal with is the adjacency matrix of a graph. Given a graph with vertices $v_1, \ldots, v_n$ we can construct the respective adjacency matrix by setting the entry at position (i, j) to 1 if the vertices v_i and v_j are joined by an edge and 0 otherwise. This definition of the adjacency matrix depends on the chosen vertex order. The eigenvalues of the adjacency matrix, however, do not and can therefore be interpreted as a property of the graph itself. The same applies to the eigenspaces if only we attribute the entries of an eigenvector to the corresponding vertices of the graph (by matching indices).

Apart from introductory results and some remarks on eigenvector iteration, each chapter of this thesis concentrates on a certain graph class and predominantly studies its eigenspace stucture.

Starting with the eigenspace relation between a graph and its complement it will be shown that the dimension of the kernel of a graph differs from the dimension of the eigenspace for eigenvalue -1 of the complement by at most one. If the dimensions are not equal, then the smaller space will be contained in the larger one. For undirected graphs equal dimension implies identical eigenspaces. These results are based on more general matrix theoretical findings.

Subsequently, our main concern are trees and distance powers of paths and circuits. Besides studying the special eigenspaces mentioned above we also derive spectral bounds, determine the occurence or multiplicities of certain eigenvalues, search for common eigenvectors of two graphs from the same class, and construct simply structured bases of certain graph eigenspaces.

2 Basics

In the following sections we will introduce basic concepts that will be used in later chapters.

2.1 Linear algebra

Linear algebra provides tools used frequently in algebraic graph theory. We will therefore introduce some notation found throughout the following sections and briefly quote some theorems that will be used in the context of graphs later on. For more details consult any standard book on linear algebra.

Let K be a field. Let $K^{n\times m}$ denote the set of $n \times m$ matrices with entries from K and $K^n = K^{n\times 1}$. This means we will not strictly distinguish between a column vector and a matrix with only one column.

Let $J_{k,l} \in \mathbb{R}^{k\times l}$ be the all ones matrix, $\mathbb{1}_n = J_{n,1} \in \mathbb{R}^n$ the all ones vector, $N_{k,l} \in \mathbb{R}^{k\times l}$ the null matrix, and $I_k \in \mathbb{R}^{k\times k}$ the identity matrix. The column vectors $e_1, \dots, e_k$ of the identity matrix I_k are called the *standard unit vectors* and form the *standard basis* of $\mathbb{R}^k$.

Occasionally, we will write $J_k = J_{k,k}$ and $N_k = N_{k,k}$.

Further, let $L_k, U_k \in \mathbb{R}^{k\times k}$ be all ones lower and upper triangular matrices, respectively. Also, let $\tilde{L}_k = L_k - I_k$ and $\tilde{U}_k = U_k - I_k$ be the corresponding strictly lower and upper triangular matrices.

If the dimensions are clear from the context, we will occasionally omit the subscripts to improve readability. We may even write $0 = N_k$, especially within block matrices.

A matrix in which the i-th column vector can be derived from the first column vector by means of a downward rotation by $i - 1$ entries is called a *circulant* matrix.

In the following, consider a matrix $A = (a_{ij}) \in K^{n\times n}$. We call matrix A *normal* if it represents a normal endomorphism, i.e. $AA^T = A^T A$. A matrix $P \in \mathbb{R}^n$ is called a *permutation matrix* if its column vectors form the standard basis of $\mathbb{R}^n$. Permutation matrices are orthogonal, i.e. $P^{-1} = P^T$.

The *characteristic polynomial* χ of A is defined by

$$\chi(x; A) = \det(A - xI). \tag{1}$$

Lemma 2.1. The constant term of the characteristic polynomial $\chi(x; A)$ equals the determinant of A. □

Proof. Note that $\chi(0;A) = \det A$. ■

Note that by some sources alternatively $\det(xI - A)$ is considered the characteristic polynomial.

It is easy to see that

$$\chi(\lambda; A) = 0 \;\Leftrightarrow\; \operatorname{Ker}(A - \lambda I) \neq \{0\}. \tag{2}$$

The zeros of the characteristic polynomial of a matrix A are called the *eigenvalues* of A. The set of all eigenvalues is referred to as the *spectrum* of A. For any eigenvalue λ we call

$$\operatorname{Eig}(\lambda; A) = \operatorname{Ker}(A - \lambda I) \tag{3}$$

the corresponding *eigenspace*.

Theorem 2.2. Let A be symmetric. Then all eigenvalues of A are real numbers. □

Throughout, we tacitly assume that angles between vectors are measured using the standard inner product.

Different eigenspaces are disjoint (neglecting the null vector) and may even be mutually perpendicular.

Theorem 2.3. If $Av_1 = \lambda_1 v_1$ and $Av_2 = \lambda_2 v_2$ holds for two vectors $v_1, v_2 \neq 0$ and eigenvalues $\lambda_1 \neq \lambda_2$, then v_1 and v_2 are linearly independent. □

Theorem 2.4. Let A be normal. If $Av_1 = \lambda_1 v_1$ and $Av_2 = \lambda_2 v_2$ holds for two vectors v_1, v_2 and eigenvalues $\lambda_1 \neq \lambda_2$, then v_1 and v_2 are perpendicular. □

We turn our attention to integer matrices and will comment on their rational eigenvalues. But first we need the following well-known lemma on polynomials:

Lemma 2.5. Let

$$a_n x^n + \ldots + a_1 x + a_0 = 0$$

for $x = \frac{p}{q}$ with $\gcd(p,q) = 1$ and integer coefficients a_i. Then,

$$p | a_0 \;\wedge\; q | a_n.$$

□

Proof. Substitute $x = \frac{p}{q}$ into the polynomial equation and multiply by q^n. Rearranging the result, we get

$$\begin{aligned} 0 &= a_n p^n + q\left(a_{n-1}p^{n-1}q^0 + \ldots + a_0 p^0 q^{n-1}\right) \\ &= a_0 q^n + p\left(a_n p^{n-1} q^0 + \ldots + a_1 p^0 q^{n-1}\right). \end{aligned} \tag{4}$$

Because of $\gcd(p, q) = 1$ the result follows immediately. ■

Lemma 2.6. Every rational eigenvalue of an integer matrix is integer. □

Proof. Consider Lemma 2.5 for the characteristic polynomial of an integer matrix. It is easy to see that all coefficients are integer and that $a_n = (-1)^n$. Consequently, for every eigenvalue $\lambda = \frac{p}{q}$ with $\gcd(p, q) = 1$ we have $q|(-1)^n$ so that λ must be integer. ■

A different proof technique can be found in [29]. It relies on the fact that for any rational eigenvalue of an integer matrix there would exist an integer eigenvector.

We will call a matrix *positive* or *non-negative* if all its entries are positive or non-negative, respectively. A matrix A is called *reducible* if there exists a permutation matrix P such that

$$P^{-1}AP = \begin{pmatrix} X & 0 \\ Y & Z \end{pmatrix} \tag{5}$$

with square matrices X, Z. Otherwise, we say that A is *irreducible*.

The following theorems are concerned with non-negative matrices. For a thorough treatment the reader is referred to [16].

Theorem 2.7. (PERRON, FROBENIUS)
Let A be a non-negative irreducible matrix. Then all eigenvalues of A of largest modulus are simple and among them there is always a positive real eigenvalue λ_{max}. The eigenspace for λ_{max} contains a positive eigenvector.

Moreover, the spectrum of A, considered as a set of points in the complex plane, is mapped onto itself under a rotation around the origin by the angle $\frac{2\pi}{k}$ if k denotes the number of eigenvalues of A of largest modulus.

If $k > 1$, then there exists a permutation matrix P such that

$$P^{-1}AP = \begin{pmatrix} 0 & B_1 & & & \\ & 0 & B_2 & & \\ & & \ddots & \ddots & \\ & & & 0 & B_{h-1} \\ B_0 & & & & 0 \end{pmatrix}$$

with square blocks along the main diagonal (omitted blocks are zero). □

Since λ_{max} is uniquely determined, we will refer to it as the *largest* or *maximum* eigenvalue of A.

Theorem 2.8. Let A be non-negative. Let λ'_{max} be the largest eigenvalue of any principal submatrix $A' \neq A$ of A. Then,

$$\lambda'_{max} \leq \lambda_{max}.$$

If A is irreducible, then the inequality is strict. If A is reducible, then equality holds for at least one principal submatrix. □

Theorem 2.9. Let A be non-negative. Increase any entry of A to get the non-negative matrix A'. Then,

$$\lambda_{max} \leq \lambda'_{max}.$$

The inequality is strict if A is irreducible. □

The final theorem in this section describes a phenomenon called *eigenvalue interlacing.*

Theorem 2.10. Let A be symmetric and A' be one of its principal submatrices. Let $\lambda_1 \leq \ldots \leq \lambda_n$ and $\lambda'_1 \leq \ldots \leq \lambda'_m$ be the eigenvalues of A and A', respectively. Then the inequality

$$\lambda_i \leq \lambda'_i \leq \lambda_{n-m+i}$$

holds for all $i = 1, \ldots, m$. □

Historically, the original notion of interlacing was only used for the case $m = n - 1$.

2.2 Algebraic graph theory

For the general basics of graph theory, the reader is referred to sources like [9], [24], [2], or [13].

Throughout, we will only consider finite, simple, loopless graphs. Unless stated otherwise all graphs are undirected. Our definitions and notation mainly follow [17]. However, we will speak of the *degree* $\gamma(v)$ of a vertex v instead of its valency. The maximum and minimum degree of a graph G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. Further, we will not strictly distinguish between isomorphic graphs and even write $G = H$ if the graphs G and H are isomorphic. Basically, any two isomorphic graphs differ only by the labelling of their respective vertex sets.

The *neighbourhood* $N(v)$ is the set of all vertices adjacent to v. The set $N(v) \cup \{v\}$ will be called the *closed neighbourhood*.

Note that for a set $M \setminus \{x\}$ we will frequently write $M - x$. Likewise, $G - x$ denotes the subgraph of $G = (V, E)$ induced by the vertices $V - x$ and $G - e$ is derived from G by removing edge $e \in E$.

If $\overline{G}$ is the complement of G, we will use $\overline{\gamma}(v)$ for the degree of v in $\overline{G}$. The same principle applies to other notation.

Recall that the *distance* $\mathrm{d}_G(u, v)$ is the length of a shortest path in G from vertex u to vertex v (or ∞ if no such path exists). Further, the *diameter* $\mathrm{diam}(G)$ of a graph G is the length of a longest path in G.

The *k-th distance power* $G^{(k)}$ of a graph G has the same vertex set as G. Two vertices u, v of $G^{(k)}$ are adjacent if and only if $\mathrm{d}_G(u, v) \leq k$. Note that $G^{(k)}$ is complete if $k \geq \mathrm{diam}(G)$.

2.2.1 Essentials

Let $G = (V, E)$ be a graph with $V = \{x_1, \ldots, x_n\}$ and write $x_i \sim x_j$ if the vertices x_i and x_j are adjacent. Then we define the *adjacency matrix* $A(G) = (a_{ij})$ by

$$a_{ij} = \begin{cases} 1 & \text{if } x_i \sim x_j \\ 0 & \text{else} \end{cases}.$$

Note that for an undirected graph the matrix $A(G)$ is symmetric.

The adjacency matrix of a graph therefore allows to look up if an edge leads from vertex x_i to x_j. The powers of the adjacency matrix have a similar property:

Theorem 2.11. [3] Let A be the adjacency matrix of the directed graph G. Then the entry at position (i, j) of A^r equals the number of directed walks of length r from vertex x_i to vertex x_j. □

From this point, we will assume that all graphs mentioned are **undirected** (unless stated otherwise).

We are interested in eigenvalues and eigenvectors of $A(G)$. Obviously, the matrix $A(G)$ depends on the actual ordering of the vertices of G. But the effect of any reordering of the vertices on the adjacency matrix can be reproduced by a basis transformation $P^{-1}A(G)P$ with a suitable permutation matrix P. Hence, all possible adjacency matrices of an isomorphy class of graphs are similar and therefore have the same eigenvalues and eigenvalue multiplicities. This justifies that we may speak of the eigenvalues of a graph regardless of the representation chosen.

Note that for K_n all adjacency matrices are the same whereas for P_n we have several possibilities. Since we will frequently exploit the structure of special choices of the adjacency matrix we will introduce canonical vertex orderings for some graph classes. In particular, we will assume a sequential vertex order both for paths P_n and circuits C_n.

The eigenvalues of a graph G are the roots of the *characteristic polynomial*

$$\chi(x; G) = \det(A(G) - \lambda x).$$

The set of all eigenvalues is called the *spectrum* of G. We see from Theorem 2.2 that all eigenvalues of a graph are real. The maximum modulus of all eigenvalues of G is called the *spectral radius* $\rho(G)$.

The eigenspace of eigenvalue λ is denoted by $\mathrm{Eig}(\lambda; G)$. If there is no risk of confusion we will frequently write $E_\lambda = \mathrm{Eig}(\lambda; G)$ and $\overline{E}_\lambda = \mathrm{Eig}(\lambda; \overline{G})$.

Since $A(G)$ is symmetric and therefore diagonalisable we see that the multiplicity of a root of $\chi(x; G)$ equals the dimension of the corresponding eigenspace.

Example 2.12. (Spectrum of K_n)

The adjacency matrix of the complete graph K_n is $J - I$. Since J has eigenvalues n and 0 with multiplicities 1 and $n - 1$, respectively, we see that K_n has eigenvalues $n - 1$ and -1 with multiplicities 1 and $n - 1$. □

It should be observed that any graph can be reconstructed if its eigenvalues and a basis of eigenvectors are known (conduct a simple basis transformation). However, it is not generally possible to reconstruct a graph from its spectrum only. In fact, there exist constructions to obtain arbitrarily many cospectral graphs [25].

Owing to the following reconstruction theorem, the characteristic polynomial of a graph can be almost entirely reconstructed from the characteristic polynomials of its one-vertex-deleted subgraphs:

Theorem 2.13. (Clarke, cf. [7], [5])

$$\chi'(\lambda; G) = - \sum_{v \in V(G)} \chi(\lambda; G - v).$$

□

In order to fully reconstruct the characteristic polynomial it suffices to know one of the eigenvalues of G.

Many of the results we present next are direct consequences of the theorems from section 2.1. For more details see [17] or [3].

Theorem 2.14. The eigenspaces of a graph are mutually perpendicular. □

Lemma 2.15. Every rational eigenvalue of a graph is necessarily integer. □

Proof. See Lemma 2.6. ■

The diameter of a graph can be used to provide a lower bound for the number of distinct eigenvalues of a graph:

Theorem 2.16. [3] Let G be a graph with diameter d. Then G has at least $d+1$ distinct eigenvalues. □

An important interpretation of eigenvectors is as follows. Consider a graph $G = (V, E)$, $V = \{v_1, \ldots, v_n\}$, with adjacency matrix A and let $w = (w_i)$ be an eigenvector of A for eigenvalue λ. Now assign the *weight* $w(v_i) = w_i$ to each vertex v_i. Looking at the system $Aw = \lambda w$ row by row we see that for every vertex v_i the sum of the weights of its neighbours equals λ times its own weight w_i, i.e.

$$\sum_{v_j \in N(v_i)} w(v_j) = \lambda w_i \tag{6}$$

for $i = 1, \ldots, n$. We will refer to this equation as the *summation rule*.

The automorphisms of a graph provide a simple but often effective device to explore the structure of eigenvectors:

Theorem 2.17. [3] Let σ be an automorphism of a graph G with adjacency matrix A and x any eigenvector of G for eigenvalue λ. If P is the permutation matrix that transforms A into the adjacency matrix $P^{-1}AP$ of $\sigma(G)$, then $P^{-1}x$ is an eigenvector of $\sigma(G)$ for eigenvalue λ. □

2.2.2 Consequences of the Perron-Frobenius theorem

We will now turn our attention to some important consequences of the Perron-Frobenius Theorem 2.7 and the theory of non-negative matrices [16]. In this context it is important to note that a graph G is connected if and only if its adjacency matrix is irreducible, i.e. there exists no permutation matrix P such that

$$A(G) = P^{-1} \begin{pmatrix} B_1 & 0 \\ B_2 & B_3 \end{pmatrix} P$$

with square matrices B_1 and B_3. For a directed graph irreducibility of the adjacency matrix means strong connectivity.

Theorem 2.18. Let G be a directed graph. Then G has a non-negative real eigenvalue λ_{max} of largest modulus. For λ_{max} there exists a non-negative eigenvector. The deletion of vertices from G does not increase the spectral radius.

If G is strongly connected and has at least one edge, then λ_{max} is positive and simple with a positive eigenvector. The maximum eigenvalue of every strict subgraph of G is strictly smaller than λ_{max}.

Otherwise, the maximum eigenvalue of at least one strong component of G equals λ_{max}. □

Since the adjacency matrix of an undirected graph also yields a directed graph we can deduct the following corollaries:

Corollary 2.19. Let G be an undirected graph. Then the eigenvalues of G are real and the maximum eigenvalue λ_{max} is non-negative. Further, the moduli of all other eigenvalues do not exceed λ_{max}. If G is connected and has at least one edge, then λ_{max} is positive and simple.

Finally, we have

$$\lambda_{max}(H) \leq \lambda_{max}(G)$$

for every subgraph H of G with $H \neq G$. The inequality is strict if G is connected. □

Remark 2.20. Parts of both Theorem 2.18 and Corollary 2.19 are consequences of Theorem 2.8. The principal submatrices of the adjacency matrix of G are exactly the adjacency matrices of the induced subgraphs of G. Owing to Theorem 2.9 we see that the eigenvalue inequalities remain valid even for non-induced subgraphs. □

Theorem 2.21. Any two positive eigenvectors of a connected graph G are linearly independent. □

A direct consequence of this theorem and the corollary before is that for a connected graph only the eigenvalue λ_{max} affords a positive eigenvector.

Finally, the PERRON-FROBENIUS theorem can be applied to investigate the spectra of bipartite graphs. Recall that a graph is bipartite if its vertex set can be split into sets V_1 and V_2 such that these sets induce null graphs. Equivalently, there exists a vertex ordering for which the adjacency matrix assumes the block diagonal form

$$\begin{pmatrix} 0 & B_1 \\ B_2 & 0 \end{pmatrix}.$$

With the help of Theorem 2.7 we arrive at a characterisation of bipartite graphs:

Theorem 2.22. A connected graph is bipartite if and only if $-\lambda_{max}$ is one of its eigenvalues. □

It is easy to see that the spectrum of a bipartite graph exhibits even stricter symmetry:

Theorem 2.23. Let $G = (V, E)$ be bipartite with bipartition $V = V_1 \cup V_2$. If v is an eigenvector for eigenvalue λ, then the vector $\tilde{v}$ obtained by inverting the signs of all components of v associated with vertices from V_1 is an eigenvector for eigenvalue $-\lambda$ with the same multiplicity. □

Corollary 2.24. The spectrum of a bipartite graph is symmetric around zero. □

2.2.3 Eigenvalue bounds

We will now provide some eigenvalue bounds, in particular for the the largest eigenvalue λ_{max}, that will be used in later chapters.

Lemma 2.25. Let G be a connected graph on $n \geq 2$ vertices. Then,

$$\lambda_{max}(G) \geq 1.$$

□

Proof. Since G has at least one edge it contains an induced K_2 whose maximum eigenvalue is one. Therefore, the result follows by Corollary 2.19. ■

Theorem 2.26. [17] If H is an induced subgraph of G, then

$$\lambda_{\min}(G) \leq \lambda_{\min}(H) \leq \lambda_{\max}(H) \leq \lambda_{\max}(G).$$

□

It is interesting to compare this result to Corollary 2.19.

We can extend this result if we apply the notion of interlacing to graphs. The following theorem is a simple rewrite of Theorem 2.10:

Theorem 2.27. Let G be a graph and H an induced subgraph such that $|V(G)| = n$ and $|V(H)| = m$. Let $\lambda_1 \leq \ldots \leq \lambda_n$ and $\lambda'_1 \leq \ldots \leq \lambda'_m$ be the eigenvalues of G and H, respectively. Then the inequality

$$\lambda_i \leq \lambda'_i \leq \lambda_{n-m+i}$$

holds for all $i = 1, \ldots, m$. □

Corollary 2.28. Every multiple eigenvalue of $G - v$ is also an eigenvalue of G. □

This corollary provides a complementary tool for the reconstruction Theorem 2.13.

Eigenvalue interlacing is also observed if a matrix is block partitioned and each block is replaced by the average of its entries ([23], [12]). As an immediate application we see that the maximum eigenvalue of a graph is bounded from below by the average row sum of its adjacency matrix (which in turn equals the average node degree):

Lemma 2.29. Let G be a graph and $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ its adjacency matrix. Then,

$$\lambda_{max}(G) \geq \frac{1}{n}\sum_{i,j=1}^{n} a_{ij}.$$

□

On the other hand, the maximum eigenvalue of a graph is bounded from above by the maximum row sum of its adjacency matrix:

Lemma 2.30. Let G be a graph and $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ its adjacency matrix. Then,

$$\lambda_{max}(G) \leq \max_{j=1,\ldots,n} \sum_{i=1}^{n} a_{ji}.$$

□

Proof. Let $v = (v_i)$ be an eigenvector of A such that $\lambda_{max} v = Av$ and

$$\max_{i=1,\ldots,n} v_i = 1. \tag{7}$$

Choose an index j such that $v_j = 1$. Then we get

$$\lambda_{max} = \lambda_{max} v_j = \sum_{i=1}^{n} a_{ji} v_i \leq \sum_{i=1}^{n} a_{ji} \leq \max_{j=1,\ldots,n} \sum_{i=1}^{n} a_{ji}. \tag{8}$$

■

Another useful bound is due to YUAN:

Theorem 2.31. [45] If G is a graph with n vertices and m edges, then

$$\lambda_{max}(G) \leq \sqrt{2m - n + 1}$$

with equality if and only if G is isomorphic to K_n or $K_{1,n-1}$. □

2.2.4 Circulant graphs

In subsequent chapters we will frequently encounter circulant graphs. A *circulant* graph is a graph whose adjacency matrix is circulant. Note that this definition is invariant under isomorphisms. The spectrum of a circulant graph exhibits very strict structural properties as we will see below.

In the following, we will abbreviate $\omega = e^{\frac{2\pi i}{n}}$.

Theorem 2.32. [3] Let $(0, a_2, \ldots, a_n)^T$ be the first column of a real circulant matrix A. Then the eigenvalues of A are exactly

$$\lambda_r = \sum_{j=2}^{n} a_j \omega^{(j-1)r}, \quad r = 0, \ldots, n-1.$$

□

Corollary 2.33. Let G be a circulant graph. Let $(0, a_2, \ldots, a_n)^T$ be the first column of a circulant adjacency matrix of G. Then the eigenvalues of G are exactly

$$\lambda_r = \sum_{j=2}^{n} a_j \omega^{(j-1)r}, \quad r = 0, \ldots, n-1.$$

□

Theorem 2.34. The eigenvalues of C_n are

$$\lambda_r = \omega^r + \omega^{-r}, \quad r = 0, \ldots, n-1.$$

□

Proof. The canonical adjacency matrix (entries not specified are zero)

$$A(C_n) = \begin{pmatrix} 0 & 1 & & & 1 \\ 1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 0 & 1 \\ 1 & & & 1 & 0 \end{pmatrix} \tag{9}$$

of C_n is obviously circulant. Using Corollary 2.33 we obtain the claimed eigenvalues. ■

2.2.5 Regular graphs

For regular graphs there exist a number of special results that make it easier to deal with their spectra and eigenvectors. For example, the class of regular graphs is characterised by the maximum eigenvalue or its accompanying eigenspace:

Theorem 2.35. [3],[17] If G is regular of degree r, then r is an eigenvalue of G. Its eigenspace is spanned by the all ones vector. Further, the spectral radius $\sigma(G)$ equals r.

Conversely, if the all ones vector is an eigenvector of a graph G or if the maximum degree is an eigenvalue of G, then G must be regular. □

The complements of regular graphs can be easily analysed using the following theorem:

Theorem 2.36. [7],[17] Let G be regular of degree k. Further let

$$f_G(x) = \frac{\chi(x;G)}{x-k}, \quad f_{\overline{G}}(x) = \frac{\chi(x;\overline{G})}{x-n+1+k},$$

i.e. we omit from each characteristic polynomial the linear factor of the respective degree of regularity. Then,

$$f_G(-x-1) = (-1)^{n-1} f_{\overline{G}}(x).$$

Moreover, if G has eigenvalues $k, \lambda_2, \ldots, \lambda_n$, then its complement $\overline{G}$ has eigenvalues $n-k-1, -1-\lambda_2, \ldots, -1-\lambda_n$ with the same respective eigenvectors. □

Corollary 2.37. Let G be regular and neither a complete nor a null graph. Then,

$$E_0 = \overline{E}_{-1}, \quad E_{-1} = \overline{E}_0.$$

□

Proof. The omitted linear factors for f_G and $f_{\overline{G}}$ cannot be x or $(x+1)$. Therefore, from Theorem 2.36 we see that the multiplicities and the corresponding eigenvectors are as claimed. ■

Corollary 2.38. Let G be regular of degree k. If x is an eigenvector for eigenvalue $\lambda \neq k$, then the sum over its components vanishes. □

Proof. The sum over the components of x is zero if and only if x is perpendicular to the all ones vector. This vector spans the eigenspace of the degree of regularity k. The eigenspaces of a graph, however, are mutually perpendicular (cf. Theorem 2.14). ■

The last two corollaries will be relied on frequently.

Note that Corollary 2.38 can be easily extended to arbitrary matrices:

Lemma 2.39. Let $A \in \mathbb{R}^{n \times n}$ be symmetric. If the all ones vector is an eigenvector of A for eigenvalue λ, then for every eigenvalue $\mu \neq n - \lambda$ of $J - A$ the component sum vanishes. □

Proof. Let $A\mathbb{1} = \lambda\mathbb{1}$ and consider the matrix $B = J - A - \mu I$. If $x \in \operatorname{Ker} B$, then $Bx = 0$ and also $JBx = 0$. Thus,

$$JJx - JAx - \mu JIx = 0. \tag{10}$$

But from $JJ = nJ$, $JA = \lambda J$ and $JI = J$ we get

$$(n - \lambda - \mu)Jx = 0, \tag{11}$$

which means that the component sum of x is necessarily zero. ■

3 Graph complements

This chapter is dedicated to the relation between the eigenspaces of a graph and its complement. In particular, the eigenspaces E_0 and $\overline{E}_{-1}$ exhibit a tight connection.

In the following, let A be an $n \times n$ matrix over fixed field K and $\lambda \in K$. We begin by showing a number of results on general matrices, to be precise, we consider matrices of the form $A - \lambda J$ and study their relationship with matrix A.

Theorem 3.1. Let $\lambda \neq 0$. Then

$$\begin{aligned}\operatorname{Ker} A \cap \operatorname{Ker}(A - \lambda J) &= \{x \in \operatorname{Ker} A : \ \mathbb{1}^T x = 0\} \\ &= \{x \in \operatorname{Ker}(A - \lambda J) : \ \mathbb{1}^T x = 0\}.\end{aligned}$$

□

Proof. Let $x \in \operatorname{Ker} A \cap \operatorname{Ker}(A - \lambda J)$. Then both $Ax = 0$ and $(A - \lambda J)x = 0$. Because of

$$(A - \lambda J)x = Ax - \lambda Jx = -\lambda Jx = 0 \tag{12}$$

it follows that $Jx = 0$ and hence $\mathbb{1}^T x = 0$. This proves

$$\operatorname{Ker} A \cap \operatorname{Ker}(A - \lambda J) \subseteq \{x \in \operatorname{Ker} A : \ \mathbb{1}^T x = 0\}. \tag{13}$$

Now let $x \in \operatorname{Ker} A$ and $\mathbb{1}^T x = 0$. Then by $0 = Ax - \lambda Jx = (A - \lambda J)x$ it follows that $x \in \operatorname{Ker}(A - \lambda J)$. Conversely, if $x \in \operatorname{Ker}(A - \lambda J)$ and $\mathbb{1}^T x = 0$ we immediately get $Ax = (A - \lambda J)x = 0$ and therefore $x \in \operatorname{Ker} A$.

■

Theorem 3.2. Let $\dim \operatorname{Ker} A = d_1$ and $\dim \operatorname{Ker}(A - \lambda J) = d_2$. Then

$$\dim(\operatorname{Ker} A \cap \operatorname{Ker}(A - \lambda J)) \geq \max\{d_1, d_2\} - 1.$$

□

Proof. For $\lambda = 0$ the result is obvious. Let $\lambda \neq 0$.

Consider the matrix

$$A' = \begin{pmatrix} A \\ \mathbb{1}^T \end{pmatrix} \in K^{(n+1) \times n}. \tag{14}$$

By Theorem 3.1 the intersection of the two kernels exactly consists of all vectors x with $Ax = 0$ and $\mathbb{1}^T x = 0$. It is therefore equal to $\operatorname{Ker} A'$. Obviously, $\operatorname{rk} A' \leq \operatorname{rk} A + 1$. Thus,

$$\dim \operatorname{Ker} A' = n - \operatorname{rk} A' \geq n - (\operatorname{rk} A + 1) = \dim(\operatorname{Ker} A) - 1. \tag{15}$$

Also, for

$$A'' = \begin{pmatrix} A - \lambda J \\ \mathbb{1}^T \end{pmatrix} \in K^{(n+1)\times n} \tag{16}$$

we get

$$\dim \operatorname{Ker} A'' \geq \dim(\operatorname{Ker}(A - \lambda J)) - 1. \tag{17}$$

■

Remark 3.3. The same result can be obtained by reasoning as follows. From Theorem 3.1 we know that any vector from one of the two kernels also belongs to the other kernel exactly if the sum over all its entries is zero. Given an arbitrary basis of one of the kernels, we can construct a basis such that at least all but one of its vectors have component sum zero. Therefore, the dimensions of the two kernels cannot differ by more than one. □

Theorem 3.4.

1. $|\operatorname{rk} A - \operatorname{rk}(A - \lambda J)| \leq 1$
2. $\operatorname{rk} A < \operatorname{rk}(A - \lambda J) \;\Rightarrow\; \operatorname{Ker}(A - \lambda J) \subsetneqq \operatorname{Ker} A$
3. $\operatorname{rk} A > \operatorname{rk}(A - \lambda J) \;\Rightarrow\; \operatorname{Ker} A \subsetneqq \operatorname{Ker}(A - \lambda J)$

□

Proof. Let d_1, d_2 be as described in Theorem 3.2. Suppose $d_1 \geq d_2$. Then by Theorem 3.2 we get

$$d_1 - 1 \leq \dim(\operatorname{Ker} A \cap \operatorname{Ker}(A - \lambda J)) \leq \dim \operatorname{Ker}(A - \lambda J)) = d_2. \tag{18}$$

Thus $d_1 \leq d_2 + 1$. Analogously, $d_2 \leq d_1 + 1$ if $d_1 \leq d_2$.

Now let $\operatorname{rk} A < \operatorname{rk}(A - \lambda J)$. It follows that $d_1 = d_2 + 1$. We can choose a basis of $\operatorname{Ker} A$ such that at least $d_1 - 1$ basis vectors have zero component sum. But then by Theorem 3.1 we have found a basis for $\operatorname{Ker}(A - \lambda J)$. Hence

$$\operatorname{Ker}(A - \lambda J) \subsetneqq \operatorname{Ker} A. \tag{19}$$

Analogously, the third result follows.

■

At this point we know that if the two kernels have different dimensions the smaller kernel is contained in the other one. But in the case of equal dimensions the kernels need not necessarily be identical. We give a simple example.

Example 3.5. Consider the matrix

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

Then we have

$$\operatorname{Ker} A = \operatorname{Span}\{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\}, \qquad \operatorname{Ker}(A - J) = \operatorname{Span}\{\begin{pmatrix} -2 \\ 1 \\ -2 \end{pmatrix}\}.$$

□

If however we know that the matrix A is symmetric, then the two kernels must be identical:

Theorem 3.6. Let $A = A^T$ and $\operatorname{rk} A = \operatorname{rk}(A - \lambda J)$. Then

$$\operatorname{Ker} A = \operatorname{Ker}(A - \lambda J),$$

□

Proof. For $\lambda = 0$ this is obvious. Let $\lambda \neq 0$. Assume that

$$\operatorname{Ker} A \neq \operatorname{Ker}(A - \lambda J). \tag{20}$$

Since the kernels have equal dimension it cannot be that one kernel contains the other because then they would be identical. Therefore, there exists a vector

$$b \in \operatorname{Ker}(A - \lambda J) \setminus \operatorname{Ker} A. \tag{21}$$

Let $s = \lambda \mathbb{1} b$. Then

$$Ab = (A - \lambda J)b + \lambda Jb = \lambda Jb = s\mathbb{1}. \tag{22}$$

We see that necessarily $s \neq 0$ because otherwise $b \in \operatorname{Ker} A$ by Theorem 3.1. Let

$$\tilde{A} = \left(\, A \mid \mathbb{1} \, \right). \tag{23}$$

Then,

$$\mathbb{1} \in \operatorname{Im} A \;\Leftrightarrow\; \operatorname{rk} \tilde{A} = \operatorname{rk} A. \tag{24}$$

But $A(\frac{1}{s}b) = \mathbb{1}$, therefore $\operatorname{rk} \tilde{A} = \operatorname{rk} A$.

Let $A' = \tilde{A}^T$. Then $\operatorname{Ker} A' \subseteq \operatorname{Ker} A$. By $\operatorname{rk} A' = \operatorname{rk} \tilde{A}^T = \operatorname{rk} \tilde{A} = \operatorname{rk} A$ we even see that $\operatorname{Ker} A' = \operatorname{Ker} A$. Hence $\mathbb{1}^T x = 0$ for all $x \in \operatorname{Ker} A$. By Theorem 3.1 this means that

$$\operatorname{Ker} A \subseteq \operatorname{Ker}(A - \lambda J). \tag{25}$$

Since we have assumed that the kernels have equal dimension the theorem follows. ■

Theorem 3.7. Let $A = A^T$ and $\operatorname{rk}(A - \lambda_0 J) = \operatorname{rk} A$ for a some $\lambda_0 \neq 0$. Then for any $\lambda \in K$ we have either

$$\operatorname{rk}(A - \lambda J) = \operatorname{rk} A$$

or

$$\operatorname{rk}(A - \lambda J) = \operatorname{rk} A - 1.$$

□

Proof. Let $x \in \operatorname{Ker} A$. Then $\operatorname{Ker} A = \operatorname{Ker}(A - \lambda_0 J)$ and therefore $\mathbb{1}^T x = 0$ by Theorem 3.6 so that $x \in \operatorname{Ker}(A - \lambda J)$ by Theorem 3.1. Consequently, $\operatorname{Ker} A \subseteq \operatorname{Ker}(A - \lambda J)$ and $\operatorname{rk}(A - \lambda J) \leq \operatorname{rk} A$ for all $\lambda \in K$. By Theorem 3.2 the result immediately follows. ■

Consider the following congruence relation. Given a fixed matrix M, we will say that two matrices A and B are congruent modulo M, written $A \equiv B$, if there exists $\lambda \in K$ such that $A - B = \lambda M$. Now let $M = J$. Then $K^{n \times n}$ gets partitioned into congruence classes $C(A) = \{A - \lambda J : \lambda \in K\}$.

It turns out that only a very restricted number of possible ranks occur within each congruence class:

Theorem 3.8.

1. Let $R = \{\operatorname{rk}(A') : A' \in C(A)\}$. Then
   (a) $R = \{\operatorname{rk}(A)\}$ or
   (b) $R = \{\operatorname{rk}(A) - 1, \operatorname{rk}(A)\}$ or
   (c) $R = \{\operatorname{rk}(A), \operatorname{rk}(A) + 1\}$.
2. If $A = A^T$ then either
   (a) $\operatorname{rk} A' = \operatorname{rk} A$ for all $A' \in C(A)$ or
   (b) there exists $A'' \in C(A)$ such that

$$\operatorname{rk} A' = \operatorname{rk} A'' + 1$$

   for all $A' \in C(A)$, $A' \neq A''$.

□

Proof. The first part immediately follows from Theorem 3.4.

Now let $A = A^T$ and suppose that more than one rank occurs within $C(A)$. Then there exist matrices $\tilde{A}$, $A'' \in C(A)$ such that

$$\operatorname{rk} A'' < \operatorname{rk} \tilde{A}. \tag{26}$$

Suppose there exists a matrix $A' \in C(A)$, $A' \neq A''$ with $\operatorname{rk} A' = \operatorname{rk} A''$. Then by Theorem 3.7

$$\operatorname{rk} B \leq \operatorname{rk} A'' \tag{27}$$

for all $B \in C(A'') = C(A)$. In particular this means $\operatorname{rk} \tilde{A} \leq \operatorname{rk} A''$, a contradiction. Hence,

$$\operatorname{rk} A' = \operatorname{rk} \tilde{A} \tag{28}$$

for all $A' \in C(A)$, $A' \neq A''$. ■

The second part of Theorem 3.8 strengthens Theorem 3.7. It tells us that if two ranks exists within a class, then the smaller rank is only achieved for one single matrix of the class.

Example 3.9. Let

$$A_1 = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then any easy check on the determinant shows that $\operatorname{rk}(A_1 - \lambda J) = 2$ for all $\lambda \in \mathbb{R}$.

Let

$$A_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then for $\lambda_0 = \frac{1}{2}$ we have $A_2 - \lambda_0 J = \lambda_0 J$ so that

$$1 = \operatorname{rk}(A_2 - \lambda_0 J) < \operatorname{rk} A_2 = 2.$$

By Theorem 3.8 we know that $\operatorname{rk}(A_2 - \lambda J) = 2$ for all $\lambda \neq \lambda_0$.

□

We will now apply our results to eigenspaces of graphs and their complements.

Let $G = (V, E)$ be a graph with adjacency matrix A. Observe that

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

is the adjacency matrix of $\overline{G}$ that corresponds to the same vertex ordering. Recall the abbreviations $\overline{E}_{-1} = \operatorname{Eig}(-1; \overline{G})$ and $E_0 = \operatorname{Eig}(0; G) = \operatorname{Ker} A$.

Lemma 3.10.

$$\overline{E}_{-1} = \mathrm{Ker}(J - A).$$

□

Proof. It suffices to note that

$$\overline{E}_{-1} = \mathrm{Ker}(\overline{A} + I) = \mathrm{Ker}(J - A). \tag{29}$$

■

By virtue of this lemma and the symmetry of A, our previous results can be immediately applied to eigenspaces of graphs:

Theorem 3.11.

1. $|\dim \overline{E}_{-1} - \dim E_0\,| \leq 1$,
2. $\dim \overline{E}_{-1} < \dim E_0 \;\Rightarrow\; \overline{E}_{-1} \subsetneqq E_0$.
3. $\dim \overline{E}_{-1} = \dim E_0 \;\Rightarrow\; \overline{E}_{-1} = E_0$.

□

For regular graphs there already exist stronger results, e.g. Theorem 2.36 and Corollary 2.37.

It is interesting to note that Theorem 3.11 partly overlaps with the following known Theorem:

Theorem 3.12. [7] Let λ be a multiple eigenvalue of G. Then,

$$|\dim \overline{E}_{-\lambda-1} - \dim E_\lambda\,| \leq 1.$$

□

4 Trees

This chapter is dedicated to the study of eigenspaces of trees and their line graphs. Note that the subclass of paths will be paid special attention in a separate chapter.

The characteristic polynomial of a tree can be computed in linear time by an algorithm described in [27] and [14]. The same algorithm can also compute the rank of the adjacency matrix of a tree which for trees is twice the size of a maximum matching [8]. A fast algorithm for the direct computation of eigenvectors of trees can be found in [28]. Its ideas are based on results published in [1].

Theorem 2.16 states that the number of distinct eigenvalues of a graph is at least its diameter plus one. In [32] this result is generalised to tree pattern matrices, i.e. to general symmetric matrices whose zero/nonzero pattern represents a given tree.

An interesting result on the signs of the entries of eigenvectors of trees has been obtained in [18]. Take an eigenvector for the k-th largest eigenvalue of a tree and interpret its components as vertex weights. Then there exist at least $k-1$ edges whose endpoints have weights with opposite signs.

The spectral radius of a tree may range between that of a path and a star:

Theorem 4.1. [33] Let T be a tree on n vertices. Then,

$$2\cos\frac{\pi}{n+1} = \lambda_{max}(P_n) \leq \lambda_{max}(T) \leq \lambda_{max}(K_{1,n-1}) = \sqrt{n-1}.$$

□

The idea of the proof is to define a partial ordering of cospectral trees which preserves the ordering of the maximum eigenvalue. The relation $\lambda_{max}(P_n) \leq \lambda_{max}(B) \leq \lambda_{max}(K_{1,n-1})$ can also be obtained for the Laplacian spectrum of a tree [37].

Another way to bound the spectral radius is in terms of the maximum degree [18]:

$$\sqrt{\Delta} \leq \lambda_{max}(T) < 2\sqrt{\Delta - 1}. \tag{30}$$

Since for any graph there exists an eigenvalue λ with

$$-\sqrt{\delta} \leq \lambda \leq \sqrt{\delta} \tag{31}$$

it follows immediately that at least one eigenvalue of a forest lies in the interval $[-1, 1]$ (cf. [18]).

Counting all possible matchings of a given forest F, it is immediately possible to state its characteristic polynomial. Let $m(G, k)$ be the number of matchings of size

k of a graph G. Let formally $m(F, 0) = 1$ and

$$\mu(x; G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(G, k) x^{n-2k} \tag{32}$$

be the *matching polynomial* of G.

Theorem 4.2. [18], [20], [10] Let F be a forest. Then,

$$\chi(x; F) = (-1)^n \mu(x; F).$$

□

In particular, we see that a forest is nonsingular if and only if it contains a one-factor. Note that this relation between the characteristic and the matching polynomial even characterises the class of forests [18].

From Theorems 4.2 and 2.27 we conclude that the zeros of the matching polynomial of a forest are real and that they interlace the spectrum of any one vertex deleted induced subforest. These properties also hold for arbitrary graphs [19].

In the following, let T be a tree with vertex set $V = V(T) = \{x_1, \ldots, x_n\}$ and adjacency matrix A. If $w = (w_i)$ is an eigenvector of T, we will interpret its components as weights on the vertices of T, writing $w(x_i) = w_i$.

4.1 Eigenspaces E_0, E_{-1}, $\overline{E}_0$, and $\overline{E}_{-1}$

Theorem 3.11 implies that for an arbitrary graph at least one of the eigenspaces E_0 and $\overline{E}_{-1}$ is contained in the other one. The main result of this section is that for trees, however, the eigenspace E_0 always contains $\overline{E}_{-1}$.

It is useful to note that instead of using the summation rule (6) on the complement of a graph one can operate on the graph itself and simply let each sum comprise the values of all non-neighbours.

Further, for the sake of brevity and simplicity let us introduce the following shorthand notation:

$$\sum_M = \sum_{x_i \in M} w(x_i),$$
$$\sum_M f = \sum_{x_i \in M} w(x_i) f(x_i),$$
$$\sum_{N(M)} = \sum_{v \in M} \sum_{N(v)}$$

with $f : V \to \mathbb{R}$.

Lemma 4.3. Let G be a graph and $w = (w_i) = w(x_i)$. Then $w \in \mathrm{Eig}(-1; \overline{G})$ if and only if

$$\sum_{N(x_j)} = \sum_{V} \qquad \forall x_j \in V(G).$$

□

Proof. Let $x_j \in V(G)$. Then

$$\overline{N}(x_j) = V - N(x_j) - x_j \tag{33}$$

and therefore

$$\sum_{\overline{N}(x_j)} = \sum_{V} - \sum_{N(x_j)} - w_j. \tag{34}$$

But -1 is an eigenvalue of $\overline{T}$ if and only if

$$\sum_{\overline{N}(x_j)} = -w_j \tag{35}$$

and therefore the result follows from equation (34). ■

Remark 4.4. Application of Lemma 4.3 to trees yields some further interesting summation rules for the components of eigenvectors for the eigenvalue -1 of trees.

Let $x \in V$ be a leaf of the tree T and y its neighbour. Then we have $\overline{N}(x) = V - x - y$ and therefore

$$w(y) = \sum_{V}. \tag{36}$$

Suppose there exists an inner node z of T that is adjacent only to neighbours of leaves. Then,

$$\sum_{N(z)} = \gamma(z) \sum_{V} = \sum_{V}. \tag{37}$$

But because of $\gamma(z) \geq 2$ this means

$$\sum_{V} = 0. \tag{38}$$

□

Theorem 4.5. It holds

$$\overline{E}_{-1} \subseteq E_0$$

for all trees. □

Proof. Choose a leaf $x \in V$ and partition the vertex set into sets $M_0, M_1, \ldots, M_N$ such that (cf. figure 1)

$$\mathrm{d}(x, z) = j \forall z \in M_z. \tag{39}$$

Further, let B_i denote the leaves contained in the set M_i.

For the following computations note that

$$\sum_{M_i} (\gamma - 1) = \sum_{M_i - B_i} (\gamma - 1), \quad i \geq 1, \tag{40}$$

since leaves have degree one. Also, keep in mind that multiple neighbours in $N(M_i)$ contribute multiple times to a sum over $N(M_i)$.

Let $w \in \mathrm{Eig}(-1; \overline{T})$. We need to show that the component sum of w vanishes (cf. Theorem 3.1). Apply Lemma 4.3 for each distance level to get

$$\begin{aligned}
\sum_{N(M_0)} &= \sum_{M_1} &&= |M_0| \sum_V, \\
\sum_{N(M_1)} &= \sum_{M_2} + \sum_{M_0} &&= |M_1| \sum_V, \\
\sum_{N(M_i)} &= \sum_{M_{i+1}} + \sum_{M_{i-1}} (\gamma - 1) &&= |M_i| \sum_V, \quad 2 \leq i \leq N-1, \\
\sum_{N(M_N)} &= \sum_{M_{N-1}} (\gamma - 1) &&= |M_N| \sum_V .
\end{aligned} \tag{41}$$

The idea is that the multiset $N(M_i)$ consists of the set M_{i+1} (each of these nodes has exactly one predecessor in M_i) and the multiset derived from the predecessors of M_i (each of which has degree minus one successors in M_i). Summation of the equations (41) yields

$$\sum_{M_0} + \sum_{M_1} \gamma + \ldots + \sum_{M_{N-1}} \gamma + \sum_{M_N} = |V| \sum_V \tag{42}$$

and further

$$\sum_V \gamma = |V| \sum_V \tag{43}$$

since M_0 and M_N contain only vertices of degree one. Now assume that the component sum of w does not vanish. Let w.l.o.g. $\sum w_i = 1$. Then from equation (43) we deduce

$$n = \sum_{x_i \in V} \gamma(x_i) w(x_i) \leq (n-1) \sum_{x_i \in V} w(x_i) = n - 1, \tag{44}$$

which is impossible. ■

Corollary 4.6. It holds

$$\overline{E}_{-1} \subseteq E_0$$

for all forests. □

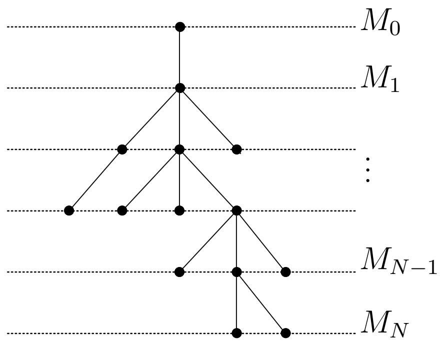


Figure 1: Partitioning tree vertices by their distance from a fixed leaf

Proof. Let G be a forest and $w \in \text{Eig}(-1; G)$. Then the restriction of w to a component of G is either the null vector or an eigenvector of the component for the same eigenvalue. Apply Theorem 4.5 on each component separately. Since the component sums of the restrictions vanish the component sum of w itself also does. ■

Remark 4.7. For graphs that are not trees it is easy to find counterexamples to Theorem 4.5, cf. figure 2. Ordering the vertices according to their labels we have

$$E_0 = \text{Span}\{(0,0,0,0,0,0,1,-1)^T\},$$
$$\overline{E}_{-1} = \text{Span}\{(0,0,0,0,0,0,1,-1)^T, (-1,2,1,-1,1,1,-1,0)^T\}.$$

□

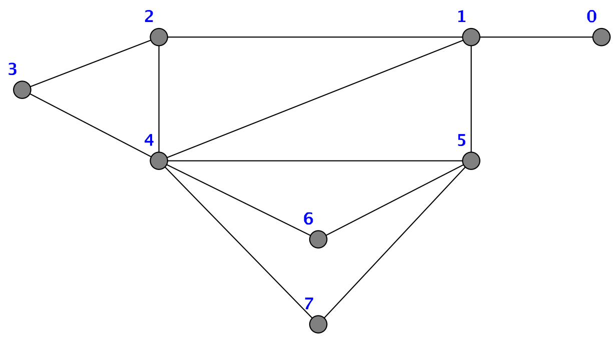


Figure 2: Graph with $\overline{E}_{-1} \not\subseteq E_0$

Remark 4.8. The relation between the eigenspaces E_{-1} and $\overline{E}_0$ can be arbitrary even for trees. In figure 3 the representative example trees are shown. □

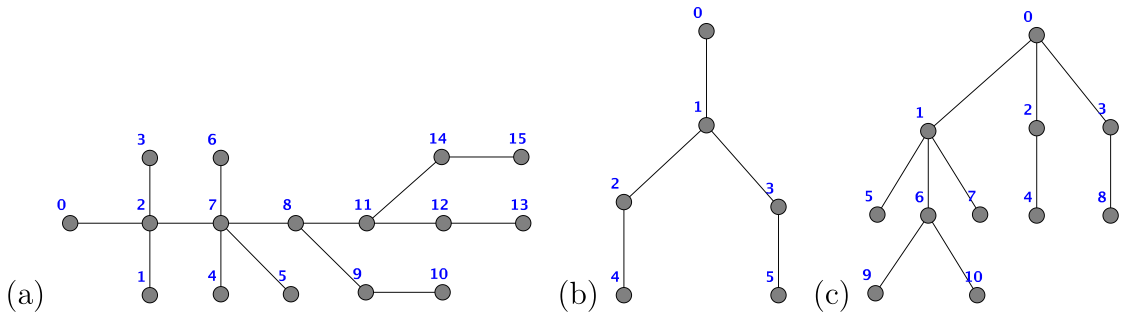


Figure 3: Example trees with (a) $E_{-1} \supsetneq \overline{E}_0$, (b) $E_{-1} = \overline{E}_0$ and (c) $E_{-1} \subsetneq \overline{E}_0$

The next theorem presents a relation between the size of the kernel of a tree and the chromatic number of the complement of its line graph. Since the rank of the adjacency matrix of a tree can be computed in linear time this offers an interesting way to determine the chromatic number $\chi(\overline{L(T)})$.

Theorem 4.9. Let T be a tree on n vertices. Then,

$$\dim E_0 = n - 2\chi(\overline{L(T)}).$$

□

Proof. To obtain a valid colouring of the vertices of T we may assign the same colour to two vertices of $\overline{T}$ only if they are adjacent in T. Since the clique number ω of T is at most 2 it is not possible to have more than two vertices in the same colour class of $\overline{T}$. Therefore, to find a colouring of $\overline{T}$ with minimal number of colours simply determine a maximum set of independent edges of T. Then the endpoints of each edge become the two-element colour classes whereas the remaining vertices form one-element colour classes.

Let c_1 and c_2 denote the numbers of the one-element and two-element colour classes, respectively. Then c_2 by construction is the independence number α of the intersection graph of all subgraphs K_2 in T (which is simply the line graph of T). Therefore,

$$c_2 = \alpha(L(T)). \tag{45}$$

We now make use of some results on perfect graphs. Remember that a graph is perfect if and only if its clique number equals the chromatic number for every induced subgraph. According to [43] a line graph is perfect if and only if its root does not contain an odd circuit of size at least 5. Further, a graph is perfect if and only its complement is perfect [9]. Hence, it follows from the acyclicity of T that $L(T)$ is perfect so that

$$\alpha(L(T)) = \omega(\overline{L(T)}) = \chi(\overline{L(T)}). \tag{46}$$

Combining equations (45) and (46) yields

$$c_2 = \chi(\overline{L(T)}). \tag{47}$$

But since c_2 is the size of a maximum matching of T we have [8]

$$c_2 = \frac{1}{2}\operatorname{rk} A = \frac{1}{2}(n - \dim E_0) \tag{48}$$

so that the result readily follows. ■

Computer experiments suggest that there always exists a basis of the kernel of a forest with a particularly simple structure:

Conjecture 4.10. For every forest there exists a basis of E_0 such that all vectors contained in this basis only have entries 0, 1, or -1. □

We provide a proof for the special case that $\dim E_0 = 1$. But beforehand we need to provide some notation and preliminary theory.

Lemma 4.11. Let F be a forest. Then,

$$\det F \in \{-1, 0, 1\}.$$

□

Proof. If F is singular we have $\det F = 0$. Let therefore F be nonsingular. Then by Theorem 4.2 and the definition (32) of the matching polynomial the number n of vertices of F is even and the constant term of $\chi(x; F)$ is exactly $\det F = (-1)^{\frac{n}{2}} m(F, \frac{n}{2}) \neq 0$. But $m(F, \frac{n}{2})$ is the number of one-factors of F. We conclude that F contains a one-factor. On the other hand, a forest may only contain a single one-factor. To see this we observe that the edges incident to leaves of F are necessarily contained in a one-factor. Removing their endpoints and all incident edges we get a smaller tree that necessarily also contains a one-factor. Repeat the procedure until all vertices have been covered by matching edges. Consequently, $\det F = (-1)^{\frac{n}{2}}$. ■

The *adjugate* $A^* = (a^*_{ij})$ of a given matrix $A = (a_{ij})$ is defined as follows. Let a^*_{ij} be the cofactor of a_{ij} in the determinant of A, i.e. $a^*_{ij} = (-1)^{i+j} \det A_{[j,i]}$ with $A_{[j,i]}$ being the matrix obtained by deleting row j and column i from A.

We will call the matrix $B(\lambda) = A - \lambda I$ derived from the adjacency matrix A of a graph G the *characteristic matrix* of G.

Let T be a tree with vertices $v_1, \ldots, v_n$. Then by P_{ij} we denote the unique path in T that joins v_i and v_j. The graph $T - P_{ij}$ is formed by removing the vertices of P_{ij} and all incident edges from T.

Theorem 4.12. [18] Let T be a tree with characteristic matrix $B(x) \in \mathbb{R}^{n \times n}$ Then,

$$b^*_{ij} = (-1)^{i+j}\chi(x; T - P_{ij}), \quad i, j = 1, \ldots, n$$

holds for the entries of the adjugate $B^*(x) = (b^*_{ij})$ of B. □

Note that [18] states this theorem for forests although the path P_{ij} does not exist if v_i and v_j lie in different components. However, the theorem holds if in this case we formally let $F - P_{ij} = \emptyset$ and therefore $\chi(x; F - P_{ij}) = 0$. This is necessary because the adjugate assumes block diagonal form if we consider a forest.

Corollary 4.13. If λ is an eigenvalue of F, then every nonzero column vector of $B^*(\lambda)$ is an eigenvector of F for the eigenvalue λ. □

Proof. Since $\chi(\lambda; F) = 0$ the result follows directly from the fact that [16]

$$B(x)B^*(x) = \chi(x; F)I. \tag{49}$$

■

Note that due to the block diagonal form of the adjugate every such eigenvector is zero on all but one of the components of F.

Lemma 4.14. Let F be a forest with adjacency matrix $A \in \mathbb{R}^{n \times n}$. Then,

$$a^*_{ij} \in \{-1, 0, 1\}$$

holds for the entries of the adjugate A^* of A. □

Proof. Observe $A^* = B^*(0)$ and apply Lemma 4.11 and Theorem 4.12 for each tree T of F. The result follows readily from $\chi(0; T - P_{ij}) = \det(T - P_{ij}) \in \{-1, 0, 1\}$ and the fact the A^* is block diagonal. ■

Lemma 4.15. If F is a simply singular forest with adjacency matrix $A \in \mathbb{R}^{n \times n}$, then

$$\operatorname{rk} A^* = 1.$$

□

Proof. Since $\lambda = 0$ is an eigenvalue of F we have

$$AA^* = B(0)B^*(0) = \chi(0; F)I = 0 \tag{50}$$

from equation (49) so that

$$\operatorname{Ker} A \supseteq \operatorname{Im} A^*. \tag{51}$$

But $\dim \operatorname{Ker} A = 1$ so that $\operatorname{rk} A^* \leq 1$.

Now let

$$\chi(x; F) = \sum_{i=0}^{n} a_i x^i. \tag{52}$$

Then we have $a_0 = 0$ and $a_1 \neq 0$. We conclude that n must be odd and that F possesses an almost perfect matching that only misses a single vertex v_i.

But then $F - v_i$ has a perfect matching i.e. a one-factor so that by Theorem 4.2 we find

$$\chi(0; F - P_{ii}) = \det(F - P_{ii}) = \det(F - v_i) \neq 0. \tag{53}$$

Hence, $A^* \neq 0$ by Theorem 4.12 and therefore $\operatorname{rk} A^* \geq 1$. ■

Theorem 4.16. Let F be a simply singular forest. Then $E_0 = \operatorname{Ker} F$ is spanned by a vector $x = (x_i)$ with entries $x_i \in \{-1, 0, 1\} \forall i$. □

Proof. Lemma 4.15 guarantees that $B^*(0)$ contains at least one nonzero column vector x. By Corollary 4.13 the vector x is an eigenvector from E_0 and by Lemma 4.14 it only contains entries 0, 1, or -1. ■

Remark 4.17. The technique we have used fails for multiply singular forests. It has been shown [18] for every tree T and induced path P that the function

$$f : x \mapsto \frac{\chi(x; T - P)}{\chi(x; T)}$$

has only simple poles. This means that by removing the path P from T each eigenvalue loses at most one degree of multiplicity. Now consider a multiply singular forest F and recall that its characteristic polynomial is the product of the characteristic polynomial of its trees.

Case 1. If F contains a multiply singular component T, then depending on whether P lies in T or not this component becomes either T or $T - P$ in $F - P$. But both are singular so that $F - P$ is singular as well.

Case 2. If all components of F are at most simply singular, then there exist at least two simply singular components in F. Therefore, after the removal of a path P there remains at least one singular component so that $F - P$ is still singular.

Overall, in view of Theorem 4.12 we see that the adjugate $B^*(0)$ of the forest F is the null matrix. We cannot use Corollary 4.13 to construct eigenvectors for $\operatorname{Ker} F$. □

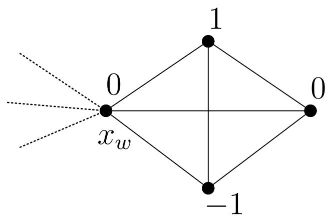
4.2 Eigenspaces of line graphs of trees

In this section we will be chiefly concerned with lower bounds in connection with the eigenvalue -1 of the line graph of a tree.

In the following, let T' denote the intersection graph of the maximum cliques of $L(T)$. It is easy to see that T' is a tree. The leaves of T' represent the *terminal cliques* of $L(T)$.

Lemma 4.18. Assign to every node of T' the size of its associated maximum clique in $L(T)$ as a node weight. Then every leaf of T' with weight $w \geq 3$ contributes $w-2$ to the multiplicity of the eigenvalue $\lambda = -1$ of $L(T)$. □

Proof. Choose a leaf of T' and let Q be its associated terminal clique in $L(T)$. Let $V(Q) = \{x_1, \ldots, x_w\}$ such that x_w is the cut vertex of Q. Now construct $w-2$ linearly independent eigenvectors $v^{(k)}$ $(k = 2, \ldots, w-1)$ for eigenvalue -1 as follows.



Let $Q' = Q - x_w$. Assign value 1 to a fixed vertex of Q', in turn -1 to one other vertex of Q' and 0 to all other vertices of $L(T)$. ■

Remark 4.19. The construction from Lemma 4.18 can be applied to arbitrary graphs G in the sense that each maximum clique Q of $L(G)$ with homogeneous exterior neighbourhood (i.e. $N(x) \setminus V(Q)$ is the same for every vertex $x \in V(Q)$) contributes to the multiplicity of the eigenvalue $\lambda = -1$ of $L(G)$. □

Lemma 4.20. Let $x = (x_i) \in \operatorname{Eig}(-1; L(T))$ and M be the nodes of a maximum clique of $L(T)$. If M contains not only cut vertices, then

$$\sum_{v_i \in M} x_i = 0.$$

□

Proof. Let $v_j \in M$ not be a cut vertex. Then $N(v_j) = M - v_j$. For $x = (x_i) \in \mathrm{Eig}(-1; L(T))$ we have in particular

$$\sum_{v_i \in N(v_j)} x_i = -x_j \tag{54}$$

so that we get

$$0 = \sum_{v_i \in N(v_j)+v_j} x_i = \sum_{v_i \in M} x_i. \tag{55}$$

■

Theorem 4.21. Let $x = (x_i) \in \mathrm{Eig}(-1; L(T))$ such that for every every cut vertex $v_j \in L(T)$ we have $x_j = 0$. Then,

$$x \in \mathrm{Eig}(-1; L(T)^{(k)}) \ \forall k \in \mathbb{N}.$$

□

Proof. Let $d \in \mathbb{N}$ and let $x = (x_i)$ be as described. For every maximum clique of $L(T)$ the sum over the corresponding entries of x vanishes because either Lemma 4.20 can be applied or by the prerequisites of the theorem the concerned entries of x are zero anyway.

Let $v \in L(T)$ and consider the sum S_k over the entries of x that correspond to vertices z with $\mathrm{d}(z, v) \leq k$. For $k = 1$ we have the closed neighbourhood $N(v) + v$.

If v is a cut vertex we see that its closed neighbourhood comprises exactly two maximum cliques of $L(T)$, otherwise only one maximum clique. Now consider $S_2, S_3, \ldots, S_d$. Each time, the range of the sum is extended by a number of maximum cliques, excluding some of the cut vertices which may already have been in the sum. But since the values of cut vertices are zero anyway we may split the overall sum into partial sums that each range over a single maximum clique. Therefore, all partial sums except the initial sum S_1 vanish. The summation rule (6) thus yields the same result both for $L(T)$ and for every distance power. ■

It should be remarked that, in general, for the linegraph of a tree there exist many vectors x that fulfil the prerequisites of Theorem 4.21. According to Lemma 4.18, each terminal clique of $L(T)$ with $w \geq 3$ vertices gives rise to $w - 2$ linearly independent eigenvectors that vanish on the cut-vertices of $L(T)$.

Note that the closed neighbourhood of a vertex $v \in L(T)$ corresponds to an induced K_1 or K_2 in T'. The extension of the sums can be interpreted as the inclusion of the next distance level from this induced subgraph using a breadth first search on T'.

Corollary 4.22. The construction from the proof of Lemma 4.18 can be used to obtain a basis of E_{-1} for any distance power of $L(T)$. □

We will conclude this section by quoting some interesting results on the eigenvalues 0 and -1 of line graphs of trees.

Theorem 4.23. [22] The eigenvalue $\lambda = 0$ is at most simple for the graph $L(T)$. Attach a new vertex v to the tree T to obtain the graph $T + v$. Then for exactly one of the graphs $L(T)$ and $L(T + v)$ the eigenvalue $\lambda = 0$ is simple. □

The preceding theorem allows to deduce a number of properties of the kernel of $L(T)$. For instance, it can be shown that for singular $L(T)$ there exists no vertex from T' such that an eigenvector from $\text{Ker}(L(T))$ contains exactly two nonzero entries within the corresponding maximum clique in $L(T)$.

Theorem 4.24. [41] If $L(T)$ is singular, then T necessarily has an even number of vertices. □

Theorem 4.25. [41] Let $L(T)$ be singular. Then a vertex v can be removed from $L(T)$ such that at least $\lambda = 0$ or $\lambda = -1$ is a multiple eigenvalue of $L(T) - v$. □

This theorem allows a partition of all trees into two classes.

Conversely, note that by Theorems 2.13 and 2.27 every multiple eigenvalue of $L(T) - v$ is also an eigenvalue of $L(T)$.

5 Paths

In this chapter we will investigate the spectrum of paths P_n. We will start with recursion formulae for the calculation of the characteristic polynomial, then we will analyse the structure of eigenvectors of paths and proceed to the complete determination of the spectrum and all associated eigenvectors. Finally, the relation between the eigenspaces for eigenvalues 0 and -1 for paths and their complements will be examined.

5.1 Recursion formulae for $\chi(x)$

Recursions for the calculation of the characteristic polynomial $\chi(x)$ of paths have long been known [15],[6],[39], although not necessarily connected to the notion of graphs.

In the following, let $a_n(x) = \chi(x; P_n)$ and formally $a_0(x) = 1$.

Theorem 5.1. [25]

$$a_n(x) = -xa_{n-1}(x) - a_{n-2}(x) \quad \text{for } n \geq 2.$$

□

Proof. We have

$$a_n(x) = \begin{vmatrix} -x & 1 & 0 & \dots & 0 \\ 1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \dots & 0 & 1 & -x \end{vmatrix}. \tag{56}$$

Expanding along the last row yields

$$a_n(x) = -xa_{n-1} - \begin{vmatrix} -x & 1 & 0 & \dots & 0 \\ 1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & 1 & 0 \\ \vdots & \ddots & \ddots & -x & 0 \\ 0 & \dots & 0 & 1 & 1 \end{vmatrix}. \tag{57}$$

The result now follows by expanding the remaining determinant along the last column. ■

An especially interesting algorithmic proof can be found in [27]. It relies on the fact that the characteristic polynomial of a tree can be elegantly determined in linear time by a symbolic algorithm that works directly on the graph.

The following generalisation reveals an even deeper connection between the characteristic polynomials of paths:

Theorem 5.2.

$$a_n(x) = a_i(x)a_{n-i}(x) - a_{i-1}(x)a_{n-i-1}(x) \quad \text{for } 1 \leq i \leq n-1.$$

□

Proof. For $n = 2$ the result is clear. Therefore let $n \geq 3$. For the sake of readability we will omit the function argument of the a_i. By Theorem 5.1 we have

$$a_0 = -xa_1 - a_2 \tag{58}$$

and

$$a_{n-1} = -xa_{n-2} - a_{n-3}. \tag{59}$$

Rewriting Theorem 5.1 as

$$a_n = a_1a_{n-1} - a_0a_{n-2} \tag{60}$$

and substituting equations (58) and (59) we arrive at

$$\begin{aligned} a_n &= -xa_1a_{n-2} - a_1a_{n-3} - (-x)a_1a_{n-2} + a_2a_{n-2} \\ &= -a_1a_{n-3} + a_2a_{n-2}. \end{aligned} \tag{61}$$

The result now follows by repeated application of this technique. ■

Remark 5.3. Phrasing Theorem 5.2 in terms of matching polynomials, the same recursion has been found in [10] already. □

5.2 The spectrum of P_n

Lemma 5.4. [3] P_n has exactly n distinct and simple eigenvalues. □

Proof. Since P_n has diameter $n-1$ we conclude from Theorem 2.16 that P_n has at least n distinct eigenvalues. Adding up the minimum dimensions of the eigenspaces we see that all eigenvalues must be simple. ■

Lemma 5.5. If $n \in \mathbb{N}$, then for the spectral radius of P_n we have

$$\rho(P_n) \leq 2.$$

□

Proof. Since P_n is a subgraph of C_n the spectral radius of P_n does not exceed the degree of regularity 2 of a circuit (cf. Theorem 2.35 and Corollary 2.19). Alternatively, the result also follows from Lemma 2.30 since the maximum row sum of any adjacency matrix of P_n equals 2. ■

We will now determine the complete spectrum of P_n which can be found by a number of different approaches ([39],[33],[7]). For example, by deleting any vertex from a circuit C_{n+1} we get a path P_n. Therefore we can use Theorem 2.13 to derive the spectrum of P_n from the spectrum of C_{n+1} (cf. Theorem 7.3). We will, however, simply describe the eigenvectors and eigenvalues of P_n ([6]) and restrict ourselves to direct verification:

Theorem 5.6. For $j = 1, \ldots, n$ let $x^{(j)} = (x_k^{(j)}) \in \mathbb{R}^n$ with

$$x_k^{(j)} = \sin\left(\frac{jk\pi}{n+1}\right), \quad k = 1, \ldots, n.$$

Then the set $\{x^{(1)}, \ldots, x^{(n)}\}$ forms a basis of $\mathbb{R}^n$ consisting of eigenvectors of P_n with the respective eigenvalues

$$\lambda_j = 2\cos\left(\frac{j\pi}{n+1}\right).$$

Moreover, we have $\lambda_1 > \lambda_2 > \ldots > \lambda_n$. □

Proof. Consider the k-th entries ($k = 2, \ldots, n-1$) of $Ax^{(j)}$ and $x^{(j)}$ for the canonical adjacency matrix A of P_n. Their ratio is

$$\frac{\sin\left(\frac{j(k-1)\pi}{n+1}\right) + \sin\left(\frac{j(k+1)\pi}{n+1}\right)}{\sin\left(\frac{jk\pi}{n+1}\right)}. \tag{62}$$

Applying the formula [4]

$$\sin\alpha + \sin\beta = 2\sin\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right) \tag{63}$$

for $\alpha = c(k+1)$ and $\beta = c(k-1)$ with $c = \frac{j\pi}{n+1}$ we see that the above ratio equals λ_j. Alternatively, Taylor expansion at $k = 0$ also immediately leads to the same result.

To show that $\lambda_j > \lambda_{j+1}$ we consider λ_j as a continuous function of $j \in \mathbb{R}$. It is easy to see that its derivative

$$\frac{-2\pi}{n+1} \sin\left(\frac{j\pi}{n+1}\right) \tag{64}$$

is always negative for $1 \leq j \leq n$.

The reasoning so far is also formally valid for $k = 1$ and $k = n$.

Linear independence of the vectors $x^{(1)}, \ldots, x^{(n)}$ is obvious as they represent eigenvectors of pairwise different eigenvalues (cf. Theorem 2.3). ■

For the determinant of these eigenvectors of P_n we can find a surprisingly simple formula:

Theorem 5.7. Let $A = (a_{jk}) \in \mathbb{R}^{n\times n}$ with $a_{jk} = \sin\left(\frac{jk\pi}{n+1}\right)$. Then

$$\det A = \left(\frac{n+1}{2}\right)^{\frac{n}{2}}.$$

□

Proof. Consider the matrix $B = (b_{pq}) = A^2$. Then we have

$$b_{pq} = \sum_{j=1}^{n} \sin\frac{jp\pi}{n+1} \sin\frac{jq\pi}{n+1}. \tag{65}$$

Using the equality

$$\sin x \sin y = \frac{1}{2}(\cos(x-y) - \cos(x+y)) \tag{66}$$

from [4] we find

$$\begin{aligned} b_{pq} &= \frac{1}{2}\sum_{j=1}^{n}\left(\cos\frac{j(p-q)\pi}{n+1} - \cos\frac{j(p+q)\pi}{n+1}\right) \\ &= \frac{1}{2}\sum_{j=0}^{n}\cos\frac{j(p-q)\pi}{n+1} - \frac{1}{2}\sum_{j=0}^{n}\cos\frac{j(p+q)\pi}{n+1} \\ &= \frac{1}{2}\sum_{j=0}^{n}\cos\frac{j(p-q)\pi}{n+1}. \end{aligned} \tag{67}$$

For $p = q$ this sum consists only of ones, whereas for $p \neq q$ we have a complete sum of real parts of roots of unity. Consequently, it follows that

$$b_{pq} = \begin{cases} 0 & \text{for } p \neq q \\ \frac{n+1}{2} & \text{for } p = q \end{cases}. \tag{68}$$

To complete the proof it suffices to observe that

$$(\det A)^2 = \det A^2 = \left(\frac{n+1}{2}\right)^n.$$

■

In particular, this again ensures the linear independence of the vectors constructed in Theorem 5.6.

In figure 4 the spectrum of the graphs $P_2, \ldots, P_{22}$ is plotted as points. They lie on the curves we get from viewing the λ_i as continuous functions of $n \in \mathbb{R}$. Observe the interlacing of the spectra of P_n and P_{n+1} (cf. Theorem 2.27).

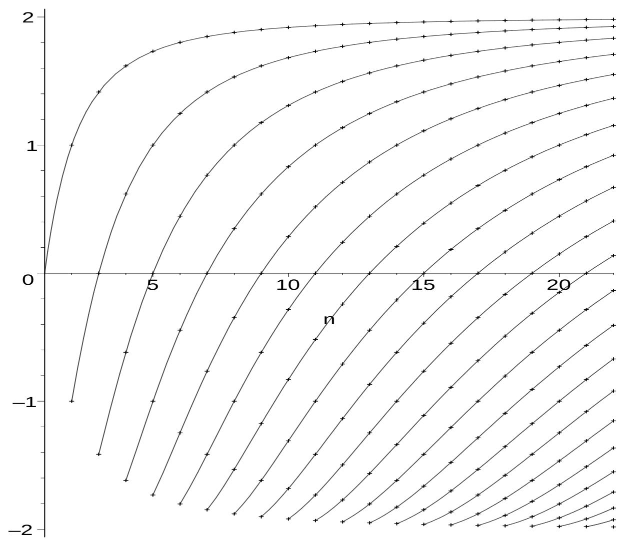


Figure 4: The spectrum of the paths $P_2, \ldots, P_{22}$

Remark 5.8. Of all graphs on n vertices the path P_n has the smallest spectral radius (i.e. maximum eigenvalue) [7]. □

Having computed the entire spectrum of P_n, it is now also possible to give an explicit formula for its characteristic polynomial, e.g. by assembly of linear factors. But other formulations are also possible:

Theorem 5.9. [7]

$$\chi(x; P_n) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^{n-k} \binom{n-k}{k} x^{n-2k} = \frac{\sin\left((n+1)\arccos\left(-\frac{x}{2}\right)\right)}{\sqrt{1-\frac{x^2}{4}}}.$$

□

Proof. Both representations follow by straightforward induction on n (use Theorem 5.1). ■

Note that the same result can be obtained in the context of matching polynomials, e.g. by using generating functions [10].

To conclude this section, we present an interesting result on continued fractions that is closely related to the spectra of paths.

Theorem 5.10. Given $n \in \mathbb{N}$ there exists a real number $c > 0$ such that the first n members of the sequence

$$c, \; -\frac{1}{c} + c, \; -\frac{1}{-\frac{1}{c} + c} + c, \; -\frac{1}{-\frac{1}{-\frac{1}{c} + c} + c} + c, \; \ldots$$

have strictly alternating signs. □

Proof. Let $n \in \mathbb{N}$ and A be the canonical adjacency matrix of P_n. We conduct an LU decomposition [21] of the matrix $B = A + cI$. To construct the upper triangular matrix U, we proceed as follows. For $i = 1, \ldots, n-1$, multiply row i of $B = (b_{ij})$ by $-\frac{b_{i+1,i}}{b_{ii}}$ and add it to row $i+1$. As a result, U contains the continued fraction on its main diagonal, the upper diagonal contains all ones, and the remaining entries of U are zero.

It is clear that for P_i with $1 \leq i \leq n-1$ the respective upper triangular matrices of the LU decomposition are principal submatrices of the matrix U we get for P_n. Now choose $c > 0$ such that it is smaller than every positive eigenvalue of the paths $P_1, \ldots, P_{n-1}$. Since paths are bipartite, by Corollary 2.24 their spectrum is symmetrical around zero. Therefore, comparing matrices A and B for our choice of c, we see that a spectral shift has been conducted that has only changed exactly one eigenvalue sign, namely the eigenvalue 0 has become $c > 0$.

Now consider the sets $M_s = \{b_{11}, b_{22}, \ldots, b_{ss}\}$ for $s = 1, \ldots, n$. Keeping in mind the spectral shift, we can use M_s to reconstruct the inertia of P_s because any principal submatrix of U has the same inertia as a principal submatrix of B with the same size. But as a result of the spectral shift, we see that for even s we have as many positive as negative elements in M_s, whereas for odd s the number of positive members exceeds the number of negative elements by exactly one. Consequently, because of $M_1 \subseteq M_2 \subseteq \ldots \subseteq M_s$ we see that the signs of the b_{ii} must be strictly alternating along the main diagonal of B. ■

5.3 Eigenvector structure

Although we already have completely determined the eigenvectors of P_n it is worthwhile to take a closer look to reveal interesting structural properties. In particular, in this section we will see that the entries of an eigenvector of P_n can be determined by evaluation of the characteristic polynomials $a_0, \ldots, a_{n-1}$. Also the nature of any zero entries is exposed.

In the following, let $x = (x_i) \in \mathbb{R}^n$ be an eigenvector of P_n for eigenvalue λ. Let A be the tridiagonal adjacency matrix of P_n.

Theorem 5.11. Let $x_{j-1} = 0$ for some $j \in \{3, \ldots, n-1\}$. Then,

$$c \cdot x^T = (-a_{j-3}, \ldots, -a_1, -a_0, 0, a_0, a_1, \ldots, a_{n-j})\,(-\lambda)$$

for some $c \in \mathbb{R}$, $c \neq 0$. □

Proof. First note that $Ax = \lambda x$ translates to the equations

$$x_{i-1} + x_{i+1} = \lambda x_i, \qquad i = 2, \ldots, n-1. \tag{69}$$

Let $x_{j-1} = 0$. Assume $x_j = 0$. Then by eq. (69) it would follow that $x_{j+1} = 0$ and so on, yielding $x = 0$, which is a contradiction. Therefore, w.l.o.g. let $x_j = 1$. In this case eq. (69) yields $x_{j+1} = \lambda$. Therefore,

$$x_j = a_0(-\lambda), \tag{70}$$

$$x_{j+1} = a_1(-\lambda). \tag{71}$$

Now assume that

$$x_{i-1} = a_{k-1}(-\lambda), \tag{72}$$

$$x_i = a_k(-\lambda) \tag{73}$$

holds for a pair i, k of integers with $2 \leq i \leq n-1$ and $k \geq 0$.

Then by eq. (69) we see that

$$a_{k-1}(-\lambda) + x_{i+1} = \lambda a_k(-\lambda). \tag{74}$$

Using Theorem 5.1 for $x = -\lambda$, we get

$$x_{i+1} = a_{k+1}(-\lambda). \tag{75}$$

Hence by repeated application of this step we conclude that x is a multiple of the vector

$$(*, 0, a_0(-\lambda), a_1(-\lambda), \ldots, a_{n-j}(-\lambda)).$$

The remaining entries can be determined in a similar manner by observing that eq. (69) yields

$$x_{j-1} = -a_0(-\lambda). \tag{76}$$

■

Remark 5.12. Note that neither $x_1 = 0$ nor $x_n = 0$ can occur as this would automatically lead to $x = 0$. □

Theorem 5.13. We have

$$\begin{aligned} c \cdot x^T &= (a_0, a_1, \ldots, a_{n-1})\,(-\lambda) \\ &= (a_{n-1}, a_{n-2}, \ldots, a_0)\,(-\lambda) \end{aligned}$$

for some $c \in \mathbb{R}$, $c \neq 0$. □

Proof. From $Ax = \lambda x$ we can derive the equations

$$x_2 = \lambda x_1, \tag{77}$$

$$x_{n-1} = \lambda x_n. \tag{78}$$

Setting $x_0 = 0$ and $x_{n+1} = 0$, these equations attain the same formal structure as in eq. (69). So formally the proof of Theorem 5.11 remains valid for this case. ■

Both theorems reveal a tight relationship between the characteristic polynomials a_i and the eigenvectors of P_n.

We can expose even more structure due to symmetry:

Lemma 5.14.

1. If $n = 2k$, then we have

   $$c \cdot x^T = (a_0, a_1, \ldots, a_{k-1}, a_{k-1}, \ldots, a_1, a_0)\,(-\lambda)$$

   for some $c \in \mathbb{R}$, $c \neq 0$.

2. If $n = 2k + 1$, then either we have

   $$c \cdot x^T = (a_0, a_1, \ldots, a_{k-1}, a_k, a_{k-1}, \ldots, a_1, a_0)\,(-\lambda)$$

   or

   $$c \cdot x^T = (a_0, a_1, \ldots, a_{k-1}, 0, -a_{k-1}, \ldots, -a_1, -a_0)\,(-\lambda)$$

   for some $c \in \mathbb{R}$, $c \neq 0$.

□

Proof. Having assumed that we number the vertices of P_n from one end to the other, we will now reverse the vertex numbering. This automorphism transforms any eigenvector z_1 of P_n into another eigenvector z_2 of P_n, belonging to the same eigenvalue (see Theorem 2.17). Lemma 5.4 states that P_n has exactly n distinct and simple eigenvalues. So z_1 and z_2 must be linearly dependent, and the result follows from Theorem 5.13. ■

Note that the equation $a_k(-\lambda) = 0$ from the second alternative of the second case implies that $-\lambda$ is an eigenvalue of P_k.

Having determined the entries around any zero entry of an eigenvector, we will continue our investigation of the role of the zero entries.

Theorem 5.15. Let $n \equiv j \mod j+1$. If w is an eigenvector of P_j, then

$$x^T = (w, 0, -w, 0, w, \ldots)$$

yields an eigenvector x of P_n for the same eigenvalue. □

Proof. The summation rules derived for the adjacency matrix of P_j are also valid for the adjacency matrix of P_n. Therefore, the summation for any vertex that is not one of the inserted zero weight vertices yields a common multiple. For the remaining zero weight vertices, however, we get a zero sum by construction. ■

Corollary 5.16. Any eigenvector w of P_k gives rise to an eigenvector

$$x = (w, 0, -w)^T$$

of P_{2k+1} for the same eigenvalue. Therefore, the spectrum of P_k is contained in the spectrum of P_{2k+1} (cf. [14]). □

Proof. We have $2k+1 \equiv k \mod k+1$. ■

Corollary 5.17. The path P_{2k+1} is always singular with eigenvector

$$(1, 0, -1, 0, 1, 0, \ldots)^T.$$

□

The construction from Theorem 5.15 gives rise to zero entries in eigenvectors of paths. The following theorem states that this is the only way to introduce zero entries.

Theorem 5.18. If $x = (x_i)$ is an eigenvector of P_n for eigenvalue λ and $x_{j+1} = 0$, then

$$n \equiv j \mod j+1.$$

□

Proof. From Theorem 5.13 we conclude that $a_j(-\lambda) = x_{j+1} = 0$. But because of Theorem 5.11 this must be also the value of x_{2j+1}. Therefore, from $x = (w, 0, -w, *)^T$ with $w = (x_1, \ldots, x_{j-1})^T$ it follows that in fact $x = (w, 0, -w, 0, *)^T$. Repeat this conclusion for the newly discovery zero entry. We finally get r copies of $\pm w$ and $r-1$ zero entries between them, which means that $n \equiv j \mod j+1$. ■

We now know exactly under what circumstances path eigenvectors contain zero entries. It is therefore very easy to state their exact number:

Corollary 5.19. If $x = (x_i)$ is an eigenvector of P_n and k the smallest index for which $x_k = 0$, then x contains exactly $\frac{n-k+1}{k}$ zero entries. □

5.4 Eigenspaces E_0, E_{-1}, $\overline{E}_0$, and $\overline{E}_{-1}$

We have seen in section 3 that there exist interesting relations between the eigenspaces for the eigenvalues 0 and -1 of a graph and its complement. We will therefore study these eigenspaces for paths and a number of derived graph classes.

First we will study the eigenspace E_0 of P_n. The following theorem summarises some results that have already been discovered and characterises the relation between E_0 and $\overline{E}_{-1}$.

Theorem 5.20.

1. P_n is singular if and only if n is odd.
2. For $n \geq 2$, n odd, E_0 is spanned by the vector

$$(1, 0, -1, 0, 1, 0, -1, \ldots)^T.$$

3. If $n \equiv 3 \mod 4$, then $E_0 = \overline{E}_{-1}$, otherwise $\overline{E}_{-1} = \{0\}$.

□

Proof.

1. Checking Theorem 5.6 it is immediately clear that $\lambda_j = 0$ occurs if and only if n is odd.
2. This is Corollary 5.17.
3. Since P_n is a tree, Theorem 4.5 implies $\overline{E}_{-1} \subseteq E_0$. But for even n the path P_n is nonsingular and therefore $\overline{E}_{-1} = \{0\}$. Let $n \geq 2$ be odd. Then we see that exactly for $n \equiv 3 \mod 4$ the eigenvector $(1, 0, -1, 0, 1, 0, -1, \ldots)^T$ that spans E_0 has component sum zero. Consequently, by Theorem 3.1 we have $\overline{E}_{-1} \supseteq E_0$, which proves equality. For $n \equiv 1 \mod 4$ we have $\overline{E}_{-1} = \{0\}$ because no other vector from the superspace E_0 has component sum zero.

■

Remember that if P_n is singular, the eigenvalue $\lambda = 0$ is only simple.

Now we will focus on the eigenspace E_{-1} of P_n and its relation to $\overline{E}_0$.

Lemma 5.21.

1. $E_{-1} \neq \{0\}$ if and only if $n \equiv 2 \mod 3$. In this case the eigenspace is spanned by the vector
$$(-1, 1, 0, -1, 1, 0, -1, 1, \ldots, 0, -1, 1)^T.$$
2. $E_{-1} \subseteq \overline{E}_0$.

□

Proof.

1. From Theorem 5.6 it follows easily that $\lambda_j = -1$ is an eigenvalue of P_n if and only if
$$j = \frac{2}{3}(n+1) \in \mathbb{N}. \tag{79}$$
This happens exactly for $n \equiv 2 \mod 3$. Summing over all adjacent vertices of P_n, it is readily checked that
$$(-1, 1, 0, -1, 1, 0, -1, 1, \ldots, 0, -1, 1)^T.$$
is an eigenvector of P_n for eigenvalue -1. It spans E_{-1} because all eigenvalues of P_n are simple.

2. E_{-1} is spanned by a vector with component sum zero, so by Theorem 3.1 the claim follows.

■

Theorem 5.22.

1. Let $x = (x_i) \in \overline{E}_0$. Then x has the form

$$(a, b, 0, a, b, 0, \ldots)^T$$

with numbers $a, b \in \mathbb{R}$.

2. Let $n \geq 4$. Then $\overline{E}_0 = E_{-1}$.

□

Proof.

1. Let A be the canonical adjacency matrix of P_n. Consider a vector $x = (x_i)$ from the kernel of the adjacency matrix $B = J - A - I$ of $\overline{P_n}$. For $j = 2, \ldots, n-2$ we form the differences of the components j and $j+1$ of $Bx = 0$. We see that

$$x_i = x_{i+3} \tag{80}$$

for $i = 1, \ldots, n-3$ so that $x = (a, b, c, a, b, c, \ldots)^T$. Taking the difference for $j = 1$ yields $x_3 = 0$.

2. Let $n \geq 4$ and $x \in \overline{E}_0$. We will show that $x = (x_i)$ has component sum zero, then by Lemma 5.21 the result follows. Assume w.l.o.g. that

$$\sum_{i=1}^{n} x_i = 1. \tag{81}$$

From the first component of $Bx = 0$ we see that

$$\sum_{i=3}^{n} x_i = 0 \tag{82}$$

and therefore

$$x_1 + x_2 = 1. \tag{83}$$

We will now consider three cases:

Case 1. Let $n = 3k$. Then by the first part of the theorem and equations (81), (83) we have

$$1 = \sum_{i=1}^{n} x_i = k(x_1 + x_2 + x_3) = k. \tag{84}$$

But this would mean $n = 3$, a contradiction.

Case 2. Let $n = 3k + 1$. Then from the last component of $Bx = 0$ we deduce

$$0 = \sum_{i=1}^{n-2} x_i = (k-1)(x_1 + x_2 + x_3) + x_1 + x_2 = (k-1) + 1 = k. \tag{85}$$

But this would mean $n = 1$, a contradiction.

Case 3. Let $n = 3k + 2$. Then in a similar fashion as in case 1 we find

$$1 = \sum_{i=1}^{n} x_i = k(x_1 + x_2 + x_3) + x_1 + x_2 = k + 1. \tag{86}$$

But this would mean $n = 2$, a contradiction.

■

Table 1 conveys an impression of what we have found out up to this point of the section. The remaining cases for $n \leq 3$ can be checked by hand.

n	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
$\dim E_0$	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
$\dim \overline{E}_{-1}$	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0
$\dim E_{-1}$	1	0	0	1	0	0	1	0	0	1	0	0	1	0	0	1	0	0	1
$\dim \overline{E}_0$	2	1	0	1	0	0	1	0	0	1	0	0	1	0	0	1	0	0	1

Table 1: Dimensions of E_0, E_{-1}, $\overline{E}_0$ and $\overline{E}_{-1}$ for the paths $P_2, \ldots, P_{20}$

Our reasoning so far can be applied to unions of paths and their complements. Keep in mind that the restriction of an eigenvector of a union of graphs to one of the components trivially yields an eigenvector on that component for the same eigenvalue. Conversely, arbitrary eigenvectors for a common eigenvalue can be determined for every component and then be combined into an eigenvector of the union for the same eigenvalue. We may also choose null vectors on the components as long as at least one vector is not the null vector.

Theorem 5.23. Consider the union $2P_n$.

1. If n is even, then $E_0 = \overline{E}_{-1} = \{0\}$.

2. If $n \equiv 3 \mod 4$, then $E_0 = \overline{E}_{-1}$ and $\dim E_0 = 2$.
3. If $n \equiv 1 \mod 4$, then $E_0 \supsetneq \overline{E}_{-1}$ and $\dim E_0 = 2$.

□

Proof. First note that Corollary 4.6 ensures $\overline{E}_{-1} \subseteq E_0$.

1. From Theorem 5.20 we see that P_n and therefore also $2P_n$ is nonsingular if and only if n is even. In this case we have $E_0 = \overline{E}_{-1} = \{0\}$.
2. If $n \equiv 3 \mod 4$ we get an eigenvector for eigenvalue 0 on each component, their component sum being zero. Therefore they span E_0 so that $\dim E_0 = 2$. But by Theorem 3.1 they also span the subspace $\overline{E}_{-1}$.
3. If $n \equiv 1 \mod 4$ we also get an eigenvector for eigenvalue 0 on each component, but we have non-vanishing component sums. Combining them into a basis of E_0 we see that $\dim E_0 = 2$. Since E_0 contains a vector with non-vanishing component sum we may find a basis of E_0 that contains only exactly one such vector. Hence, by Theorem 3.1 we have $\dim \overline{E}_{-1} = 1$.

■

Corollary 5.24. $2P_n$ is nonsingular if and only if n is even. □

Theorem 5.25. Consider the union $2P_n$. Then, $E_{-1} = \overline{E}_0$ and

$$\dim E_{-1} = \begin{cases} 2 & \text{if } n \equiv 2 \mod 3 \\ 0 & \text{otherwise} \end{cases}.$$

□

Proof. Remembering Lemma 5.21, we find that for $n \equiv 2 \mod 3$ we have $\dim E_{-1} = 2$ with a basis of eigenvectors with vanishing component sums. Also, $E_{-1} = \{0\}$ for all other choices of n.

We will now show that $\overline{E}_0$ is nontrivial only for $n \equiv 2 \mod 3$ and that in this case we get a basis of two eigenvectors with vanishing component sum. This will prove $E_{-1} = \overline{E}_0$.

Let A be the canonical adjacency matrix of $2P_n$, i.e. the block diagonal matrix consisting of two canonical adjacency matrices of P_n. Let $x \in \overline{E}_0 = \mathrm{Ker}(J - A - I)$, i.e. $Bx = 0$ for $B = J - A - I$.

Taking the difference of the n-th and $(n+1)$-th components of $Bx = 0$, we find

$$x_{n-1} + x_n = x_{n+1} + x_{n+2}. \tag{87}$$

Further, the difference of components $n-1$ and n as well as $n+1$ and $n+2$ yields

$$x_{n-2} = x_{n+3} = 0. \tag{88}$$

Using a technique similar to that in Theorem 5.22 on the first and second n components, we can deduct the following structure of the vector x:

$$x = (a, b, 0, a, b, 0, a, \ldots, c, 0, d, c, 0, d, c)^T. \tag{89}$$

We now need to consider three different cases.

Case 1. Let $n = 3k$. Then the center of x is

$$x = (*, a, b, 0, 0, d, c, *)^T. \tag{90}$$

Equations (87) and (88) imply that

$$a = c = 0 \ \wedge \ b = d. \tag{91}$$

Looking into component n of $Bx = 0$, we see that

$$\begin{aligned} 0 &= \sum_{i=1}^{n} x_i + 0 + 0 + \sum_{i=n+3}^{2n} x_i \\ &= k(a+b) + 0 + 0 + c + (k-1)(c+d) \\ &= (2k-1)b. \end{aligned} \tag{92}$$

But now from $2k - 1 \neq 0$ we conclude $b = d = 0$ and therefore $x = 0$.

Case 2. Let $n = 3k + 1$. Then the center of x is

$$x = (*, b, 0, a, c, 0, d, *)^T. \tag{93}$$

In a similar way as in case 1 we find that $x = 0$.

Case 3. Let $n = 3k + 2$. Then the center of x is

$$x = (*, 0, a, b, d, c, 0, *)^T. \tag{94}$$

Equation (87) implies that

$$a + b = c + d. \tag{95}$$

Considering component $n + 1$ of $Bx = 0$ we find that

$$0 = k(a+b) + a + b + 0 + 0 + k(c+d) = (2k+1)(a+b). \tag{96}$$

Thus, $a + b = 0 = c + d$ so that the component sum of x vanishes. ■

Examples of our findings can be found in table 2.

n	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$\dim E_0$	0	2	0	2	0	2	0	2	0	2	0	2	0	2
$\dim \overline{E}_{-1}$	0	2	0	1	0	2	0	1	0	2	0	1	0	2
$\dim E_{-1}$	2	0	0	2	0	0	2	0	0	2	0	0	2	0
$\dim \overline{E}_0$	2	0	0	2	0	0	2	0	0	2	0	0	2	0

Table 2: Dimensions of E_0, E_{-1}, $\overline{E}_0$ and $\overline{E}_{-1}$ for the graphs $2P_2, \ldots, 2P_{15}$

Theorem 5.26. Consider the graph $G = P_n \cup P_{n+1}$.

1. For all $n \in \mathbb{N}$ we have $\dim E_0 = 1$.
2. We have $\overline{E}_{-1} = \{0\}$ unless $n \equiv 2$ or $n \equiv 3 \mod 4$, in which case $E_0 = \overline{E}_{-1}$.
3. $E_{-1} = \{0\}$ if and only if $3|n$ (i.e. $|G| \equiv 1 \mod 6$). Otherwise, $\dim E_{-1} = 1$.
4. $E_{-1} = \overline{E}_0$.

□

Proof.

1. Exactly one of the graphs P_n and P_{n+1} is singular, therefore $\dim E_0 = 1$.
2. We have vanishing component sums within E_0 if and only if

$$n \equiv 3 \mod 4 \ \vee \ n+1 \equiv 3 \mod 4, \tag{97}$$

that is if

$$n \equiv 2 \mod 4 \ \vee \ n \equiv 3 \mod 4. \tag{98}$$

Since G is a forest, this completely determines $\overline{E}_{-1}$.

3. We get an eigenvector with component sum zero that spans E_{-1} exactly for

$$n \equiv 2 \mod 3 \ \vee \ n+1 \equiv 2 \mod 3. \tag{99}$$

Otherwise, $3|n$ and we have $E_{-1} = \{0\}$.

4. It can be easily seen that $\overline{E}_0$ is spanned by a single vector with component sum zero if

$$n \equiv 2 \mod 3 \ \vee \ n+1 \equiv 2 \mod 3. \tag{100}$$

$\overline{E}_0$ is trivial otherwise. Therefore we have $E_{-1} = \overline{E}_0$.

■

n	1	2	3	4	5	6	7	8	9	10	11	12
$\dim E_0$	1	1	1	1	1	1	1	1	1	1	1	1
$\dim \overline{E}_{-1}$	0	1	1	0	0	1	1	0	0	1	1	0
$\dim E_{-1}$	1	1	0	1	1	0	1	1	0	1	1	0
$\dim \overline{E}_0$	1	1	0	1	1	0	1	1	0	1	1	0

Table 3: Dimensions of E_0, E_{-1}, $\overline{E}_0$ and $\overline{E}_{-1}$ for $P_n \cup P_{n+1}$, $n = 1, \ldots, 12$

The respective eigenspace dimensions have been compiled in table 3.

A cocktail party graph $CP(2n)$ is formed by removal of a one-factor from K_{2n}. In particular, this graph is regular so that by Corollary 2.37 we have $E_0 = \overline{E}_{-1}$ and $E_{-1} = \overline{E}_0$. The complement of a cocktail party graph is nP_2 so that we can use our findings about paths to study eigenspaces E_0 and E_{-1} of cocktail party graphs.

Theorem 5.27. Consider $G = CP(2n)$. Then,

1. $\dim E_0 = n$,
2. $E_{-1} = \{0\}$.

□

Proof. The complement of $G = CP(2n)$ is nP_2. It has eigenvalues 1 and -1 with multiplicity n each, which means that 0 is an eigenvalue of G with multiplicity n. Also, nP_2 is never singular so that $E_{-1} = \{0\}$. ■

Note that the spectrum of $CP(2n)$ can be completely determined by Theorem 2.33 because the graph is circulant with generating vector $(0, 1, \ldots, 1, 0, 1, \ldots, 1)^T$ (zeros at positions 1 and $n+1$). We find that $\lambda_0 = 2n - 2$ and $\lambda_r = -1 - \omega^{rn}$ for $1 \leq r \leq 2n - 1$, proving the previous theorem a second time.

6 Distance powers $P_n^{(d)}$ of paths

In this section we deal with distance powers of paths. We will be concerned with a number of different topics, among them recursion formulae of the characteristic polynomial, multiple eigenvalues, and common eigenvectors.

Let $\lceil \frac{n}{2} \rceil \leq d < n$. Then the canonical adjacency matrix A of $P_n^{(d)}$ derived from the canonical adjacency matrix of P_n takes the form of a banded matrix with a zero main diagonal and both d upper and lower bands containing all ones.

To start with, we look at the distribution of the eigenvalues of $P_n^{(d)}$.

Theorem 6.1. Let $\lceil \frac{n}{2} \rceil \leq d < n$ and $s = n - d - 1$. Let $\lambda_1 \leq \ldots \leq \lambda_n$ be the eigenvalues of $P_n^{(d)}$. Then

$$\begin{gathered} \lambda_1, \ldots, \lambda_{s+1} < -1, \\ \lambda_{s+2} = \ldots = \lambda_{n-s} = -1, \\ \lambda_{n-s+1}, \ldots, \lambda_n > -1. \end{gathered}$$

□

Proof. Applying a sequence of symmetrical row and column operations, we will perform a principal axis transformation on $A+I$ so that we obtain a diagonal matrix with the same inertia.

Step 1. Iterate $j = 1, \ldots, s+1$ and nest $i = j+1, \ldots, n-s$. Each time, subtract row j from row i and after that column j from column i. Then our matrix takes the form:

$$\begin{pmatrix} J_{1,1} & N_{1,s} & N_{1,n-2s-1} & N_{1,s} \\ N_{s,1} & N_{s,s} & N_{s,n-2s-1} & I_s \\ N_{n-2s-1,1} & N_{n-2s-1,s} & N_{n-2s-1,n-2s-1} & N_{n-2s-1,s} \\ N_{s,1} & I_s & N_{s,n-2s-1} & J_{s,s} \end{pmatrix}. \tag{101}$$

Remove the first row and column from matrix (101) because we can already see that they hint at a positive eigenvalue in $A+I$. Note that this effects a shift in row and column indices.

Step 2. Iterate $j = 1, \ldots, s$ and nest $i = 1, \ldots, s$. Each time, subtract row j divided by two from row $d+i$ (columns likewise). Then the lower right block becomes null so that the matrix takes the form:

$$\begin{pmatrix} N_{s,s} & N_{s,n-2s-1} & I_s \\ N_{n-2s-1,s} & N_{n-2s-1,n-2s-1} & N_{n-2s-1,s} \\ I_s & N_{s,n-2s-1} & N_{s,s} \end{pmatrix}. \tag{102}$$

Step 3. For $i = 1, \dots, s$ add row $n-1-s+i$ divided by two to row i (columns likewise). This yields

$$\begin{pmatrix} I_s & N_{s,n-2s-1} & I_s \\ N_{n-2s-1,s} & N_{n-2s-1,n-2s-1} & N_{n-2s-1,s} \\ I_s & N_{s,n-2s-1} & N_{s,s} \end{pmatrix}. \tag{103}$$

Step 4. Now we eliminate the upper left and lower right unit blocks. For $i = 1, \dots, s$ subtract row i from row $n-1-s+i$ (columns likewise). Then we finally reach the form

$$\begin{pmatrix} I_s & N_{s,n-2s-1} & N_{s,s} \\ N_{n-2s-1,s} & N_{n-2s-1,n-2s-1} & N_{n-2s-1,s} \\ N_{s,s} & N_{s,n-2s-1} & -I_s \end{pmatrix}. \tag{104}$$

Keeping in mind the additional positive eigenvalue and the initial spectral shift, we see that the proof is complete. ■

Note that hereafter similar requirements on d will be encountered repeatedly, as most proof techniques applied rely decisively on the fact that there exist vertices of $P_n^{(d)}$ that are adjacent to all other vertices. In particular, $P_n^{(n-1)} = K_n$.

6.1 Distance squares $P_n^{(2)}$ of paths

Remembering Theorem 5.1 one may ask if equally elegant recursion formulae exist for arbitrary distance powers of paths. Although this is possible, such formulae are somewhat tedious to derive, as we can already see for $P_n^{(2)}$:

Theorem 6.2. Let $p_i(x) = \chi(P_i^{(2)}; x)$ and formally $p_0(x) = 1$. Then for $n \geq 5$ the following equality holds:

$$p_n(x) = -(x+1)\left(p_{n-1}(x) + p_{n-2}(x) - p_{n-3}(x) - p_{n-4}(x)\right) + p_{n-5}(x).$$

□

Proof. Let A_k be the canonical adjacency matrix of $P_k^{(2)}$. Then we define the matrices

$$R_k = A_k - xI \tag{105}$$

and

$$Q_1 = (1), \; Q_2 = \begin{pmatrix} -x & 1 \\ 1 & 1 \end{pmatrix}, \; Q_k = \begin{pmatrix} R_{k-1} & e_{k-1} + e_{k-2} \\ e_{k-1}^T & 1 \end{pmatrix}, k \geq 3, \tag{106}$$

where e_i denotes the i-th unit vector of appropriate size.

We observe that

$$\det Q_k = \det R_{k-1} - \det Q_{k-1} \tag{107}$$

for $k \geq 2$.

Expanding along the last row of R_n we see that

$$\det R_n = -x \det T_1 - \det T_2 + \det T_3 \tag{108}$$

with $T_1 = R_{n-1}$ and

$$T_2 = \begin{pmatrix} R_{n-2} & e_{n-2} \\ e_{n-2}^T + e_{n-3}^T & 1 \end{pmatrix}, \; T_3 = \begin{pmatrix} R_{n-3} & e_{n-3} & 0 \\ e_{n-4}^T + e_{n-3}^T & 1 & 1 \\ e_{n-3}^T & -x & 1 \end{pmatrix}. \tag{109}$$

We see $T_2 = Q_{n-1}^T$ so that

$$\det T_2 = \det Q_{n-1} = \det R_{n-2} - \det Q_{n-2}. \tag{110}$$

Expand T_3 along its last column to get

$$\det T_3 = \det T_{31} - \det T_{32} \tag{111}$$

with $T_{31} = Q_{n-2}^T$ and

$$T_{32} = \begin{pmatrix} R_{n-3} & e_{n-3} \\ e_{n-3}^T & -x \end{pmatrix}. \tag{112}$$

We now expand T_{32} along its last column so that

$$\det T_{32} = -x \det T_{321} - \det T_{322} \tag{113}$$

with $T_{321} = R_{n-3}$ and

$$T_{322} = \begin{pmatrix} R_{n-4} & e_{n-4} + e_{n-5} \\ 0^T & 1 \end{pmatrix}. \tag{114}$$

But by expanding T_{322} along its last row it follows immediately that $\det T_{322} = \det R_{n-4}$.

Collecting the results we arrive at

$$\det R_n = -x \det R_{n-1} - \det R_{n-2} + x \det R_{n-3} + \det R_{n-4} + 2 \det Q_{n-2}. \tag{115}$$

Repeated use of the recursion (107) to eliminate all occurrences of Q_i yields

$$\begin{aligned} \det R_n = &- x \det R_{n-1} - \det R_{n-2} + x \det R_{n-3} + \det R_{n-4} \\ &+ 2 \sum_{j=0}^{n-3} (-1)^{n-j-1} \det R_j. \end{aligned} \tag{116}$$

Writing $\det R_i$ as $p_i(x)$, we get

$$p_n(x) = -xp_{n-1}(x) - p_{n-2}(x) + xp_{n-3}(x) + p_{n-4}(x) + 2\left(\sum_{j=0}^{n-3}(-1)^{n-j-1}p_j(x)\right). \quad (117)$$

Use the previous equation to compute $p_n(x)$ and $p_{n-1}(x)$. Then for the sum we have

$$\begin{aligned} p_n(x) + p_{n-1}(x) = &- xp_{n-1}(x) - (x+1)p_{n-2}(x) + (x-1)p_{n-3}(x) \\ &+ (x+1)p_{n-4}(x) + p_{n-5}(x) + 2p_{n-3}(x). \end{aligned} \quad (118)$$

The result now follows by solving for $p_n(x)$. ■

Corollary 6.3. Let $n \in \mathbb{N}$. Then,

$$\det P_n^{(2)} = \begin{cases} \frac{n}{3} + 1 & \text{if } n \equiv 0 \mod 3 \\ 0 & \text{if } n \equiv 1 \mod 3 \\ -\frac{n-2}{3} - 1 & \text{if } n \equiv 2 \mod 3 \end{cases}$$

i.e. the sequence $(\det P_n^{(2)})_{n \in \mathbb{N}_0}$ reads

$$1, 0, -1, 2, 0, -2, 3, 0, -3, 4, 0, -4, \ldots$$

if we formally let $\det P_0^{(2)} = 1$. □

Proof. For $n \in \{1, 2, 3, 4\}$ the theorem is easily checked by hand.

So let $n \geq 5$. We proceed by induction. Assume that the theorem has been proven for the determinants of $P_0^{(2)}, \ldots, P_{n-1}^{(2)}$.

Abbreviating $c_i = \det P_i^{(2)}$ and noting that $c_i = \chi(0; P_i^{(2)})$, we evaluate the recursion formula from Theorem 6.2 at $x = 0$ to get

$$c_n = -c_{n-1} - c_{n-2} + c_{n-3} + c_{n-4} + c_{n-5}. \quad (119)$$

Note that by assumption

$$(c_0, c_1, c_2, c_3, \ldots, c_{n-1}) = (1, 0, -1, 2, 0, -2, \ldots). \quad (120)$$

We need to consider three cases:

Case 1. Let $n = 3q$ and prove $c_n = q + 1$.
Case 2. Let $n = 3q + 1$ and prove $c_n = 0$.
Case 3. Let $n = 3q + 2$ and prove $c_n = -(q + 1)$.

Since these cases are all alike we will only prove the first case. Let therefore $n = 3q$.

From (120) we conclude that

$$c_{n-1} = -q, \quad c_{n-2} = 0, \quad c_{n-3} = q, \quad c_{n-4} = -(q-1), \quad c_{n-5} = 0. \tag{121}$$

Inserting these values into equation (119), the result $c_n = q+1$ follows immediately. ■

Since we can compute $\det P_n^{(2)}$ it is now possible to reconstruct the characteristic polynomial of $P_n^{(2)}$ from the characteristic polynomials of its one vertex deleted subgraphs:

Theorem 6.4. Let $V(P_n^{(2)}) = \{v_1, \ldots, v_n\}$. Assume that

$$\chi(x; P_n^{(2)} - v_i) = a_{i,n-1}x^{n-1} + \ldots + a_{i,1}x + a_{i,0}.$$

Then,

$$\chi(x; P_n^2) = -\frac{1}{n}\left(\sum_{i=1}^{n} a_{i,n-1}\right)x^n - \ldots - \frac{1}{2}\left(\sum_{i=1}^{n} a_{i,1}\right)x^2 - \left(\sum_{i=1}^{n} a_{i,0}\right)x + \det P_n^{(2)}.$$

□

Proof. This is a direct consequence of Theorem 2.13 and Lemma 2.1. ■

6.2 Bounds for the maximum eigenvalue of $P_n^{(d)}$

In this section we will develop bounds for the maximum eigenvalue of $P_n^{(d)}$ and analyse their quality. We start with an upper bound:

Theorem 6.5. Let $1 \leq d < n-1$. Then,

$$\lambda_{max}(P_n^{(d)}) \leq \sqrt{-(d + d^2 - 2nd) - n + 1}.$$

□

Proof. For $d < n-1$ the graph $P_n^{(d)}$ has exactly

$$m = \sum_{i=1}^{d}(n-i) = dn - \frac{1}{2}d(d+1) \tag{122}$$

edges. By virtue of Theorem 2.31 the result now follows. ■

Remark 6.6. Another upper bound is given by the maximum row sum of the canonical adjacency matrix (cf. Theorem 2.30), that is

$$\lambda_{max}(P_n^{(d)}) \leq \min(n-1, 2d). \tag{123}$$

Since $P_n^{(d)}$ is a subgraph of the graph $C_n^{(d)}$ which is regular of degree $\min(n-1, 2d)$ we can also derive this bound by means of Corollary 2.19. □

Theorem 6.7. Let $1 \leq d < n-1$ and

$$b(n,d) = -\frac{d + d^2 - 2nd}{n}.$$

Then,

$$\lambda_{max}(P_n^{(d)}) \geq b(n,d).$$

□

Proof. Remembering that the sum s of all entries of an adjacency matrix equals twice the number of edges, we can use equation (122) to find $s = d(2n - d - 1)$ so that the result follows by Lemma 2.29. ■

Remark 6.8. In order to prove Theorem 6.7 we have basically used the block quotient technique described in [23] on a single block. One may ask if a less trivial partition of the matrix may yield a better bound. For even n a straightforward choice would be a partition of the adjacency matrix into four equally sized blocks. The eigenvalues of the resulting 2×2 quotient matrix could be computed directly. It turns out, however, that this approach leads to exactly the same bound as in Theorem 6.7. □

Figure 5 exemplifies the bounds we have derived. The maximum eigenvalues of $P_{14}^{(d)}$ have been plotted as points and whereas the bounds are shown as continuous functions. In particular, we see that for small values of d the simple piecewise linear upper bound from equation (123) is tighter than the upper bound from Theorem 6.5. The lower bound appears to be tighter than any of the two upper bounds.

We proceed with an analysis of the lower bound.

Theorem 6.9. Let $\lambda_1 \leq \ldots \leq \lambda_n$ be the eigenvalues of $P_n^{(d)}$, $1 \leq d < n-1$. If $b(n,d)$ denotes the bound from Theorem 6.7, then

$$\lambda_i \leq b(n,d)$$

holds for $i = 1, \ldots, d+1$. □

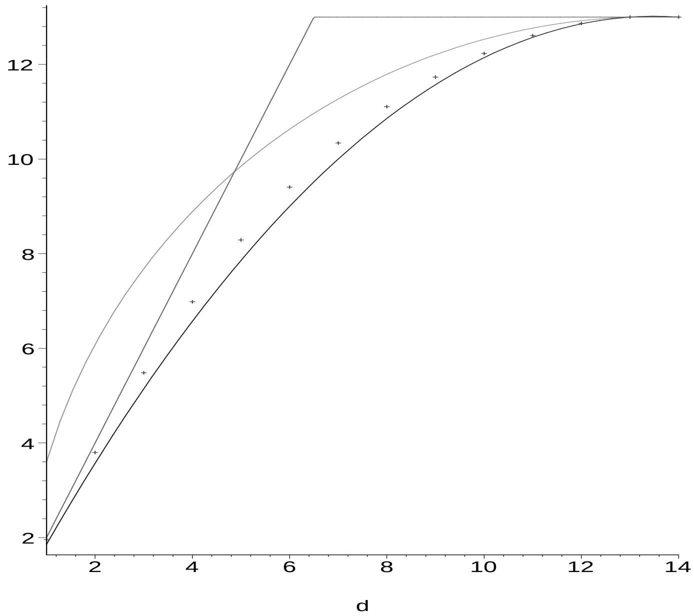


Figure 5: Bounds for the maximum eigenvalue of $P_{14}^{(d)}$

Proof. Let A be the canonical adjacency matrix of $P_n^{(d)}$. The main idea is as follows. Shift the spectrum of A to the left by the value of the bound to test. Then determine the inertia of the resulting matrix $A + cI$ to see how many eigenvalues have been separated by the bound. For this purpose we will compute an LDL^T decomposition ([35],[16]) of the symmetric matrix $A + cI$ such that D is diagonal and L is a lower triangular matrix with an all ones main diagonal. Since $U = DL^T$ is an upper triangular matrix we see that this is basically an LU decomposition. But U has the same main diagonal as D, so it has the same inertia. To compute the triangular matrix U it suffices to conduct a Gauss forward elimination procedure without pivoting.

First observe that the upper left $(d + 1) \times (d + 1)$ principal submatrix of the A is the canonical adjacency matrix of $P_{d+1}^{(d)} = K_{d+1}$. It is straightforward to verify that LU decomposition of this principal submatrix of $A + cI$ yields an upper triangular matrix $U = (u_{ij}) \in \mathbb{R}^{(d+1)\times(d+1)}$ with

$$u_{ij} = \begin{cases} 0 & \text{if} \quad i > j \\ \frac{(c-1)(c-1+i)}{c-2+i} & \text{if} \quad i = j \\ \frac{c-1}{c-2+i} & \text{if} \quad i < j \end{cases} . \tag{124}$$

Since this matrix is a principal submatrix of the upper triangular matrix computed for the full matrix $A + cI$, we can check the signs of the main diagonal entries u_{ii} to get lower bounds for the number of separated eigenvalues. Substituting

$$-c = b(n, d) = -\frac{d + d^2 - 2nd}{n} \tag{125}$$

we get

$$u_{ii} = \frac{(d + d^2 - 2nd - n)(d + d^2 - 2nd - n + in)}{n(d + d^2 - 2nd - 2n + in)}. \tag{126}$$

For the numerator we see that

$$d + d^2 - 2nd - n = -(d + 1)(n - d) - nd < 0 \tag{127}$$

and

$$d + d^2 - 2nd - n + in = d(d + 1) - (2d + 1 - i)n < 0 \tag{128}$$

since $d \leq 2d + 1 - i$ (remember $1 \leq i \leq d + 1$) and $d + 1 < n$. On the other hand, the denominator is negative:

$$\begin{aligned} d + d^2 - 2nd - 2n + in &= (d - 2n)(d + 1) + in \\ &< -n(d + 1) + in \\ &= (i - (d + 1))n \\ &\leq 0. \end{aligned} \tag{129}$$

Hence, $u_{ii} < 0$ for $i = 1, \ldots, d + 1$. But this means that for $-c = b(n, d)$ the matrix $A + cI$ has at least $d + 1$ negative eigenvalues. ■

Note that the bound $b(n, d)$ is always positive for $d \in \mathbb{N}$. Therefore, the above theorem blends with Theorem 6.1 which for sufficiently large values of d guarantees a number of negative eigenvalues of $P_n^{(d)}$.

However, we can prove much better separation even for smaller values of d than those demanded by Theorem 6.1.

Theorem 6.10. Let $d \geq n - \frac{1}{2}\left(1 + \sqrt{2n^2 + 1}\right)$. Then the bound from Theorem 6.7 separates λ_{max} from the rest of the spectrum of $P_n^{(d)}$. □

Proof. Let $\lambda_1 > \ldots > \lambda_r$ be the different eigenvalues of $P_n^{(d)}$. In [38] is was shown that

$$\lambda_2 \leq \frac{n}{2} - 1. \tag{130}$$

Keeping in mind that $1 \leq d \leq n - 1$, it is straightforward to check that this upper bound for the second largest eigenvalue is strictly smaller than the lower bound $b(n, d)$ for that largest eigenvalue if and only if

$$d > n - \frac{1}{2}\left(1 + \sqrt{2n^2 + 1}\right). \tag{131}$$

■

Corollary 6.11. Let $d \geq \frac{1}{3}n$. Then the bound from Theorem 6.7 separates λ_{max} from the rest of the spectrum of $P_n^{(d)}$. □

Proof. It suffices to note that

$$\frac{1}{3}n \geq \left(1 - \frac{1}{2}\sqrt{2}\right) n \geq n - \frac{1}{2}\left(1 + \sqrt{2n^2+1}\right). \tag{132}$$

■

Figure 6 illustrates the separation property of the bound $b(n,d)$. In fact, it seems that the lower bound $b(n,d)$ provides a good estimate for the largest eigenvalue of $P_n^{(d)}$.

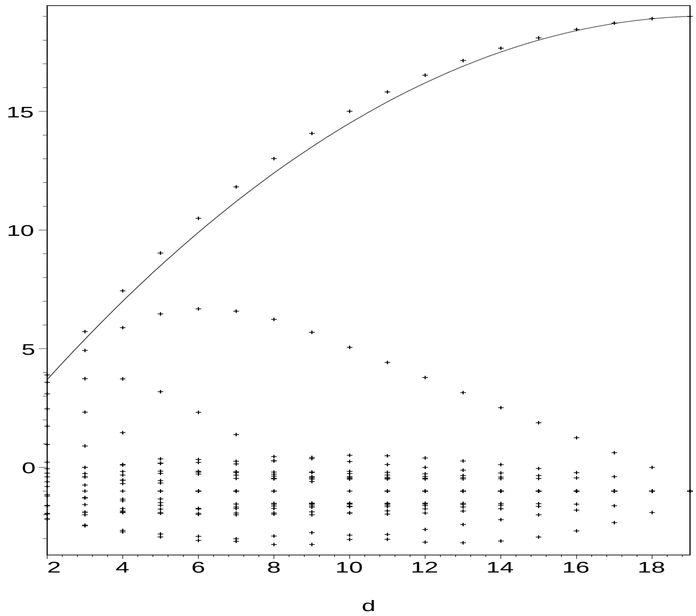


Figure 6: Separation of the maximum eigenvalue of $P_{20}^{(d)}$

Remark 6.12. Note that $P_n^{(d)}$ is an induced subgraph of $C_{n+d}^{(d)}$. Therefore, we know by Theorem 2.27 that the eigenvalues of $P_n^{(d)}$ interlace those of $C_{n+d}^{(d)}$. Since the eigenvalues of $C_{n+d}^{(d)}$ are well-known (cf. section 8) one would expect to derive usable eigenvalue bounds from the interlacing property. But especially for the larger eigenvalues the interlacing may prove too loose to be of much use. On the other hand, if λ is an eigenvalue of $C_{n+d}^{(d)}$ with multiplicity k, the interlacing property guarantees us that λ is also an eigenvalue of $P_n^{(d)}$ with multiplicity at least $k - d$.

Both issues can be seen in figure 7 where the eigenvalues of $P_n^{(d)}$ are denoted by circuits that lie in the interlacing intervals predicted from the eigenvalues of $C_{n+d}^{(d)}$. □

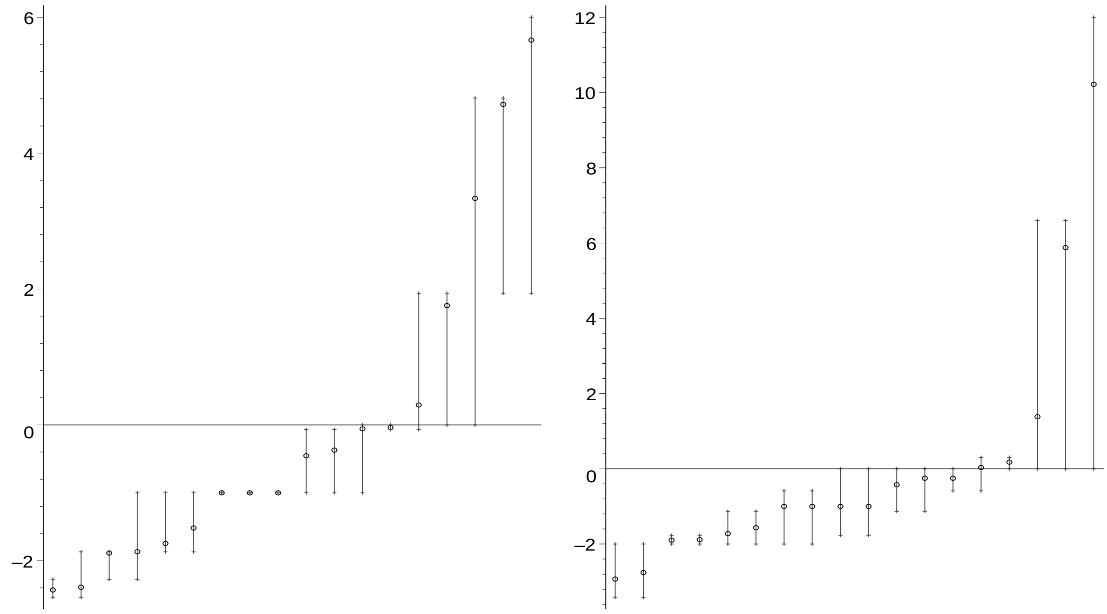


Figure 7: Eigenvalue interlacing of $P_n^{(d)}$ and $C_{n+d}^{(d)}$ for $P_{18}^{(3)}$ and $P_{18}^{(6)}$

To conclude this section we will use the previous results to check under what circumstances the maximum eigenvalue of a path power cannot be rational.

Theorem 6.13. Let $d \in \mathbb{N}$. Then $\lambda_{max}(P_n^{(d)}) \notin \mathbb{Q}$ if $n > d^2 + d$. □

Proof. Let $d \in \mathbb{N}$ and $n > d^2 + d$. Then from Theorem 6.7 we deduct

$$\lambda_{max}(P_n^{(d)}) > 2d - 1.$$

On the other hand, from Remark 6.6 and Corollary 2.19 it follows that

$$\lambda_{max}(P_n^{(d)}) < 2d.$$

Therefore, $\lambda_{max}(P_n^{(d)})$ cannot be integer. But assuming $\lambda_{max}(P_n^{(d)})$ to be rational would then contradict Lemma 2.15. ■

6.3 Multiple eigenvalues

In this section we will study the occurrence of eigenvalues with multiplicity greater than one. We will see that for sufficiently large d all eigenvalues of $P_n^{(d)}$ except $\lambda = -1$ must be simple.

To start with, we study the structure of eigenvectors belonging to simple eigenvalues of $P_n^{(d)}$.

Lemma 6.14. Let λ be a simple eigenvalue of $P_n^{(d)}$ and v a corresponding eigenvector.

1. If n is even, then v either has the form
$$(\dots, a_2, a_1, a_0, -a_0, -a_1, -a_2, \dots)^T$$
or
$$(\dots, a_2, a_1, a_0, a_0, a_1, a_2, \dots)^T.$$
2. If n is odd, then v either has the form
$$(\dots, a_2, a_1, 0, -a_1, -a_2, \dots)^T$$
or
$$(\dots, a_2, a_1, a_0, a_1, a_2, \dots)^T.$$

□

Proof. Let P be the permutation matrix that reverses the canonical vertex ordering of $P_n^{(d)}$. Then by Theorem 2.17 the product Pv is also an eigenvector for eigenvalue λ. Since λ is simple we have
$$Pv = \mu v \tag{133}$$
for some $\mu \in \mathbb{R}$. But P is an involution so that $P^2 = I$. Hence,
$$v = P^2 v = \mu P v = \mu^2 v \tag{134}$$
and therefore
$$\mu = \pm 1. \tag{135}$$
Consequently, $Pv = v$ or $Pv = -v$ so that vector v possesses the claimed form. ■

In the following, two values s, t will be associated with a given graph $P_n^{(d)}$ as follows:
$$s = 2d + 2 - n, \quad t = n - d - 1. \tag{136}$$
Because of
$$n = t + s + t \tag{137}$$
we will write eigenvectors of $P_n^{(d)}$ as
$$(a \mid b \mid c) = (a_1, \dots, a_t, b_1, \dots, b_s, c_1, \dots, c_t)$$
with $a = (a_i) \in \mathbb{R}^t$, $b = (b_i) \in \mathbb{R}^s$ and $c = (c_i) \in \mathbb{R}^t$.

Note that for $\frac{n}{2} < d < n - 1$ we have $s \geq 2$ and $t \geq 1$. In this case, the canonical adjacency matrix of $P_n^{(d)}$ looks like
$$A(P_n^{(d)}) = \begin{pmatrix} J_t - I_t & J_{t,s} & \tilde{L}_t \\ J_{s,t} & J_s - I_s & J_{s,t} \\ \tilde{R}_t & J_{t,s} & J_t - I_t \end{pmatrix}. \tag{138}$$

Theorem 6.15. Let $\frac{n}{2} < d < n-1$. Then

1. $\dim \mathrm{Eig}(-1; P_n^{(d)}) = s-1$,
2. the vectors

$$\{(0 \mid e_1 - e_2 \mid 0)^T, (0 \mid e_1 - e_3 \mid 0)^T, \ldots, (0 \mid e_1 - e_s \mid 0)^T\},$$

   constitute a basis of $\mathrm{Eig}(-1; P_n^{(d)})$ ($e_i \in \mathbb{R}^s$ is the i-th unit vector).

□

Proof. Let $\frac{n}{2} < d < n-1$ and A the canonical adjacency matrix of $P_n^{(d)}$. From equation (138) it is clear that

$$\mathrm{rk}(A+I) \leq \mathrm{rk}\begin{pmatrix} J_t & J_{t,s} & \tilde{L}_t \\ \mathbb{1}^T & \mathbb{1}^T & \mathbb{1}^T \\ \tilde{R}_t & J_{t,s} & J_t \end{pmatrix} = 2t+1 = s-1. \tag{139}$$

On the other hand, it is easy to see that the $s-1$ vectors

$$\begin{pmatrix} 0 \\ \hline 1 \\ -1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hline 1 \\ 0 \\ -1 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 \\ \hline 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ -1 \\ \hline 0 \end{pmatrix}. \tag{140}$$

are linearly independent and indeed eigenvectors of $P_n^{(d)}$ for eigenvalue $\lambda = -1$. Therefore, they form a basis of $\mathrm{Eig}(-1; P_n^{(d)})$. ■

Remark 6.16. According to Theorem 6.15 the set $\mathrm{Eig}(-1; P_n^{(d)}) \setminus \{0\}$ contains exactly those vectors $v = (x \mid z \mid y)^T$ such that not all components of z are identical. Therefore we can distinguish between two types of eigenvectors of $P_n^{(d)}$ for $\lambda \neq -1$:

$$v^T = (x \mid 0 \mid y) \qquad \text{type I}$$

and

$$cv^T = (x \mid \mathbb{1}^T \mid y) \qquad \text{type II}$$

for some $c \in \mathbb{R}$, $c \neq 0$. □

Lemma 6.17. Let $v = (x \mid 0 \mid y)^T \in \mathrm{Eig}(\lambda; P_n^{(d)})$. Assume that any other vector from this eigenspace that has the same form is a multiple of v.

Then

$$v = (x_1, x_2, \ldots, x_t, 0, \ldots, 0, x_t, \ldots, x_2, x_1)^T$$

or

$$v = (x_1, x_2, \ldots, x_t, 0, \ldots, 0, -x_t, \ldots, -x_2, -x_1)^T$$

for some vector $x = (x_i) \in \mathbb{R}^t$. □

Proof. Use a symmetry argument like in the proof of Lemma 5.14. ■

Note that Lemma 6.17 holds in particular if λ is simple.

Theorem 6.18. Any eigenspace basis of $P_n^{(d)}$ affords at most one vector of type I. □

Proof. Let A be the canonical adjacency matrix of $P_n^{(d)}$ and let $v = (x \mid 0 \mid y)^T$ be a type I eigenvector. Then we have

$$(A + I)v = \lambda v \tag{141}$$

for some $\lambda \neq 0$ (cf. Remark 6.16) and therefore

$$J_t x + J_{t,s} 0 + \tilde{L}_t y = \lambda x, \tag{142a}$$

$$J_{s,t} x + J_{s,s} 0 + J_{s,t} y = 0, \tag{142b}$$

$$\tilde{R}_t x + J_{t,s} 0 + J_t y = \lambda y. \tag{142c}$$

Since all components of equation (142b) are identical, we can also write

$$J_t x + J_t y = 0 \tag{143}$$

and substitute this equation into (142a) and (142c) to get

$$(\tilde{L}_t - J_t) y = \lambda x, \tag{144a}$$

$$(\tilde{R}_t - J_t) x = \lambda y. \tag{144b}$$

Solving for x and y yields

$$x = \frac{1}{\lambda} (\tilde{L}_t - J_t) y, \tag{145a}$$

$$y = \frac{1}{\lambda} (\tilde{R}_t - J_t) x. \tag{145b}$$

Substituting (145a) into (144b) and (145b) into (144a) we find

$$(\tilde{R}_t - J_t)(\tilde{L}_t - J_t)y = \lambda^2 y, \tag{146a}$$

$$(\tilde{L}_t - J_t)(\tilde{R}_t - J_t)x = \lambda^2 x. \tag{146b}$$

Let $M_1 = (\tilde{R}_t - J_t)(\tilde{L}_t - J_t)$. Then

$$M_1 = \begin{pmatrix} 1 & \dots & \dots & \dots & 1 \\ \vdots & 2 & \dots & \dots & 2 \\ \vdots & \vdots & 3 & \dots & 3 \\ \vdots & \vdots & \vdots & \text{etc.} & \\ 1 & 2 & 3 & & t \end{pmatrix}. \tag{147}$$

We will show that M_1 has only simple eigenvalues, which means that for given λ the vector y is completely determined up to a factor.

Translating $M_1 y = \lambda^2 y$ from (146a) into a system of equations, we get

$$\begin{aligned} (1,1,1,\dots,1)^T y &= \lambda^2 y_1 \\ (1,2,2,\dots,2)^T y &= \lambda^2 y_2 \\ (1,2,3,\dots,3)^T y &= \lambda^2 y_3 \\ &\vdots \end{aligned} \tag{148}$$

and, further, by subtracting adjacent rows

$$\begin{aligned} (1,1,1,\dots,1,1)^T y &= \lambda^2 y_1 \\ (0,1,1,\dots,1,1)^T y &= \lambda^2 (y_2 - y_1) \\ (0,0,1,\dots,1,1)^T y &= \lambda^2 (y_3 - y_2) \quad . \\ &\vdots \\ (0,0,0,\dots,0,1)^T y &= \lambda^2 (y_t - y_{t-1}) \end{aligned} \tag{149}$$

Since the coefficient matrix is regular and $\lambda \neq 0$ we can solve this system uniquely by backward substitution provided that $y_t \neq 0$ is known (the case $y_t = 0$ leads to $y = 0$). As a consequence, M_1 has only simple eigenvalues.

Due to the fact that $M_2 = (\tilde{L}_t - J_t)(\tilde{R}_t - J_t)$ can be constructed from M_1 by reversing the order of all row and column indices it has the same eigenvalues as M_1. Therefore, x is also completely determined up to a factor (which is identical to the factor for y). ■

By now we have discovered enough structure to formulate a first result on the size of an eigenspace of $P_n^{(d)}$.

Theorem 6.19. Let $\frac{n}{2} < d < n-1$. Then every multiple eigenvalue $\lambda \neq -1$ of $P_n^{(d)}$ has multiplicity 2. □

Proof. Assume $\dim \operatorname{Eig}(\lambda; P_n^{(d)}) \geq 2$ for some $\lambda \neq -1$. Since for any pair of type II vectors there exists a linear combination that yields a type I vector we may assume w.l.o.g. that any basis B of $\operatorname{Eig}(\lambda; P_n^{(d)})$ contains at least one type I vector v_1 and a type II vector v_2. By Theorem 6.18 the vector v_1 is the only type I vector in B. Hence, if B contained another type II vector $v_3 \neq v_2$, the set $\{v_1, v_2, v_3\}$ would be linearly dependent because there exists a type I linear combination of v_2 and v_3. ■

As the main result of this section we will see that there are, in fact, no multiple eigenvalues $\lambda \neq -1$ of $P_n^{(d)}$ for $\frac{n}{2} < d < n-1$. But before we can prove this, we need to provide some more structural results on type I and II eigenvectors.

Theorem 6.20. Let $\frac{n}{2} < d < n-1$. Then every type II eigenvector $v = (x \mid z \mid y)^T$ of $P_n^{(d)}$ for eigenvalue $\lambda \neq -1$ takes the form

$$c \cdot v^T = (x_1, x_2, \ldots, x_t, 1, \ldots, 1, x_t, \ldots, x_2, x_1)$$

for some $c \in \mathbb{R}$, $c \neq 0$. □

Proof. Let w.l.o.g. $v_2 = (\tilde{x} \mid \mathbb{1} \mid \tilde{y})^T$ be a given type II eigenvector of $P_n^{(d)}$ for eigenvalue $\lambda \neq -1$. Choose P as the permutation matrix that reverses the canonical vertex order of $P_n^{(d)}$. Then $v_3 = Pv_2 - v_2$ is of type I.

Suppose that λ is simple. Then $v_3 = 0$ because otherwise v_2 and v_3 would be a pair of linearly independent vectors in a one-dimensional vector space. Therefore $Pv_2 = v_2$ so that v_2 takes the claimed form.

Now assume that λ is a multiple eigenvalue. We can find a corresponding type I eigenvector $v_1 = (x \mid 0 \mid y)^T$. But then by Theorem 6.18,

$$Pv_2 - v_2 = \mu v_1 \tag{150}$$

and therefore

$$\begin{pmatrix} \tilde{x}_t - \tilde{x}_1 \\ \tilde{x}_{t-1} - \tilde{x}_2 \\ \vdots \\ \tilde{x}_1 - \tilde{x}_t \end{pmatrix} = \mu \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_t \end{pmatrix}. \tag{151}$$

Summing up all components in equation (151) yields

$$0 = \mu \sum_{i=1}^{t} x_i. \tag{152}$$

Assume that $\mu \neq 0$. Then from the previous equation and by similar reasoning for y we get

$$J_t x = 0, \tag{153a}$$

$$J_t y = 0. \tag{153b}$$

Substituting equations (153a) and (153b) into equations (142a) and (142c), respectively, we deduce

$$\tilde{L}_t y = \tilde{\lambda} x, \tag{154a}$$

$$\tilde{R}_t x = \tilde{\lambda} y. \tag{154b}$$

with $\tilde{\lambda} = \lambda + 1$. We may rearrange these equations as follows,

$$(\tilde{R}_t \tilde{L}_t) y = \tilde{\lambda}^2 y, \tag{155a}$$

$$(\tilde{L}_t \tilde{R}_t) x = \tilde{\lambda}^2 x. \tag{155b}$$

We observe that

$$\tilde{L}_t \tilde{R}_t = \begin{pmatrix} 0 & \dots & \dots & \dots & 0 \\ \vdots & 1 & \dots & \dots & 1 \\ \vdots & \vdots & 2 & \dots & 2 \\ \vdots & \vdots & \vdots & \text{etc.} & \\ 0 & 1 & 2 & & t-1 \end{pmatrix}. \tag{156}$$

The matrix $\tilde{R}_t \tilde{L}_t$ can be derived from $\tilde{L}_t \tilde{R}_t$ by reversing the order of all row and column indices.

Exploiting the structure (156), the first component of equation (155b) reads

$$0 = \lambda^2 x_1 \tag{157}$$

so that $x_1 = 0$. The second component reads

$$J_t x - x_1 = \lambda^2 x_2 \tag{158}$$

so that $x_2 = 0$. Now subtract the second component from the third to get

$$J_t x - x_1 - x_2 = \lambda^2 (x_3 - x_2) \tag{159}$$

and therefore $x_3 = 0$. If we continue the subtraction of adjacent components we finally find $x = 0$. Likewise, we can show $y = 0$ so that we arrive at a contradiction.

We may therefore assume $\mu = 0$ so that $v_3 = 0$. But now again, we have $P v_2 = v_2$ so that the proof is complete. ■

Lemma 6.21. Let $\frac{n}{2} < d < n-1$ and $v = (x \mid 0 \mid y)^T$ with $x = (x_i)$ be a type I eigenvector of $P_n^{(d)}$ for eigenvalue $\lambda \neq 1$. Then,

$$x_1 \neq 0 \neq x_t.$$

□

Proof. Let $\frac{n}{2} < d < n-1$ and A be the canonical adjacency matrix of $P_n^{(d)}$. Consider an eigenvector v of $\tilde{A} = A + I$ for eigenvalue $\tilde{\lambda} = \lambda + 1 \neq 0$. Looking at component $t+1$ of

$$\tilde{A}v = \tilde{\lambda}v \tag{160}$$

it becomes clear that the component sum of v equals zero.

From Theorem 6.18 and Lemma 6.17 we derive that v may only assume two possible forms.

We therefore need to consider four cases:

Case 1. Assume $x_1 = 0$ and $v = (x_1, \dots, x_t, 0, \dots, 0, x_t, \dots, x_1)^T$.
Case 2. Assume $x_t = 0$ and $v = (x_1, \dots, x_t, 0, \dots, 0, x_t, \dots, x_1)^T$.
Case 3. Assume $x_1 = 0$ and $v = (x_1, \dots, x_t, 0, \dots, 0, -x_t, \dots, -x_1)^T$.
Case 4. Assume $x_t = 0$ and $v = (x_1, \dots, x_t, 0, \dots, 0, -x_t, \dots, -x_1)^T$.

We will only prove the first case because the remaining cases can be treated analogously.

Let $x_1 = 0$ and $v = (x_1, \dots, x_t, 0, \dots, 0, x_t, \dots, x_1)^T$. Consider the components $t, 2, t-1, 3, \dots$ of equation (160):

$$\begin{array}{lll} \tilde{\lambda}x_t & = 2\sum x_i - x_1 & \Rightarrow x_t = 0 \\ \tilde{\lambda}x_2 & = \sum x_i + x_t & \Rightarrow x_2 = 0 \\ \tilde{\lambda}x_{t-1} & = 2\sum x_i - x_1 - x_2 & \Rightarrow x_{t-1} = 0 \\ \tilde{\lambda}x_3 & = \sum x_i + x_t + x_{t-1} & \Rightarrow x_3 = 0 \\ & \vdots & \vdots \end{array} \tag{161}$$

from which we conclude $x = 0$ and therefore $v = 0$, a contradiction. ■

Theorem 6.22. Let $\frac{n}{2} < d < n-1$. Then every eigenvalue $\lambda \neq -1$ of $P_n^{(d)}$ is simple. □

Proof. Let $\frac{n}{2} < d < n-1$ and A be the canonical adjacency matrix of $P_n^{(d)}$.

Suppose that $\lambda \neq -1$ is a multiple eigenvalue of $P_n^{(d)}$. By Theorem 6.19 its multiplicity is two. Thus, there exists a basis $B = \{v_1, v_2\}$ of $\mathrm{Eig}(\lambda; P_n^{(d)})$ with $v_1 = (x \mid 0 \mid y)^T$ and $v_2 = (\tilde{x} \mid \mathbb{1} \mid \tilde{y})^T$.

Lemma 6.21 ensures that we can find two linear combinations $v_2 + \mu v_1$ such that the first or the t-th component of the result vanishes, respectively. Since $v_2 + \mu v_1$ is a type II eigenvector it must be a multiple of v_2 by choice of our basis B. Consequently, we may assume $\tilde{x}_1 = \tilde{x}_t = 0$.

Let $\tilde{A} = A + I$ and $\tilde{\lambda} = \lambda + 1 \neq 0$. Consider component t of

$$\tilde{A}v_2 = \tilde{\lambda}v_2 \tag{162}$$

which reads

$$\left(\sum \tilde{x}_i + s + \sum \tilde{x}_i\right) - \tilde{x}_1 = \tilde{\lambda}\tilde{x}_t. \tag{163}$$

If we look at component $t+1$ of equation (162) we see that the first term on the left hand side of equation (163) equals $\tilde{\lambda}$ so that

$$0 = \tilde{x}_1 = \tilde{\lambda} \neq 0, \tag{164}$$

a contradiction. ■

Corollary 6.23. Let $\frac{n}{2} < d \leq n-1$. Then

$$\mu = 2(n-d)$$

holds for the number μ of distinct eigenvalues of $P_n^{(d)}$. □

Proof. For $d = n-1$ the graph $P_n^{(d)}$ is complete so that $\mu = 2$. Otherwise, the result follows directly from Theorems 6.15 and 6.22. ■

Now that we know that all eigenvalues $\lambda \neq -1$ of $P_n^{(d)}$ are simple, it is easy to see that any corresponding type I eigenvector takes an antisymmetric form:

Lemma 6.24. Let $\frac{n}{2} < d < n-1$ and let $v = (x \mid 0 \mid y)^T$ be an eigenvector for the simple eigenvalue $\lambda \neq -1$ of $P_n^{(d)}$. Then:

1. $v = (x_1, \ldots, x_t, 0, \ldots, 0, -x_t, \ldots, -x_1)^T$,
2. $\lambda = \frac{x_1}{x_t} - 1$,
3. $x_2 = 0 \;\Leftrightarrow\; \lambda = 0 \wedge \lambda = -2$.

□

Proof. Let $\frac{n}{2} < d < n-1$ and A be the canonical adjacency matrix of $P_n^{(d)}$. Also, let $\tilde{A} = A + I$ and $\tilde{\lambda} = \lambda + 1 \neq 0$. Then we have

$$\tilde{A}v = \tilde{\lambda}v. \tag{165}$$

Now we can reason as follows:

1. Observe Lemma 6.17 and assume to the contrary that v takes a symmetric form. Comparing components 1 and $t+1$ of equation (165) we find $x_1 = 0$, which contradicts Lemma 6.21.

2. Recalling that the component sum of x vanishes, we just have to consider component $s+t+1$ of equation (165).

3. By Lemma 6.21 we have $x_t \neq 0$. Assume w.l.o.g. that $x_t = 1$. Then we have $x_1 = \tilde{\lambda}$. The result now follows by substituting this equation into the difference of the components 1 and 2 of equation (165).

■

Example 6.25. Let $d \leq \frac{n}{2}$. Then the smallest examples of multiple eigenvalues of $P_n^{(d)}$ are shown in table 4.

n	d	λ
8	2	-1
9	3	-2
14	6	0

Table 4: Smallest examples of multiple eigenvalues of $P_n^{(d)}$, $d \leq \frac{n}{2}$

□

We have shown a number of interesting results on eigenvalues and eigenvectors of distance powers of paths. But so far we have only covered the case $\frac{n}{2} < d < n-1$. The previous example hints that for $1 \leq d \leq \frac{n}{2}$ there are only three possible multiple eigenvalues. We have confirmed this by a number of experiments and therefore close this section with the following conjecture:

Conjecture 6.26. Let $1 \leq d \leq \frac{n}{2}$. Then every eigenvalue $\lambda \notin \{-2, -1, 0\}$ of $P_n^{(d)}$ is simple. □

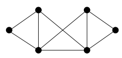
6.4 Almost complete distance powers of paths

We have already taken advantage of the fact that for $d > \lfloor \frac{n}{2} \rfloor$ there is an s-clique in $P_n^{(d)}$ whose vertices are adjacent to all other vertices of the graph. Therefore there exists a graph H such that

$$P_n^{(d)} = K_k * H, \tag{166}$$

where the asterisk denotes the complete product (*join*) of two graphs.

Example 6.27.

$$P_6^{(3)} = K_2 * P_4$$
$$P_6^{(4)} = K_4 * N_2$$
$$P_7^{(3)} = K_1 *$$ 
$$P_7^{(4)} = K_3 * P_4$$
$$P_7^{(5)} = K_5 * N_2$$

□

It is easy to see that the previous example can be generalised as follows:

Lemma 6.28.

$$\begin{aligned} P_n^{(n-3)} &= K_{n-4} * P_4 \quad \text{for } n \geq 4, \\ P_n^{(n-2)} &= K_{n-2} * N_2 \quad \text{for } n \geq 3. \end{aligned}$$

□

The following theorem allows direct computation of the characteristic polynomial of any graph that is the join of two other graphs.

Theorem 6.29. [7] Let G_1, G_2 be two graphs with n_1 and n_2 vertices, respectively. Then,

$$\begin{aligned} \chi_{G_1 * G_2}(x) =& (-1)^{n_2} \chi_{G_1}(x) \chi_{\overline{G_2}}(-x-1) \\ &+ (-1)^{n_1} \chi_{G_2}(x) \chi_{\overline{G_1}}(-x-1) \\ &- (-1)^{n_1+n_2} \chi_{\overline{G_1}}(-x-1) \chi_{\overline{G_2}}(-x-1). \end{aligned}$$

□

Corollary 6.30. [11],[40] For $i \in \{1,2\}$ let G_i be a graph on n_i vertices that is regular of degree r_i. Then,

$$\chi_{G_1 * G_2}(x) = \frac{\chi_{G_1}(x)\chi_{G_2}(x)}{(r_1 - x)(r_2 - x)} \left((r_1 - x)(r_2 - x) - n_1 n_2\right).$$

□

Proof. Use Theorem 2.36 to simplify Theorem 6.29. ■

Now we can determine the characteristic polynomial for some almost complete distance powers of paths.

Theorem 6.31. Let $n \geq 5$. Then,

$$\begin{aligned}
\chi_{P_n^{(n-2)}}(x) &= (-1-x)^{n-3}(-x)\left[(n-3-x)(-x) - 2(n-2)\right], \\
\chi_{P_n^{(n-3)}}(x) &= (-1-x)^{n-5}(x^2+x-1)\left[(n-5-x)(x^2+3x+1) - 2x(x+1)^2\right].
\end{aligned}$$

□

Proof. Observing that

$$\begin{aligned}
\chi_{K_{n-2}}(x) &= (n-3-x)(-1-x)^{n-3}, \\
\chi_{N_2}(x) &= (-x)^2,
\end{aligned} \tag{167}$$

the first part follows directly from Corollary 6.30 and Lemma 6.28 because K_{n-2} and N_2 are regular.

Noting that $\overline{K_{n-4}} = N_{n-4}$ and $\overline{P_4} = P_4$, we only need to verify that

$$\begin{aligned}
\chi_{K_{n-4}}(x) &= (n-5-x)(-1-x)^{n-5}, \\
\chi_{N_{n-4}}(x) &= (-x)^{n-4}, \\
\chi_{P_4}(x) &= (x^2-x-1)(x^2+x-1).
\end{aligned} \tag{168}$$

Then the second result follows from Lemma 6.28 and Theorem 6.29 by straightforward calculation. ■

Remark 6.32. Note that both $P_n^{(n-2)}$ and $P_n^{(n-3)}$ have some eigenvalues that depend on n and others that occur for any choice of n.

For example, $P_n^{(n-2)}$ always has the two fixed eigenvalues $\lambda_1 = 0$ and $\lambda_2 = -1$. On the other hand, its other two eigenvalues,

$$\lambda_{3,4} = \frac{1}{2}n - \frac{3}{2} \pm \sqrt{n^2 + 2n - 7},$$

depend on n. □

6.5 Eigenspaces $\boldsymbol{E_0}$, $\boldsymbol{E_{-1}}$, $\boldsymbol{\overline{E}_0}$, and $\boldsymbol{\overline{E}_{-1}}$

Lemma 6.33. Let $\frac{n}{2} < d \leq n-1$. Then for $P_n^{(d)}$ the following statements hold:

1. $\dim E_0 \leq 1$,
2. $\overline{P_n^{(d)}}$ is bipartite,
3. $\dim E_{-1} = s-1$ and $\dim \overline{E}_0 = s$.

□

Proof. For $d = n-1$ the results can be easily checked by hand.

Let therefore $\frac{n}{2} < d < n-1$. We see from Theorem 6.22 that eigenvalue $\lambda = 0$ is at most simple.

As noted in section 6.4 the graph $P_n^{(d)}$ contains an s-clique whose vertices are adjacent to all other vertices of the graph. With respect to the canonical vertex ordering, we also see that between the first t and the last t vertices there are no adjacencies. Consequently, the complement of $P_n^{(d)}$ consists of s isolated vertices and a bipartite main component that has $2t$ vertices. Overall, the complement is bipartite.

From Theorem 6.15 we already know $\dim E_{-1} = s-1$. A basis of E_{-1} necessarily only consists of vectors with vanishing component sum. Therefore, according to Theorem 3.1 we have $E_{-1} \subseteq \overline{E}_0$. Now construct a vector that is one on the isolated vertices of the complement and zero on the vertices of its main component. Obviously, this yields an eigenvector from $\overline{E}_0$ with non-vanishing component sum. Hence, because of Theorem 3.2 the proof is complete. ■

Before we proceed to our next theorem it is necessary to provide some technical lemmas which the proof of the theorem will rely on.

Lemma 6.34. The linear system

$$\left[\begin{array}{ccccccccc|c}
0 & -1 & -1 & -1 & -1 & -1 & -1 & \dots & -1 & 0 \\
-1 & -1 & -2 & -2 & -2 & -2 & -2 & \dots & -2 & -1 \\
-1 & -2 & -2 & -3 & -3 & -3 & -3 & \dots & -3 & -2 \\
-1 & -2 & -3 & -3 & -4 & -4 & -4 & \dots & -4 & -3 \\
-1 & -2 & -3 & -4 & -4 & -5 & -5 & \dots & -5 & -4 \\
\vdots & \vdots & \vdots & & & \text{etc.} & & & & \vdots \\
-1 & -2 & -3 & & & & & & & -k
\end{array}\right]$$

with coefficient matrix of dimension $(k+1)\times(k+1)$ is solvable for $k \geq 0$ if and only if $k \not\equiv 3 \mod 6$.

In this case, the solution is

$$\begin{array}{ll} (\nu, 1-\nu, \ldots, 1, \nu, -1+\nu, -1, -\nu, 1-\nu, 1, \nu)^T, \nu \in \mathbb{R} & \text{if } k \equiv 0 \mod 6, \\ (-1, 0, \ldots, 0, 1, 1, 0, -1, -1, 0, 1, 1, 0)^T & \text{if } k \equiv 1 \mod 6, \\ (-2, -1, \ldots, 1, 2, 1, -1, -2, -1, 1, 2, 1, -1)^T & \text{if } k \equiv 2 \mod 6, \\ (1, 2, \ldots, -2, -1, 1, 2, 1, -1, -2, -1, 1, 2)^T & \text{if } k \equiv 4 \mod 6, \\ (0, 1, \ldots, -1, 0, 1, 1, 0, -1, -1, 0, 1, 1)^T & \text{if } k \equiv 5 \mod 6. \end{array}$$

□

Proof. Gaussian forward elimination yields a system of the form

$$\left[\begin{array}{cccccccccccc|c} -1 & -1 & -2 & -2 & -2 & -2 & -2 & -2 & -2 & -2 & \ldots & -2 & -1 \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & \ldots & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & -1 \\ 0 & 0 & 0 & -1 & -1 & -2 & -2 & -2 & -2 & -2 & \ldots & -2 & -3 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & \ldots & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -2 & -2 & \ldots & -2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & \ldots & -1 & 0 \\ & & & & & & \text{etc.} & & & & & & \end{array}\right] \tag{169}$$

whose pattern repeats every 6 rows.

Depending on k, different situations occur for the subsequent backward substitution. It is straightforward to check that the solutions are as claimed. ■

Corollary 6.35. The homogeneous variant of the linear system from Lemma 6.34 has a nontrivial solution if and only if $3|k$. In this case, the general solution vector is

$$(\ldots, -\nu, 0, \nu, \nu, 0, -\nu, -\nu, 0, \nu)^T, \nu \in \mathbb{R}.$$

□

Proof. For $k \equiv 0 \mod 6$ we have a nontrivial solution to the non-homogeneous linear system from Lemma 6.34. Simply subtract a particular solution (e.g. for $\nu = 0$) to find the homogeneous solution. For $k \equiv 3 \mod 6$ an inconsistency arises which implies that there exists a nontrivial solution to the homogeneous linear system. This solution can be determined in a straightforward manner. Thus, the general homogeneous solution vector is

$$\begin{aligned}(\nu, -\nu, \dots, 0, \nu, \nu, 0, -\nu, -\nu, 0, \nu)^T, \nu \in \mathbb{R},\ \text{if } k \equiv 0 \mod 6,\\ (-\nu, -\nu, \dots, 0, \nu, \nu, 0, -\nu, -\nu, 0, \nu)^T, \nu \in \mathbb{R},\ \text{if } k \equiv 3 \mod 6.\end{aligned} \tag{170}$$

■

Remark 6.36. Note that the vectors from Lemma 6.34 can be constructed by a sign alternating sequence of coordinate triplets (the leftmost triplet probably being truncated),

$$(\tilde{r} \mid -r \mid \dots \mid r \mid -r \mid r)^T,$$

for example choose $r = (-1, 1, 2)$ and $\tilde{r} = (1, 2)$ for $k \equiv 4 \mod 6$. □

Lemma 6.37. Let A be adjacency matrix of $P_{2n}^{(n-1)}$, $n \in \mathbb{N}$. Then

$$\mathbb{1} \notin \operatorname{Im}(J - A)$$

if and only if $n \equiv 4 \mod 6$. Further, if $(J - A)v = \mathbb{1}$ holds for $v = (v_i)$, then

$$\sum_{i=1}^{2n} v_i = \begin{cases} -2 & \text{if } n \equiv 5 \mod 6,\\ 0 & \text{if } n \equiv 0 \mod 6,\\ 1 & \text{if } n \equiv 1 \mod 6,\\ 2 & \text{if } n \equiv 2 \mod 6,\\ 4 & \text{if } n \equiv 3 \mod 6.\end{cases}$$

□

Proof. The condition $\mathbb{1} \in \operatorname{Im}(J - A)$ translates to the linear system

$$\left[\begin{array}{cc|c} I_n & R_n & \mathbb{1}\\ L_n & I_n & \mathbb{1}\end{array}\right]. \tag{171}$$

Gaussian forward elimination of the submatrix L_n yields

$$\left[\begin{array}{cc|c} I_n & R_n & \mathbb{1}\\ N_n & M_n & x_n\end{array}\right], \tag{172}$$

$x_n \in \mathbb{R}^n$, with

$$\left[\begin{array}{c|c} M_n & x_n\end{array}\right] \tag{173}$$

resembling the system from Lemma 6.34 for $k = n - 1$. Every solution of (173) can be uniquely extended to a solution of (172) by backward substitution starting at row n of the system (172).

For $n \equiv 1 \mod 6$ it turns out that the extended solution vector takes the form

$$(r \mid -r \mid r \mid \ldots \mid -r \mid \tilde{r} \mid -r \mid r \mid -r \mid r)^T \tag{174}$$

with $r = (1-\nu, 1, \nu)$ and $\tilde{r} = (1-\nu, \nu)$. It is clear that the component sum of this vector equals the component sum of $\tilde{r}$ which in turn equals one.

Assume $n \not\equiv 1 \mod 6$. Then, given a solution vector from Lemma 6.34 the extension process simply prepends its reverse. The component sums are readily verified. ■

Lemma 6.38. Consider the graph $P_{2n}^{(n-1)}$ for $n \in \mathbb{N}$. Then,

$$\dim E_0 = \begin{cases} 2 & \text{if } n \equiv 1 \mod 6 \\ 0 & \text{else} \end{cases}.$$

For $n \equiv 1 \mod 6$ a basis of E_0 is given by two vectors as in formula (174) for $r = (1,1,0)$, $\tilde{r} = (1,0)$ and $r = (0,1,1)$, $\tilde{r} = (0,1)$ respectively. □

Proof. Let A be the canonical adjacency matrix of $P_{2n}^{(n-1)}$ and $v \in E_0$. We observe that

$$\begin{aligned} &(J - A)v = \mathbb{1} \\ \Leftrightarrow\ & Jv - \mathbb{1} = Av = 0 \\ \Leftrightarrow\ & \mathbb{1}^T v = 1. \end{aligned} \tag{175}$$

From the proof of Lemma 6.37 we see that this is the case if and only if $n \equiv 1 \mod 6$. Choosing $\nu = 1$ and $\nu = 0$, respectively, for the solution vector (cf. Lemma 6.34) we acquire the basis. ■

Theorem 6.39. Let $\lfloor \frac{n}{2} \rfloor \leq d \leq n-1$.

Then $P_n^{(d)}$ is singular if and only if either

1. $n \equiv 1 \mod 12 \wedge (d = \frac{n+1}{2} \vee d = \frac{n-1}{2})$ or
2. $n - d \equiv 2 \mod 6$ (equivalently, $t \equiv 1 \mod 6$).

In these cases we have $\dim E_0 = 1$. □

Proof. Let A be the canonical adjacency matrix of $P_n^{(d)}$.

According to Remark 6.16 there exist two possible types of eigenvectors $v \in E_0$.

Case 1. Assume w.l.o.g. that $v = (x \mid 1, \dots, 1 \mid y)$.

Consider the system $Av = 0$. We can move the center columns to the right hand side and omit redundant rows to get the linear system

$$\left[\begin{array}{cc|c} J_t - I_t & \tilde{L}_t & -s\mathbb{1} \\ \mathbb{1}^T & \mathbb{1}^T & -(s-1) \\ \tilde{R}_t & J_t - I_t & -s\mathbb{1} \end{array}\right]. \tag{176}$$

Now we subtract the center row from every other row and then remove the center row from the system so that it forms a separate condition. Finally invert the sign of the system. This yields the equations

$$(J_{2t} - \tilde{A})\tilde{x} = \mathbb{1}, \tag{177a}$$

$$\mathbb{1}^T\tilde{x} = -(s-1). \tag{177b}$$

The matrix $\tilde{A}$ equals the canonical adjacency matrix of the graph $P_{2t}^{(t-1)}$. Therefore we are looking for a vector $\tilde{x}$ that fulfils the conditions of Lemma 6.37 and also has the prescribed component sum of $-(s-1)$. Because of $\lfloor \frac{n}{2} \rfloor \le d$ we have $d \ge \frac{n-1}{2}$ and therefore $s \ge 1$. For $s > 3$ the prescribed component sum is strictly less than -2, which is not possible.

Checking the cases $s \in \{1, 2, 3\}$ we see that E_0 contains a type II eigenvector if and only if either

$$s = 3 \ \wedge \ t \equiv 5 \mod 6 \tag{178}$$

or

$$s = 1 \ \wedge \ t \equiv 0 \mod 6. \tag{179}$$

But this means that either $n \equiv 1 \mod 12$ and $d = \frac{n+1}{2}$ or $n \equiv 1 \mod 12$ and $d = \frac{n-1}{2}$.

Case 2. Assume $v = (x \mid 0, \dots, 0 \mid y)$.

Consider the system $Av = 0$. We can move the center columns to the right hand side, omit redundant rows, and remove the center row from the system so that it forms a separate condition. We obtain the linear system

$$\tilde{A}\tilde{x} = 0, \tag{180a}$$

$$\mathbb{1}^T\tilde{x} = 0 \tag{180b}$$

with $\tilde{A}$ as in case one. From Lemma 6.38 it follows that $\tilde{A}$ is singular if and only if $t \equiv 1 \mod 6$, which is equivalent to $n - d \equiv 2 \mod 6$. Since both given basis vectors have component sum one, there exists a basis of $\operatorname{Ker} \tilde{A}$ that contains exactly one vector with vanishing component sum. With respect to equation (180b) we see that by inserting s zero entries in the middle we can extend this vector to an eigenvector spanning E_0 of $P_n^{(d)}$.

Note that requiring $n-d \equiv 2 \mod 6$ and $d = \frac{n\pm1}{2}$, we find that necessarily $n \equiv 3$ or $5 \mod 12$ so that the conditions derived from cases one and two are indeed mutually exclusive. ■

Corollary 6.40. Let $\lfloor \frac{n}{2} \rfloor \le d \le n-1$. Then $E_0 \neq \{0\}$ of $P_n^{(d)}$ is spanned by a type I vector if and only if the first condition of Theorem 6.39 holds.

In this case we have $E_0 \subseteq \overline{E}_{-1}$, otherwise $\overline{E}_{-1} = \{0\}$. □

In table 5 the results of Theorem 6.39 are illustrated. The boxed dimension numbers arise from the first condition of the theorem.

Remark 6.41. Note that the the proof of Theorem 6.39 is constructive so that using Lemma 6.34 we can easily determine a basis of E_0 if $P_n^{(d)}$ is singular. □

Example 6.42. The vector

$$(2,1,-1,-2,-1,1,2,1,-1,-2,-1,1,1,1,-1,-2,-1,1,2,1,-1,-2,-1,1,2)^T$$

spans E_0 for the graph $P_{25}^{(13)}$. Note that since its component sum is one it cannot be contained in $\overline{E}_{-1}$ which in turn must be trivial. □

Theorem 6.43. Let $\lfloor \frac{n}{2} \rfloor \le d \le n-1$. Then for $P_n^{(d)}$ we have

$$\dim \overline{E}_{-1} = \begin{cases} 1 & \text{if } t \equiv 1 \mod 3 \\ 0 & \text{else} \end{cases}.$$

□

Proof. Let $\lfloor \frac{n}{2} \rfloor \le d \le n-1$ and A be the canonical adjacency matrix of $P_n^{(d)}$. Then $v \in \overline{E}_{-1}$ is equivalent to $v = (v_i) = (x \mid z \mid y)^T$ being a solution of the linear system $(J-A)v = 0$ which takes the form

$$\left[\begin{array}{ccc|c} I_t & N_{t,s} & R_t & 0 \\ N_{s,t} & I_s & N_{s,t} & 0 \\ L_t & N_{t,s} & I_t & 0 \end{array}\right]. \tag{181}$$

$n \backslash d$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
2	0																								
3	1	0																							
4		1	0																						
5		0	1	0																					
6			0	1	0																				
7			0	0	1	0																			
8				0	0	1	0																		
9				0	0	0	1	0																	
10					0	0	0	1	0																
11					0	0	0	0	1	0															
12						0	0	0	0	1	0														
13						$\boxed{1}$	$\boxed{1}$	0	0	0	1	0													
14							0	0	0	0	0	1	0												
15							1	0	0	0	0	0	1	0											
16								1	0	0	0	0	0	1	0										
17								0	1	0	0	0	0	0	1	0									
18									0	1	0	0	0	0	0	1	0								
19									0	0	1	0	0	0	0	0	1	0							
20										0	0	1	0	0	0	0	0	1	0						
21										0	0	0	1	0	0	0	0	0	1	0					
22											0	0	0	1	0	0	0	0	0	1	0				
23											0	0	0	0	1	0	0	0	0	0	1	0			
24												0	0	0	0	1	0	0	0	0	0	1	0		
25												$\boxed{1}$	$\boxed{1}$	0	0	0	1	0	0	0	0	0	1	0	
26													0	0	0	0	0	1	0	0	0	0	0	1	0

Table 5: Dimensions of E_0 for $P_n^{(d)}$, $n = 2, \dots, 26$, $d = \lfloor \frac{n}{2} \rfloor, \dots, n-1$

If we consider the differences of adjacent rows and compare the results from the upper and lower t rows it becomes obvious that $v_1 = 0$ would imply $v = 0$.

Let us therefore assume that $v_1 = c \neq 0$. Use this value to move the leftmost column of system (181) to the right hand side. Also separate the first row from the rest of the system. This yields

$$\left[\begin{array}{ccc|c} I_t & N_{t,s-1} & \tilde{R}_t & 0 \\ N_{s-1,t} & I_{s-1} & N_{s-1,t} & 0 \\ \tilde{L}_t & N_{t,s-1} & I_t & -c\mathbb{1} \end{array}\right], \tag{182a}$$

$$\mathbb{1}^T y = -c. \tag{182b}$$

Next perform Gaussian forward elimination on the submatrix $\tilde{L}_t$, which gives us the system

$$\left[\begin{array}{ccc|c} I_t & N_{t,s-1} & \tilde{R}_t & 0 \\ N_{s-1,t} & I_{s-1} & N_{s-1,t} & 0 \\ N_t & N_{t,s-1} & M_t & 0 \end{array}\right]. \tag{183}$$

The matrix M_t resembles the coefficient matrix of the linear system from Lemma 6.34 for $k = t-1$. Applying Corollary 6.35 we see that the prescribed component sum (182b) can be achieved for suitable values of ν, yielding a partial solution vector y. Observe that this is possible since according to equation (170) the component sum of y is ν if $t \equiv 1 \mod 6$ and $\nu - \nu + 0 + \nu = \nu$ if $t \equiv 4 \mod 6$. To complete the proof it suffices to note that using system (183) we can completely determine v from the partial vector y. ■

Remark 6.44. From rows $t+1$ to $t+s$ of (181) it follows directly that $\overline{E}_{-1}$ only contains type I vectors.

Comparing Theorems 6.39 and 6.43 we see that for $t \equiv 1 \mod 6$ we have $\dim E_0 = \dim \overline{E}_{-1}$. Consequently, in this case they contain only vectors whose component sum vanishes.

Again, note that the proof of Theorem 6.43 is constructive. It is therefore straightforward to obtain a basis of $\overline{E}_{-1}$. □

Our combined findings are exemplified in table 6.

d	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
$t \mod 6$	2	1	0	5	4	3	2	1	0	5	4	3	2	1	0
$\dim E_0$	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0
$\dim \overline{E}_{-1}$	0	1	0	0	1	0	0	1	0	0	1	0	0	1	0
$\dim E_{-1}$	0	2	4	6	8	10	12	14	16	18	20	22	24	26	28
$\dim \overline{E}_0$	1	3	5	7	9	11	13	15	17	19	21	23	25	27	29

Table 6: Dimensions of E_0, E_{-1}, $\overline{E}_0$ and $\overline{E}_{-1}$ for $P_{29}^{(d)}$

6.6 Common eigenvectors

In this section we investigate common eigenvectors of two different distance powers of a given path.

We say that two matrices R, S have a common eigenvector v if there exist numbers $\lambda, \mu \in \mathbb{R}$ such that

$$\begin{aligned} Rv &= \lambda v, \\ Sv &= \mu v. \end{aligned} \tag{184}$$

It is possible to tell precisely when this is the case:

Theorem 6.45. [42] Two matrices R, S have a common eigenvector if and only if

$$\bigcap_{s,t\in\mathbb{N}} \mathrm{Ker}[R^s, S^t] \neq \{0\}.$$

□

Note that $[X, Y] = XY - YX$ is the LIE bracket.

If we try to solve the common eigenvector problem (184) under the constraint $\mu = 0$, the condition from the previous theorem can be substantially simplified:

Theorem 6.46. [42] Given two matrices $R, S \in \mathbb{R}^{n\times n}$ there exists a number $\lambda \in \mathbb{R}$ such that

$$Rv = \lambda v,$$
$$Sv = 0$$

if and only if

$$\bigcap_{j=0}^{n-1} \mathrm{Ker}(SR^j) \neq \{0\}.$$

□

Our next step is to apply the notion of common eigenvectors to graphs, in particular to distance powers of paths. Two graphs G, H are said to have a common eigenvector if any (and consequently every) pair of adjacency matrices $A(G), A(H)$ has a common eigenvector.

Although Theorem 6.45 provides a very powerful criterion it is very cumbersome to analyse the terms $\mathrm{Ker}[R^s, S^t]$. However, we can use the simpler criterion of Theorem 6.46 to obtain some interesting introductory properties.

Theorem 6.47. Every graph $P_n^{(d)}$ possesses an eigenvector with vanishing component sum, i.e. an eigenvector that is perpendicular to $\mathbb{1}$. □

Proof. Let A be an adjacency matrix of $P_n^{(d)}$. Choose $R = A + I$ and $S = J$.

Consider the matrices SR^j. We will prove by induction on j that for all $j = 0, 1, \ldots$ the columns of SR^j are multiples of $\mathbb{1}$ and, further, that for $i = 0, \ldots, n-1$ the columns number $s + i$ and $n - i$ of SR^j are identical.

For $j = 0$ the case is trivial. Assume that the claim is valid for some $j \in \mathbb{N}_0$. By the induction hypothesis it follows that all rows of SR^j are identical. Therefore, the inner products that form a column of $(SR^j)R$ are all identical so that the columns of SR^{j+1} are all multiples of $\mathbb{1}$. Now since column $1+i$ of the matrix A is the reverse of column $n-i$ for $i = 0, \ldots, n-1$, the inner products with rows $1+i$ and $n-i$ of SR^j, respectively, are both the same by the induction hypothesis so that the columns number $s+i$ and $n-i$ of SR^{j+1} are identical. Due to the structure of SR^j we have

$$(SR^j)(1, 0, \ldots, 0, -1)^T = 0 \tag{185}$$

for all $j \in \mathbb{N}_0$ so that $\bigcap \mathrm{Ker}(SR^j) \neq \{0\}$.

Since R has the same eigenvectors as A and because of

$$x \perp \mathbb{1} \;\Leftrightarrow\; x \in \mathrm{Ker}\, J \tag{186}$$

we see that the proof is complete. ∎

Note that this statement is clear if there exists a multiple eigenvalue (for which we can always construct an eigenvector with vanishing component sum), but far less obvious if all eigenvalues are simple.

Corollary 6.48. The graphs $P_n^{(d)}$ and $P_n^{(n-1)}$ have a common eigenvector. □

Proof. We may assume that $d < n-1$. The graph $P_n^{(n-1)} = K_n$ is regular and has the two eigenvalues -1 and $n-1$. The eigenspace corresponding to the degree of regularity is spanned by $\mathbb{1}$ so that

$$\mathbb{R}^n = \mathrm{Span}\{\mathbb{1}\} \oplus \mathrm{Eig}(-1; P_n^{(n-1)}), \tag{187}$$

i.e. the orthogonal complement of $\mathrm{Span}\{\mathbb{1}\}$ is an eigenspace of $P_n^{(n-1)}$. Since $P_n^{(d)}$ possesses an eigenvector with vanishing component sum it must therefore also be an eigenvector of $P_n^{(n-1)}$. ∎

Now we will turn our attention to the question whether two successive distance powers $P_n^{(d)}$ and $P_n^{(d+1)}$ can have a common eigenvector. Our first goal is to derive necessary conditions for the existence of a common eigenvector.

Note that by s, t we denote the values associated with $P_n^{(d)}$, not $P_n^{(d+1)}$.

Theorem 6.49. Let $n \geq 3$ and $d \geq \lfloor \frac{n}{2} \rfloor$. Suppose that $P_n^{(d)}$ and $P_n^{(d+1)}$ have a common eigenvector. Then the difference of the respective eigenvalues is either -1, 0, or 1. □

Proof. Let A_1 and A_2 be the canonical adjacency matrices of $P_n^{(d)}$ and $P_n^{(d+1)}$, respectively. Suppose that v is a common eigenvector of A_1 and A_2, i.e. $A_1 v = \lambda_1 v$ and $A_2 v = \lambda_2 v$. Then it follows that

$$(A_2 - A_1)v = (\lambda_2 - \lambda_1)v. \tag{188}$$

We see that

$$A_2 - A_1 = \begin{pmatrix} N_t & N_{t,s} & I_t \\ N_{s,t} & N_s & N_{s,t} \\ I_t & N_{t,s} & N_t \end{pmatrix}. \tag{189}$$

Let $v = (x \mid z \mid y)^T$ with $x, y \in \mathbb{R}^t$ and $z \in \mathbb{R}^s$. Then

$$(A_2 - A_1)v = (y \mid 0 \mid x)^T. \tag{190}$$

Now compare equations (188) and (190). We get

$$(\lambda_2 - \lambda_1)x = y, \tag{191a}$$

$$(\lambda_2 - \lambda_1)y = x, \tag{191b}$$

$$(\lambda_2 - \lambda_1)z = 0 \tag{191c}$$

If $z \neq 0$ we can see from equation (191c) that necessarily $\lambda_1 = \lambda_2$. Now suppose that $z = 0$. Inserting equation (191a) into equation (191b) we find

$$(\lambda_2 - \lambda_1)^2 x = x \tag{192}$$

and therefore $|\lambda_2 - \lambda_1| = 1$. This completes the proof. ■

Corollary 6.50. Let $n \geq 3$ and $d \geq \lfloor \frac{n}{2} \rfloor$. Further, let A_1 and A_2 be the canonical adjacency matrices of $P_n^{(d)}$ and $P_n^{(d+1)}$, respectively.

Then, the eigenspaces of $A_2 - A_1$ are spanned as follows:

$$\begin{aligned} \mathrm{Eig}(-1; A_2 - A_1) &= \mathrm{Span}\{(e_i \mid 0 \mid -e_i)^T : i = 1, \dots, t\}, \\ \mathrm{Eig}(1; A_2 - A_1) &= \mathrm{Span}\{(e_i \mid 0 \mid e_i)^T : i = 1, \dots, t\}, \\ \mathrm{Eig}(0; A_2 - A_1) &= \mathrm{Span}\{(0 \mid e_i \mid 0)^T : i = 1, \dots, s\}. \end{aligned}$$

□

Proof. Let $v = (x \mid z \mid y)^T$ with $x, y \in \mathbb{R}^t$ and $z \in \mathbb{R}^s$. Then v fulfils equation (188) if and only it fulfils the system (191a) to (191c). Using these equations, it is easy to check that the given (obviously linearly independent) set of vectors indeed consists only of eigenvectors. Note that these are the only eigenspaces of $A_2 - A_1$ since their dimensions sum up to n. ■

Remark 6.51. It is possible to extend Theorem 6.49 to accommodate the case $n \geq 4$ even and $d = \frac{n}{2} - 1$ as well. This requires only minor modification to the original proof. □

Theorem 6.52. Let $n \geq 3$ and $d \geq \lfloor \frac{n}{2} \rfloor$. Then $P_n^{(d)}$ and $P_n^{(d+1)}$ have exactly $s-1$ linearly independent common eigenvectors.

These vectors lie in the eigenspaces of eigenvalue -1 of both path powers. For example, choose vectors $(0 \mid e_i - e_{i+1} \mid 0)^T$ with $i = 1, \ldots, s-1$. □

Proof. Let A_1 and A_2 be the canonical adjacency matrices of $P_n^{(d)}$ and $P_n^{(d+1)}$, respectively. Since every common eigenvector of A_1 and A_2 is also an eigenvector of $A_2 - A_1$, we can use Corollary 6.50 to check which eigenspaces of $A_2 - A_1$ admit common eigenvectors of A_1 and A_2.

Consider $v \in \mathrm{Eig}(1; A_2 - A_1)$. From Corollary 6.50 we deduce that

$$v = (x \mid 0 \mid x)^T \tag{193}$$

for some $x \in \mathbb{R}^t$. Inserting this vector into $A_1 v = v$ we can use (138) to derive the homogeneous linear system,

$$\begin{bmatrix} \tilde{L}_t + J_t - 2I_t \\ 2J_{s,t} \\ \tilde{R}_t + J_t - 2I_t \end{bmatrix} \tag{194}$$

for the components of vector x. Now subtract the upper part of the system from the lower part and divide row $n-t$ by 2. If we restrict ourselves to the last $t+1$ rows of the system, we arrive at

$$\begin{bmatrix} \mathbb{1}^T \\ \tilde{R}_t - \tilde{L}_t \end{bmatrix}. \tag{195}$$

By Gaussian forward elimination we see that this is equivalent to

$$\begin{bmatrix} R_t \\ 0^T \end{bmatrix}. \tag{196}$$

But since system (196) has maximum rank and is equivalent to (195) which is part of system (194) we see that necessarily $x = 0$ and therefore $v = 0$. Consequently, $\mathrm{Eig}(1; A_2 - A_1)$ admits no common eigenvectors of A_1 and A_2.

Analogously, we come to the same conclusion for $\mathrm{Eig}(-1; A_2 - A_1)$.

By Corollary 6.50 the structure of $\mathrm{Eig}(0; A_2 - A_1)$ is such that it only admits multiples of $(0 \mid \mathbb{1} \mid 0)^T$ as type II eigenvectors and no type I eigenvectors at all. But

$$A_1(0 \mid \mathbb{1} \mid 0)^T = (s\mathbb{1} \mid (s-1)\mathbb{1} \mid s\mathbb{1})^T \neq \lambda(0 \mid \mathbb{1} \mid 0)^T \tag{197}$$

for any choice of $\lambda \in \mathbb{R}$. Recollecting Theorem 6.15 and Remark 6.16 it becomes clear that $\mathrm{Eig}(0; A_2 - A_1)$ cannot contain common eigenvectors of A_1 and A_2 for any eigenvalue other than $\lambda = -1$. Consequently, the only option that remains is to look for common eigenvectors that belong to the common eigenvalue -1.

But from Corollary 6.50 we immediately obtain

$$\mathrm{Eig}(0; A_2 - A_1) = \mathrm{Span}\{(0 \mid \mathbb{1} \mid 0)^T\} \oplus \mathrm{Eig}(-1; A_1) \tag{198}$$

since every vector can be uniquely written as the sum of a multiple of $\mathbb{1}$ and a vector with vanishing component sum.

Thus, because of $\mathrm{Eig}(-1; A_1) \subseteq \mathrm{Eig}(-1; A_2)$ we see that $\mathrm{Eig}(0; A_2 - A_1)$ affords $s-1$ linearly independent common eigenvectors as claimed. ■

Remark 6.53. For Theorem 6.52 it is also possible to modify the proof slightly such that the case $n \geq 4$ even and $d = \frac{n}{2} - 1$ is covered. It turns out that in this case $P_n^{(d)}$ and $P_n^{(d+1)}$ do not share a common eigenvector. □

Having considered consecutive distance powers of paths, we will now take a look at common eigenvectors of P_n and $P_n^{(d)}$. We start by deriving a necessary condition. As a first application we will settle the case $d = 2$ before we finally deal with the problem in full generality.

Lemma 6.54. Let $n \geq 4$. Define functions f_1 and f_2 as follows:

$$f_q(x; n, d) = \frac{\displaystyle\sum_{m=1}^{d+q} \sin\left(\frac{mx\pi}{n+1}\right)}{\sin\left(\dfrac{qx\pi}{n+1}\right)} - 1$$

Then,

$$f_1(x) = f_2(x) \quad \text{for } x = 1, 2, \ldots, n$$

is a necessary condition for P_n and $P_n^{(d)}$ sharing a common eigenvector. □

Proof. Let A be the canonical adjacency matrix of $P_n^{(d)}$. From Theorem 5.6 we can construct a basis of eigenvectors $\{v^{(1)}, \ldots, v^{(n)}\}$ of P_n. We have to check if any eigenspace of P_n allows an eigenvector of $P_n^{(d)}$. But since all eigenvalues of P_n are simple, we just need to insert each basis vector $v = v^{(j)}$ into the equation $Av = \lambda v$. From the first and second component of this system we find that

$$\lambda = f_1(j; n, d) = f_2(j; n, d) \tag{199}$$

Interpreting the terms $f_q(j; n, d)$ as continuous functions, we see that necessarily $f_1(x) = f_2(x)$ for $x = 1, 2, \ldots, n$. ■

Corollary 6.55. Let $n \geq 4$. Then P_n and $P_n^{(2)}$ have no common eigenvectors. □

Proof. We will abbreviate

$$\varphi = \frac{j\pi}{n+1}. \tag{200}$$

Let $d = 2$ and consider the functions f_1, f_2 from Lemma 6.54. Using the trigonometric equations [4]

$$\begin{aligned} \sin(2\alpha) &= 2\sin\alpha\cos\alpha, \\ \sin(3\alpha) &= 3\sin\alpha - 4\sin^3\alpha, \\ \sin(4\alpha) &= 8\cos^3\alpha\sin\alpha - 4\cos\alpha\sin\alpha. \end{aligned} \tag{201}$$

we can write

$$\begin{aligned} f_1(j;n,2) &= \frac{\sin(2\varphi) + \sin(3\varphi)}{\sin\varphi} \\ &= 2\cos\varphi + 4\cos^2\varphi - 1 \end{aligned} \tag{202}$$

and

$$\begin{aligned} f_2(j;n,2) &= \frac{\sin\varphi + \sin(3\varphi) + \sin(4\varphi)}{\sin(2\varphi)} \\ &= \frac{1}{2\cos\varphi} + \left(2\cos\varphi - \frac{1}{2\cos\varphi}\right) + \left(4\cos^2\varphi - 2\right) \\ &= 2\cos\varphi + 4\cos^2\varphi - 2. \end{aligned} \tag{203}$$

Thus, we see that

$$f_1(j;n,2) - f_2(j;n,2) = 1, \tag{204}$$

which makes it impossible to fulfil the necessary condition of Lemma 6.54. ■

Corollary 6.56. Let $2 \leq d \leq 5$ and $n \geq 4$. If P_n and $P_n^{(d)}$ have a common eigenvector, then necessarily it belongs to $\mathrm{Eig}(-1; P_n^{(d)})$. □

Proof. We will only prove the case $d = 5$. For $d \in \{2,3,4\}$ the proof technique is essentially the same but easier to carry out.

Using abbreviation (200) and equations similar to (201) we find that

$$\begin{aligned} f_1(j;n,5) &= \frac{\sin(2\varphi) + \sin(3\varphi) + \ldots + \sin(6\varphi)}{\sin\varphi} \\ &= 4\cos\varphi - 8\cos^2\varphi - 24\cos^3\varphi + 16\cos^4\varphi + 32\cos^5\varphi \end{aligned} \tag{205}$$

and

$$f_2(j;n,5) = \frac{\sin\varphi + \sin(3\varphi) + \sin(4\varphi) + \ldots + \sin(7\varphi)}{\sin\varphi} \\ = 8\cos\varphi - 12\cos^2\varphi - 32\cos^3\varphi + 16\cos^4\varphi + 32\cos^5\varphi + 1. \tag{206}$$

Let $u = \cos\varphi$. Then it follows that

$$f_1(j;n,5) - f_2(j;n,5) = -4u + 4u^2 + 8u^3 - 1, \tag{207}$$

which is a polynomial $p(u)$. To fulfil the condition of Lemma 6.54 we need to look for the roots of $p(u) = 0$, which can be computed explicitly and are all real. It is straightforward to verify that both f_1 and f_2 only take the value -1 for any of these roots. ■

In figure 8 the graphs of f_1 and f_2 are shown for some examples to illustrate Corollaries 6.55 and 6.56. From the third plot we see that the proof of Corollary 6.56 cannot be applied for $d \geq 6$.

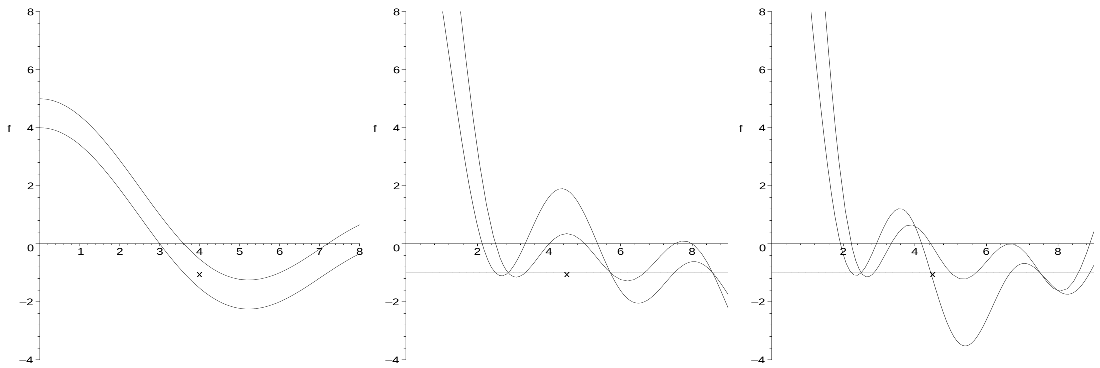


Figure 8: Graphs of $f_q(x;n,d)$ for $P_8^{(2)}$, $P_9^{(5)}$ and $P_9^{(6)}$

The next lemma shows how zero entries of eigenvectors may induce exclusion criteria.

Lemma 6.57. Let $v = (v_i)$ be an eigenvector of P_n. Suppose that $v_j = 0$ for minimal $j < \frac{n}{2}$. Then v cannot be an eigenvector of $P_n^{(j+1)}$. □

Proof. Let $v = (v_i)$ be an eigenvector of P_n with $v_j = 0$ for minimal $j < \frac{n}{2}$. By Theorem 5.11 we know that

$$v = (v_1, \ldots, v_{j-1}, 0, -v_{j-1}, \ldots, -v_1, 0, v_1, *)^T. \tag{208}$$

Let A be the canonical adjacency matrix of $P_n^{(j+1)}$. Requiring $Av = \lambda v$, we get from the j-th component of this system that

$$\lambda v_j = \left(\sum_{i=1}^{2j+1} v_i\right) - v_j \tag{209}$$

and further, by equation (208) and the fact that $v_j = 0$,

$$0 = \sum_{i=1}^{2j+1} v_i = \left(\sum_{i=1}^{j} v_i\right) + 0 + \left(\sum_{i=1}^{j}(-v_i)\right) + 0 + v_1 = v_1. \tag{210}$$

But this contradicts Remark 5.12. ■

We will now finally settle the question when a path and one of its non-complete distance powers share a common eigenvector.

Theorem 6.58. Let $\frac{n}{2} < d < n-1$. Then P_n and $P_n^{(d)}$ have no common eigenvectors. □

Proof. Let A, B be the canonical adjacency matrices of P_n and $P_n^{(d)}$, respectively. Further, let $v = (v_i)$ with $Av = \lambda v$ and $Bv = \mu v$.

First we observe that $s \geq 3$. Therefore, by Theorems 6.15 and 6.22 we see that μ is simple if and only if $\mu \neq -1$.

Suppose that μ is simple, which implies $\mu \neq -1$. Then according to Remark 6.16 the central s components of v must all be equal (again, note $s \geq 3$). Since v is also an eigenvector of P_n we know from Theorem 5.6 that w.l.o.g.

$$v_k = \sin\left(\frac{kj\pi}{n+1}\right) \tag{211}$$

for some $j \in \{1, \ldots, n\}$. Consider three consecutive central components of v. The arguments of their sine terms differ by at most

$$\sin\left(\frac{2j\pi}{n+1}\right) < 2\pi. \tag{212}$$

But since these three components are all equal, it would require the sine function to attain identical values at three different positions within an interval less than its period. This is impossible.

Now suppose that μ is a multiple eigenvalue, i.e. $\mu = -1$. By Theorem 6.15 we see that all but the central s components of v must be zero. In particular this means $v_1 = 0$, which contradicts Remark 5.12.

■

7 Circuits

In this section we will study some spectral properties of circuits C_n. These have been thoroughly studied in literature, but we receive some useful insight before we proceed to distance powers of circuits.

Throughout this section we will assume canonical vertex ordering of P_n and C_n.

Using our knowledge of paths we can easily determine eigenvectors and eigenvalues of arbitrary circuits:

Theorem 7.1. [40]. Let $\{v^{(1)}, \ldots, v^{(n)}\}$ be a basis of eigenvectors of P_n with corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$. Then, the vectors

$$\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ \vdots \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \\ 0 \\ v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \end{pmatrix}, \begin{pmatrix} v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \\ 0 \\ v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \\ 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 \\ v_1^{(n)} \\ \vdots \\ v_{n-1}^{(n)} \\ 0 \\ v_1^{(n)} \\ \vdots \\ v_{n-1}^{(n)} \end{pmatrix} \begin{pmatrix} v_1^{(n)} \\ \vdots \\ v_{n-1}^{(n)} \\ 0 \\ v_1^{(n)} \\ \vdots \\ v_{n-1}^{(n)} \\ 0 \end{pmatrix}$$

constitute a basis of eigenvectors of C_{2n+2}, the respective eigenvalues being

$$2, -2, \lambda_1, \lambda_1, \ldots, \lambda_n, \lambda_n.$$

□

Proof. The constructed vectors are obviously linearly independent (remember Remark 5.12). Using the summation rule 6 it is easy to check that they are indeed eigenvectors. ■

Theorem 7.2. Let $n \geq 3$ be odd. Let $M = \{v^{(1)}, \ldots, v^{(k)}\}$ be a maximal subset of a basis of eigenvectors of P_{n-1} for the respective eigenvalues $\lambda_1, \ldots, \lambda_k$ such that $v_1 = -v_{n-1}$ for all $v \in M$.

Then $k = \frac{n-1}{2}$ and a basis of eigenvectors of C_n is given by

$$\begin{pmatrix} 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \end{pmatrix}, \begin{pmatrix} v_1^{(1)} \\ \vdots \\ v_{n-1}^{(1)} \\ 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 \\ v_1^{(k)} \\ \vdots \\ v_{n-1}^{(k)} \end{pmatrix}, \begin{pmatrix} v_1^{(k)} \\ \vdots \\ v_{n-1}^{(k)} \\ 0 \end{pmatrix}$$

for the respective eigenvalues

$$2, \lambda_1, \lambda_1, \ldots, \lambda_k, \lambda_k.$$

□

Proof. Observe that $n-1$ is even and P_{n-1} is bipartite. We know from Theorem 2.23 and Remark 5.12 that all eigenvalues of P_{n-1} can be paired $(\lambda, -\lambda)$ and that for exactly one eigenvalue of each pair all eigenvectors $v = (v_i)$ satisfy $v_1 = -v_{n-1}$. Hence, $k = \frac{n-1}{2}$.

The constructed vectors are obviously linearly independent. Using the summation rule 6 it is easy to check that they are indeed eigenvectors.

■

Since circuits C_n are circulant graphs their spectrum is also known explicitly. The following Theorem is simply a reformulation of Theorem 2.34:

Theorem 7.3. The eigenvalues of C_n are

$$\lambda_r = 2\cos\left(\frac{2\pi r}{n}\right), \quad r = 0, 1, \ldots, n-1.$$

All eigenvalues of modulus 2 are simple, the other eigenvalues are double. □

Proof. Because of $\lambda_r \in \mathbb{R}$ it follows immediately from Corollary 2.33 that

$$\begin{aligned}
\lambda_r &= \Re\left(\sum_{j=2}^{n} a_j \omega^{(j-1)r}\right) \\
&= \sum_{j=2}^{n} a_j \cos\left(\frac{2\pi(j-1)r}{n}\right) \\
&= \cos\left(\frac{2\pi r}{n}\right) + \cos\left(\frac{2\pi(n-1)r}{n}\right) \\
&= 2\cos\left(\frac{2\pi r}{n}\right)
\end{aligned} \tag{213}$$

The multiplicities are clear from the symmetry of the cosine function. ■

We will conclude this section with an analysis of the eigenspaces E_0, $\overline{E}_{-1}$, E_{-1}, and $\overline{E}_0$. Note that $E_0 = \overline{E}_{-1}$ and $E_{-1} = \overline{E}_0$ because C_n is regular of degree 2.

Theorem 7.4. Let $n \geq 4$.

1. The circuit C_n is singular if and only if $4|n$. In this case,

$$E_0 = \text{Span}\{(1, 0, -1, 0, 1, 0, \ldots, -1, 0)^T, (0, -1, 0, 1, 0, -1 \ldots, 0, 1)^T\}.$$

2. $\lambda = -1$ is an eigenvalue of C_n if and only if $3|n$. In this case,

$$E_{-1} = \text{Span}\{(1, 0, -1, 1, 0, -1, \ldots)^T, (0, 1, -1, 0, 1, -1, \ldots)^T\}.$$

□

Proof. By Theorem 7.3,

$$0 = \lambda_r \;\Leftrightarrow\; \frac{2\pi r}{n} = \frac{\pi}{2} \;\Leftrightarrow\; r = \frac{n}{4} \in \mathbb{Z} \;\Leftrightarrow\; 4|n \tag{214}$$

Assume that $4|n$. Then C_n is singular, and we know that $\dim E_0 = 2$. Use the summation rule 6 to check that the two given vectors indeed span E_0.

With respect to the second claim of the theorem we see that

$$-1 = \lambda_r \;\Leftrightarrow\; \frac{2\pi r}{n} = \frac{\pi}{3} \;\Leftrightarrow\; r = \frac{n}{3} \in \mathbb{Z} \;\Leftrightarrow\; 3|n \tag{215}$$

Again, the summation rule verifies the validity of the given basis of E_{-1}. ■

Remark 7.5. Note that E_0 consists of all vectors $x = (x_i)$ with

$$x_1 = -x_3 = x_5 = -x_7 = \ldots$$

and

$$x_2 = -x_4 = x_6 = -x_8 = \ldots.$$

Let A be the canonical adjacency matrix of C_n. Then these conditions are reflected in rows $1, 3, 5, \ldots$ and rows $2, 4, 6, \ldots$ of the system $Ax = 0$.

By consideration of the differences of consecutive rows we also see that any vector from E_{-1} must have the form

$$(a, b, c, a, b, c, \ldots)^T$$

with numbers $a, b, c \in \mathbb{R}$. □

8 Distance powers $C_n^{(d)}$ of circuits

In this section we will investigate the eigenspaces E_0 and E_{-1} of the graphs $C_n^{(d)}$. Without further notice, we will restrict ourselves to non-complete powers, i.e. we will tacitly assume that $d < \frac{n}{2} - 1$.

Note that $E_0 = \overline{E}_{-1}$ and $E_{-1} = \overline{E}_0$ since $C_n^{(d)}$ is regular.

Distance powers of circuits are circulant, therefore we can use Corollary 2.33 to establish their spectrum.

Theorem 8.1. The eigenvalues of $C_n^{(d)}$ are exactly

$$\lambda_r = \sum_{j=1}^{d} \cos\left(\frac{2\pi rj}{n}\right) + \sum_{j=n-d}^{n-1} \cos\left(\frac{2\pi rj}{n}\right), \quad r = 0, \ldots, n-1.$$

□

Proof. Apply Corollary 2.33 for the canonical adjacency matrix of $C_n^{(d)}$. ■

Although we can explicitly compute the eigenvalues of $C_n^{(d)}$ it is somewhat intricate to predict the occurrence of a prescribed eigenvalue. In the following, we will develop criteria to determine whether 0 or -1 are eigenvalues of $C_n^{(d)}$.

Throughout, let us abbreviate $\omega = e^{2\pi i \frac{r}{n}}$.

8.1 Singularity of $C_n^{(d)}$ and $\overline{C_n^{(d)}}$

Let us abbreviate

$$S_{n,d,r} = \sum_{j=2}^{d+1} \omega^{j-1}, \quad T_{n,d,r} = \sum_{j=n+1-d}^{n} \omega^{j-1}.$$

These terms correspond to the sums that occur in Theorem 8.1.

Theorem 8.2. $C_n^{(d)}$ is singular if and only if there exists some $r \in \{1, 2, \ldots, n-1\}$ such that

$$S_{n,d,r} + T_{n,d,r} = 0.$$

Equivalently, there need to exist integers $1 \leq r < n$ and $l \in \mathbb{N}_0$ such that

$$dr = ln \ \vee \ 2(d+1)r = (2l+1)n.$$

□

Proof. We may assume $1 \le r < n$ (which implies $\omega \neq 1$).

The first claim is simply a rewrite of Theorem 8.1.

For the second claim observe that

$$S_{n,d,r} = \omega \sum_{j=0}^{d-1} \omega^j = \omega \frac{\omega^d - 1}{\omega - 1} \tag{216}$$

and

$$T_{n,d,r} = \omega \sum_{j=1}^{d} \omega^{n-j} = \omega^n \sum_{j=1}^{d} \overline{\omega}^j = \overline{\omega} \frac{\overline{\omega}^d - 1}{\overline{\omega} - 1}. \tag{217}$$

If we write

$$\Omega = \omega \frac{\omega^d - 1}{\omega - 1} \tag{218}$$

we see that

$$S_{n,d,r} + T_{n,d,r} = \Omega + \overline{\Omega}. \tag{219}$$

Consequently,

$$S_{n,d,r} + T_{n,d,r} = 0 \;\Leftrightarrow\; \Re(\Omega) = 0. \tag{220}$$

Let $\varphi = \frac{2\pi r}{n}$ so that $\omega = e^{i\varphi}$ (note that $\varphi > 0$). Substituting $x = \cos\varphi$ and $y = \sin\varphi$ it follows that

$$\frac{\omega}{\omega - 1} = \frac{x + iy}{x - 1 + iy} = \frac{(x+iy)(x-1-iy)}{(x-1)^2 + y^2} = \frac{1}{2} - \frac{y}{2(1-x)} i. \tag{221}$$

Also,

$$\omega^d - 1 = \cos(d\varphi) - 1 + i \sin(d\varphi). \tag{222}$$

Substituting equations (221) and (222) into equation (218) we get

$$\begin{aligned} \Re(\Omega) &= \frac{1}{2}\left(\cos(d\varphi) - 1\right) + \frac{y}{2(1-x)} \sin(d\varphi) \\ &= \frac{1}{2}\left(\left(\cos(d\varphi) - 1\right) + \frac{\sin\varphi}{1 - \cos\varphi} \sin(d\varphi) \right). \end{aligned} \tag{223}$$

Thus,

$$\begin{aligned} \Re(\Omega) = 0 \;&\Leftrightarrow\; \left(\cos(d\varphi) - 1\right)\left(1 - \cos\varphi\right) + \sin\varphi \sin(d\varphi) = 0 \\ &\Leftrightarrow\; \cos(d\varphi) + \cos\varphi - \cos\varphi\cos(d\varphi) + \sin\varphi\sin(d\varphi) = 1 \\ &\Leftrightarrow\; \cos(d\varphi) + \cos\varphi - \cos\left((d+1)\varphi\right) = 1 \\ &\Leftrightarrow\; \frac{\cos\left((d+1)\varphi\right) - \cos(d\varphi)}{\varphi} = \frac{\cos\varphi - \cos 0}{\varphi} \end{aligned} \tag{224}$$

The final equation of (224) allows a geometric interpretation. We require the slopes of two particular secant lines of the cosine function to be equal. In this case, due to the nature of the cosine curve there are only two possible constellations for which the slopes are the same. Either both secant lines must be apart by a nonvanishing multiple of 2π or their endpoints, if projected onto the same period of the cosine curve, must be point symmetrical with respect to $\frac{\pi}{2}$. The first condition means that $d\varphi = 2\pi l$ and the second yields $(d+1)\varphi = \pi + 2\pi l$. The result now follows by combining (220) and (224). ■

Corollary 8.3. Let $C_n^{(d)}$ be nonsingular. Then,

$$\gcd(n, d) = 1.$$

□

Proof. Assume $a = \gcd(n, d) > 1$. Then there exist integers n', d' such that $n = an'$, $d = ad'$ and $n' < n$. Choose $r = n'$ and $l = d'$. It follows that

$$dr = ad'n' = d'n = ln \tag{225}$$

and therefore by Theorem 8.2 (note $r < n$) we see that $C_n^{(d)}$ must be be singular. ■

Corollary 8.4. Let $\gcd(n, d) = 1$. Then $C_n^{(d)}$ is singular if and only if there exist numbers $r \in \{1, 2, \ldots, n-1\}$ and $l \in \mathbb{N}_0$ such that

$$2(d+1)r = (2l+1)n.$$

□

Proof. Let $\gcd(n, d) = 1$. Suppose we have found two integers that satisfy the singularity conditions of Theorem 8.2. We have to rule out the case $dr = ln$. Assuming $dr = ln$ it follows that $n|dr$. But because of $\gcd(n, d) = 1$ we get $n|r$ so that $n \leq r$, a contradiction. ■

Let $\mathrm{ord}(p, n)$ denote the order of the prime divisor p with respect to n, i.e.

$$\mathrm{ord}(p, n) = \max\{j \in \mathbb{N}_0 : p^j|n\}.$$

We will now prove that the order of 2 as a divisor of n and $d+1$ plays a crucial role for the singularity of $C_n^{(d)}$ so that Theorem 8.2 can be rephrased as follows:

Theorem 8.5. The graph $C_n^{(d)}$ is singular if and only if either

$$\gcd(n, d) > 1$$

or

$$\gcd(n, d) = 1 \ \wedge \ \mathrm{ord}(2, d+1) < \mathrm{ord}(2, n)$$

holds. □

Proof. Let $C_n^{(d)}$ be singular. Assume $\gcd(n,d)=1$. Then by Corollary 8.4 there exist integers $1 \le r < n$ and $l \in \mathbb{N}_0$ such that $2(d+1)r = (2l+1)n$. Since $2l+1$ is odd it follows that

$$1 + \operatorname{ord}(2, d+1) \le \operatorname{ord}(2, n). \tag{226}$$

For the converse statement we need to consider two cases.

Case 1. Assume that $\gcd(n,d) > 1$. Then singularity of $C_n^{(d)}$ follows from Corollary 8.3.

Case 2. Assume that $\gcd(n,d)=1$. Let $\kappa < \nu$ for $\kappa = \operatorname{ord}(2, d+1)$ and $\nu = \operatorname{ord}(2,n)$. Then there exist integers u and v such that

$$d + 1 = 2^\kappa v \ \wedge\ 2 \not| v \tag{227}$$

and

$$n = 2^\nu u \ \wedge\ 2 \not| u. \tag{228}$$

Let $a = \gcd(u,v)$ so that $u = au'$ and $v = av'$ for suitable integers u', v'. Now, if we choose

$$\begin{aligned} r &= 2^{\nu-(\kappa+1)} u', \\ l &= \frac{1}{2}(v' - 1) \end{aligned} \tag{229}$$

we get $r < n$ by virtue of $2^{\nu-(\kappa+1)} < 2^\nu$ and $u' < u$. Further,

$$2(d+1)r = 2(2^\kappa v) 2^{\nu-(\kappa+1)} u' = 2^\nu v' a u' = v'(2^\nu u) = (2l+1)n \tag{230}$$

so that by Corollary 8.4 the result follows. ■

Corollary 8.6. Let $\operatorname{ord}(2,n) \le 1$. Then $\gcd(n,d)=1$ is a necessary and sufficient condition for $C_n^{(d)}$ being nonsingular. □

Proof. Let $\operatorname{ord}(2,n) \le 1$. Then if $C_n^{(d)}$ is singular, it follows from Corollary 8.3 that $\gcd(n,d)=1$.

Conversely, assume that $\gcd(n,d)=1$. Then from Theorem 8.5 we infer that $\operatorname{ord}(2,d+1) < \operatorname{ord}(2,n)$ is a necessary and sufficient condition for the singularity of $C_n^{(d)}$. We see that $\operatorname{ord}(2,n)=0$ is impossible. Suppose that $C_n^{(d)}$ is singular and that $\operatorname{ord}(2,n)=1$. Then we have $\operatorname{ord}(2,d+1)=0$. But this means that 2 is a divisor of d, which contradicts $\gcd(n,d)=1$. ■

Our studies so far exhibit a strong link with the topic of vanishing sums of roots of unity. We will therefore take some time to investigate this matter a little further.

Let $\alpha_i \in \mathbb{C}$ denote m-th roots of unity, i.e. $\alpha_i^m = 1$. Then for $m \in \mathbb{N}$ we define

$$W(m) = \left\{ k \in \mathbb{N}_0 : \exists(\alpha_1, \ldots, \alpha_k) \sum_{i=1}^{k} \alpha_i = 0 \right\}$$

so that $W(m)$ is the set of all numbers $k \in \mathbb{N}_0$ for which there exists a vanishing sum of exactly k roots of unity.

Lemma 8.7. Let $m = p_1^{a_1} \cdot \ldots \cdot p_r^{a_r}$ be a decomposition of $m \in \mathbb{N}$ into maximal prime powers such that all exponents are strictly positive. Then,

$$p_i \in W(m)$$

and

$$\sum_{i=1}^{r} b_i p_i \in W(m)$$

for every choice of weights $b_i \geq 0$. □

Proof. Let ω_i denote the primitive p_i-th root of unity. Because of

$$\sum_{k=0}^{p_i - 1} \omega^k = \frac{1 - \omega_i^{p_i}}{1 - \omega_i} = 0 \tag{231}$$

and $p_i | m$ it follows that $p_i \in W(m)$. Consequently, every linear combination of these sums vanishes as well so that $\sum b_i p_i \in W(m)$. ■

A fundamental theorem on vanishing sums of roots of unity states that in Lemma 8.7 we have already found all elements of $W(m)$:

Theorem 8.8. [31] Let $m = p_1^{a_1} \cdot \ldots \cdot p_r^{a_r}$ be a decomposition of $m \in \mathbb{N}$ into maximal prime powers such that all exponents are strictly positive. Then,

$$W(m) = \left\{ \sum_{i=1}^{r} b_i p_i \ : \ b_i \geq 0 \forall i = 1, \ldots, r \right\}.$$

□

We will use Theorem [31] to prove the following Theorem. Note that if we omit reference to the complements of $C_n^{(d)}$, we can also show this as a corollary to Theorem 8.5.

Theorem 8.9. Let $n \geq 3$ be prime. Then the graphs $C_n^{(d)}$ and their complements are nonsingular. □

Proof. Let $n \geq 3$ be prime. Further, let $a = (a_i)$ be the first column vector of the canonical adjacency matrix of $C_n^{(d)}$. Note that $a_i \in \mathbb{N}_0$. According to Corollary 2.33 there needs to exists some integer $0 \leq r < n$ such that

$$\sum_{j=2}^{n} a_j \omega^{(j-1)r} = 0 \tag{232}$$

for $C_n^{(d)}$ to be singular. Thus, we are looking for a vanishing sum of at least one and not more than $n-1$ roots of unity. But since n is prime we see from Theorem [31] that $W(n) = \mathbb{N}_0 \forall n$, rendering it impossible to find such a vanishing sum.

The graph $C_n^{(d)}$ is regular of degree $2d$. According to Theorem 2.36, the complement $\overline{C_n^{(d)}}$ has eigenvalues

$$\begin{aligned} \mu_0 &= n - 2d - 1, \\ \mu_r &= -1 - \sum_{j=2}^{n} a_j \omega^{(j-1)r}, \quad r = 1, \ldots, n-1. \end{aligned} \tag{233}$$

Clearly, $\mu_0 \neq 0$. Let formally $a_1 = 1$. Then

$$\mu_r = \sum_{j=1}^{n} a_j \omega^{(j-1)r}, \quad r = 1, \ldots, n-1. \tag{234}$$

Since $C_n^{(d)}$ is not the complete graph at least one of the a_j must be zero. Therefore we can use the same argument as in the first part of the proof. ■

8.2 Eigenvalue multiplicities

Next we will study eigenvalue multiplicities of distance powers of circuits. The first theorem in this section states that the multiplicity of the eigenvalue $\lambda = -1$ is the same both for $C_{2n}^{(d)}$ and $C_{2n}^{(n-d-1)}$:

Theorem 8.10. Let $1 \leq d \leq n-1$. Then

$$\dim \mathrm{Eig}(-1; C_{2n}^{(d)}) = \dim \mathrm{Eig}(-1; C_{2n}^{(n-d-1)}).$$

□

Proof. Let $a = (a_i)$ and $b = (b_i)$ be the respective first columns of the canonical adjacency matrices of the graphs $C_{2n}^{(d)}$ and $\overline{C_{2n}^{(n-1-d)}}$. Setting $a_1 = 1$ we see that

$$\begin{aligned} a &= (1, \underbrace{1, \ldots, 1}_{d}, 0, \ldots, 0, \underbrace{1, \ldots, 1}_{d})^T \in \mathbb{R}^{2n}, \\ b &= (\underbrace{0, \ldots, 0}_{n-d}, \underbrace{1, \ldots, 1}_{d}, 1, \underbrace{1, \ldots, 1}_{d}, 0, \ldots, 0)^T \in \mathbb{R}^{2n}. \end{aligned} \tag{235}$$

Let $\lambda_0, \ldots, \lambda_{n-1}$ be the eigenvalues of $C_{2n}^{(d)}$ obtained from Corollary 2.33. Likewise, let $\tilde{\lambda}_0, \ldots, \tilde{\lambda}_{n-1}$ be the eigenvalues of $\overline{C_{2n}^{(n-1-d)}}$. Then,

$$\begin{aligned} \lambda_r = -1 \Leftrightarrow \sum_{j=2}^{2n} a_j \omega^{(j-1)r} = -1 \Leftrightarrow \sum_{j=1}^{2n} a_j \omega^{(j-1)r} = 0 \\ \Leftrightarrow \sum_{j=1}^{2n} a_j \omega^{(j+n-1)r} = 0 \Leftrightarrow \sum_{j=1}^{2n} b_j \omega^{(j-1)r} = 0 \Leftrightarrow \tilde{\lambda}_r = 0. \end{aligned} \tag{236}$$

The result now follows because of $E_{-1} = \overline{E}_0$ for $C_{2n}^{(n-1-d)}$. ■

Theorem 8.11.

1. Let n be odd. Then $\lambda = 2d$ is the only simple eigenvalue of $C_n^{(d)}$.
2. Let n be even. If λ is a simple eigenvalue of $C_n^{(d)}$, then

$$\lambda = 2d \ \vee \ \lambda = 2 \ \vee \ \lambda = 0.$$

If $\lambda = 0$ is a simple eigenvalue of $C_n^{(d)}$, then the number d must necessarily be even.

□

Proof. Let $v = (v_i)$ be an eigenvector for the simple eigenvalue λ of $C_n^{(d)}$. Let P be the matrix of the automorphism that shifts the vertex numbering modulo n by exactly one. Then Pv is also an eigenvector of $C_n^{(d)}$ and therefore must be a multiple of v because λ is simple. Thus,

$$\begin{pmatrix} v_1 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix} = \mu \begin{pmatrix} v_2 \\ \vdots \\ v_n \\ v_1 \end{pmatrix} \tag{237}$$

for some real number $\mu \neq 0$. By repeated substitution we get

$$v_1 = \mu v_2 = \mu^2 v_3 = \ldots = \mu^{n-1} v_n = \mu^n v_1 \tag{238}$$

so that necessarily $\mu^n = 1$. For all $n \in \mathbb{N}$ we see that $\mu = 1$ yields the eigenvector $\mathbb{1}$, which corresponds to the degree of regularity. For even n we get $\mu = -1$ as a second possible solution and the vector $(1, -1, 1, -1, \ldots)^T$ as eigenvector candidate. It is readily checked that for even d the candidate is an eigenvector for $\lambda = 0$ whereas for odd d it is an eigenvector for $\lambda = -2$. ■

Remark 8.12. The previous Theorem provides a generalisation of the result on eigenvalue multiplicites of circuits (cf. Theorem 7.3) to the class of circuit powers. □

Corollary 8.13. A distance power $C_n^{(d)}$, $d > 1$, cannot be bipartite. □

Proof. See Theorems 2.22 and 2.23. ■

8.3 Structure of E_0

In this section we will take a closer look at some properties of $E_0 = \operatorname{Ker} C_n^{(d)}$ if n is a power of two.

Let $b = \mathbb{1} \in \mathbb{R}^{2^s}$ and $n = 2^r$ with $s < r$. Then we can construct the vector

$$v_{s,r} = (b \mid -b \mid b \mid -b \mid \ldots \mid b \mid -b)^T \in \mathbb{R}^n. \tag{239}$$

Note that for the components v_j of $v_{s,r}$ this means

$$v_j = (-1)^{\lceil 2^{-s} j \rceil}. \tag{240}$$

Extend the index range of the components v_i of $v_{s,r}$ to the set of all integers by identifying $v_i = v_j$ if $i \equiv j \mod n$.

In the following, we show that such eigenvectors can be found in every kernel of $C_n^{(d)}$ if n is a power of two. The first theorem treats the case of d being odd.

Theorem 8.14. Let $n = 2^r$ and $d + 1 = 2^s \cdot (2t + 1)$ for fixed $s \in \mathbb{N}$, $t \in \mathbb{N}_0$. Then,

$$v_{s,r} \in \operatorname{Ker} C_n^{(d)}.$$

□

Proof. The sum of $2d + 2$ consecutive components of v vanishes because

$$2d + 2 = 2(2t + 1)2^s \tag{241}$$

states that we add $2(2t+1)$ blocks $\pm b$ of alternating signs (note $2d+2 \leq n$) so that

$$0 = \sum_{m=m_0+1}^{m_0+2d+2} v_m \tag{242}$$

for any $m_0 \in \mathbb{Z}$. According to (239) we have $v_{m_0+2d+2} = -v_{m_0+d+1}$ since $2^s|(d+1)$. Therefore, we may write the previous equation as

$$0 = \sum_{m=m_0+1}^{m_0+2d+1} v_m - v_{m_0+d+1}. \tag{243}$$

But the right hand side of this equation is exactly the inner product of the m_0-th row of the canonical adjacency matrix of $C_n^{(d)}$ with vector v. ■

Corollary 8.15. Every graph C_{2^r} is singular. □

Now let d be even.

Theorem 8.16. Let $n = 2^r$ and $d = 2^{s+1}t$ for fixed $s, t \in \mathbb{N}_0$.

Then,

$$v_{s,r} \in \operatorname{Ker} C_n^{(d)}.$$

□

Proof. Let w be any column of the canonical adjacency matrix of $C_n^{(d)}$. Then for the computation of $w^T v_{s,r}$ exactly two groups of d consecutive components of $v_{s,r}$ are summed up. But because of $2^{s+1}|d$ this sum contains only pairs of blocks $\pm b$ so that $w^T v_{s,r} = 0$. ■

Corollary 8.17. Let $n = 2^r$ and $d = 2^{s+1}(2t+1)$. Then,

$$v_{s',r} \in \operatorname{Ker} C_{2^r}^{(d)} \quad \forall s' = 0, 1, \ldots, s.$$

□

Experiments suggest that for any choice of n and d the eigenspace $C_n^{(d)}$ allows a basis of very simple structure. We will therefore end this section with the following conjecture:

Conjecture 8.18. For $C_n^{(d)}$ there exist bases of E_0 and E_{-1} that only contain vectors with entries 0, 1, or -1. □

9 Eigenvector iteration for λ_{max}

This section describes the iterative computation of an eigenvector for the largest eigenvalue of a given (preferably connected) graph. In [7] a theorem by T. H. Wei is quoted that describes such an iteration (cf. Theorem 9.13). Is is neither proven nor are the necessary prerequisites stated in full. The original source [44] is referenced by a number of papers on ranking theory (e.g. [26], [34]), but it is also claimed to be unpublished. But even if one of these papers offers a proof of the theorem it usually remains superficial and does not cover the prerequisites in detail, e.g. [30].

It turns out that the key to understanding is the so-callced *power method*, a standard tool in numerical linear algebra [21],[35]. The method and its geometry have been thoroughly studied [36]. Unfortunately, this fact seems to go unnoticed in literature on ranking theory.

In the following, we will clarify the matter.

To motivate the general idea of the power method let $A \in \mathbb{R}^{n\times n}$, $A \neq 0$, be diagonisable and let $B = \{x_1, \ldots, x_n\}$ be a basis of $\mathbb{R}^n$ consisting of eigenvectors of A for the respective eigenvalues $\lambda_1, \ldots, \lambda_n$. Then every vector $v \in \mathbb{R}^n$ is a unique linear combination of the x_i, say

$$v = \sum_{i=1}^{n} \mu_i x_i \tag{244}$$

with $\mu_i \in \mathbb{R}$. It follows that

$$A^k v = \sum_{i=1}^{n} \lambda_i^k \mu_i x_i. \tag{245}$$

Suppose that $\mu_i \neq 0$ for at least one eigenvalue λ_i of largest modulus. Letting $k \to \infty$ we see that only the terms containing the eigenvalues λ_i of largest modulus essentially contribute to $A^k v$, i.e.

$$\lim_{k\to\infty} \frac{\|\lambda_i^k \mu_i x_i\|}{\|A^k v\|} = 0 \tag{246}$$

if $|\lambda_i| < \max |\lambda_j|$. Note that the norm $\|\cdot\|$ may be chosen arbitrarily.

Based on this reasoning, we may define the following iterative procedure which is commonly known as the *power method*. The aim we have in mind is that the iterates generated should converge towards an eigenvector of an eigenvalue of largest modulus.

Algorithm 9.1. (Power Method)

Choose a suitable initial vector $v \neq 0$ and iterate as follows,

$$v_0 := \frac{v}{\|v\|}, \quad v_{i+1} := \frac{Av_i}{\|Av_i\|}.$$

□

Note that if A is diagonisable we have $\operatorname{Ker} A^i = \operatorname{Ker} A$ for all $i \in \mathbb{N}$. Therefore, the iteration of Algorithm 9.1 is well-defined if $v \notin \operatorname{Ker} A$.

The norm chosen for the power method gives rise to an inner product and, further, to a notion of angles, especially orthogonality. Unless stated otherwise, the norms etc. used in the remainder of this section coincide with this choice.

Let us now weaken the conditions on $A \in \mathbb{R}^{n\times n}$ and besides $A \neq 0$ only assume that the characteristic polynomial χ_A splits into linear factors over $\mathbb{R}$. To make certain that the iteration is well-defined it is necessary to require $v \notin \operatorname{Ker} A^n$.

From the theory of the JORDAN normal form we know that there exists a decomposition of $\mathbb{R}^n$ into a direct sum of A-cyclic subspaces. Let U be one of these subspaces and assume w.l.o.g. that A has JORDAN normal form. If we denote by $A|_U$ the matrix of the restriction of the endomorphism belonging to A to the subspace U (with respect to the same basis) we see that

$$A|_U = \begin{pmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix} = \lambda I + N \tag{247}$$

for some eigenvalue λ of A and a nilpotent matrix N with $N^s = 0$, $s = \dim U$.

For $\lambda \neq 0$, $k \geq s-1$ and $\tilde{v} \in U$ it follows from the binomial theorem that

$$(A|_U)^k \tilde{v} = \sum_{j=0}^{k} \binom{k}{j} \lambda^{k-j} N^j \tilde{v} = \lambda^k \sum_{j=0}^{s-1} \lambda^{-j} \binom{k}{j} N^j \tilde{v}. \tag{248}$$

If for example $\tilde{v} = (0, \dots, 0, 1)^T$, then

$$\begin{pmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix}^k \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} = \lambda^k \begin{pmatrix} \lambda^{-s+1}\binom{k}{s-1} \\ \vdots \\ \lambda^{-1}\binom{k}{1} \\ \lambda^0 \binom{k}{0} \end{pmatrix} = \lambda^k \binom{k}{s-1} \tilde{w}^{(k)} \tag{249}$$

with $\tilde{w}^{(k)} \in \mathbb{R}^s$.

For $k \to \infty$ we see that the first component of the vector $\tilde{w}^{(k)}$ becomes nonzero and that the ratio of two consecutive components is unbounded. Normalising the vectors $\tilde{w}^{(k)}$ we get a sequence that converges to the first unit vector. Since the first vector of the canonical basis of U is an eigenvector for λ we see that the application of the power method within U yields a sequence of vectors converging to an eigenvector for λ.

This argument can be extended to arbitrary vectors $\tilde{v} \in U$, $\tilde{v} \neq 0$.

Thus, we arrive at

$$(A|_U)^k \tilde{v} = \mu \lambda^k \binom{k}{\alpha} w^{(k)}, \tag{250}$$

where $0 \leq \alpha \leq s-1$ and $\mu \neq 0$. The variable μ depends only on $\tilde{v}$ and λ. Moreover, $w^{(k)}$ converges to an eigenvector $w \in U$ for the eigenvalue λ.

If the power method is applied globally, then for increasing k the weights $\lambda^k \binom{k}{\alpha}$ become negligible unless λ is an eigenvalue of largest modulus.

If both λ and $-\lambda$ are eigenvalues of largest modulus, then we obtain the following representation:

$$A^k = \lambda^k \binom{k}{\alpha} \left(\sum_{i=1}^{r} \mu_i w_i^{(k)} + (-1)^k \sum_{j=1}^{s} \nu_j u_j^{(k)} + z^{(k)} \right) \tag{251}$$

with $0 \leq \alpha \leq n-1$ and constants μ_i, ν_j that only depend on v and λ.

We see that $w_i := \lim_{k\to\infty} w_i^{(k)}$ is an eigenvector for eigenvalue λ, $u_j := \lim_{k\to\infty} u_j^{(k)}$ is an eigenvector for eigenvalue $-\lambda$, and $\lim_{k\to\infty} z^{(k)} = 0$.

If either λ or $-\lambda$ is not an eigenvalue of largest modulus, then equation (250) simplifies accordingly.

Let

$$\begin{aligned} g^{(k)} &:= \sum_{i=1}^{r} \mu_i w_i^{(k)}, \\ k^{(k)} &:= \sum_{j=1}^{s} \nu_j u_j^{(k)}, \\ g &:= \lim_{k\to\infty} g^{(k)}, \\ h &:= \lim_{k\to\infty} h^{(k)}. \end{aligned} \tag{252}$$

If $g \neq 0$, then g is an eigenvector for eigenvalue λ. But $g \neq 0$ is assured if v has a nonzero component in $\mathrm{Ker}(A - \lambda I)^n$. For h we have an analogous situation.

Using the above definitions, we have

$$v_k = \frac{A^k v}{\|A^k v\|} = \frac{g^{(k)} + (-1)^k h^{(k)} + z^{(k)}}{\|g^{(k)} + (-1)^k h^{(k)} + z^{(k)}\|}. \tag{253}$$

Several conclusions can be drawn from equation (253). Let us assume that A always satisfies the conditions stated above. Also, if by ρ we denote the spectral radius of A, then we require that the initial vector v has a nonzero component in $\mathrm{Ker}(A - \rho I)^n + \mathrm{Ker}(A + \rho I)^n$.

Denote by $\mathrm{d}(x, U)$ the distance of $x \in \mathbb{R}^n$ to the subspace $U \subseteq \mathbb{R}^n$ with respect to the given norm.

Theorem 9.2. Let $(v_i)_{i\in\mathbb{N}_0}$ be the iterates generated by the power method 9.1. Then,

$$\lim_{k\to\infty} \mathrm{d}(v_k, E_\rho + E_{-\rho}) = 0. \tag{254}$$

□

Proof. By equation (253), it follows that

$$\mathrm{d}(v_k, E_\rho + E_{-\rho}) = \frac{z^{(k)}}{\|g^{(k)} + (-1)^k h^{(k)} + z^{(k)}\|}, \tag{255}$$

which tends to zero for $n \to \infty$. [...]

DAS GILT SO NICHT! WIR K"ONNEN NICHT VORAUSSETZEN, DASS $z^{(k)}$ AUS DEM ORTHOGONALEN KOMPLEMENT DER EIGENR"AUME KOMMT. ■

Theorem 9.3. Let $A \in \mathbb{R}^{n\times n}$ be a matrix whose characteristic polynomial χ_A splits into linear factors over $\mathbb{R}$. For suitable v let $(v_i)_{i\in\mathbb{N}_0}$ be the iterates generated by the power method 9.1. Let $\mathbb{R}^n = S \oplus T$ with subspaces S, T such that S is the sum of all eigenspaces belonging to eigenvalues of largest modulus and T a suitable vector space complement. For $i \in \mathbb{N}_0$ let $v_i = x_i + y_i$ with unique vectors $x_i \in S$ and $y_i \in T$.

Then the iterates v_i converge towards S if $x_0 \neq 0$. To be more precise,

$$\lim_{k\to\infty} \|y_k\| = 0. \tag{256}$$

□

Proof. This follows directly from equation (253). ■

Theorem 9.4.

1. If v has a nonzero component in $\mathrm{Ker}(A - \rho I)^n$, but not in $\mathrm{Ker}(A + \rho I)^n$, then the sequence of the power method iterates converges to a normalised eigenvector with eigenvalue ρ.
2. If v has a nonzero component in $\mathrm{Ker}(A + \rho I)^n$, but not in $\mathrm{Ker}(A - \rho I)^n$, then the sequences of the even or odd iterates generated by the the power method each converge to a normalised eigenvector with eigenvalue $-\rho$.

□

Proof. It suffices to note that in the first case we have

$$v_k = \frac{g^{(k)} + z^{(k)}}{\|g^{(k)} + z^{(k)}\|} \to \frac{g}{\|g\|} \in E_\rho \tag{257}$$

whereas in the second case we have

$$\begin{aligned} v_{2k} &= \frac{h^{(2k)} + z^{(2k)}}{\|h^{(2k)} + z^{(2k)}\|} \to \frac{h}{\|h\|} \in E_{-\rho}, \\ v_{2k+1} &= \frac{-h^{(2k+1)} + z^{(2k+1)}}{\| - h^{(2k+1)} + z^{(2k+1)}\|} \to -\frac{h}{\|h\|} \in E_{-\rho}. \end{aligned} \tag{258}$$

■

Theorem 9.5. If v has a component in $\mathrm{Ker}(A - \rho I)^n + \mathrm{Ker}(A + \rho I)^n$, then

$$\lim_{k\to\infty} \|Av_k\| = \rho, \tag{259}$$

provided that the limit exists. □

Proof. This follows directly from the fact that

$$\begin{aligned} v_{2k} &= \frac{g^{(2k)} + h^{(2k)} + z^{(2k)}}{\|g^{(2k)} + h^{(2k)} + z^{(2k)}\|} \to \frac{g+h}{\|g+h\|}, \\ v_{2k+1} &= \frac{g^{(2k+1)} - h^{(2k+1)} + z^{(2k+1)}}{\|g^{(2k+1)} - h^{(2k+1)} + z^{(2k+1)}\|} \to \frac{g-h}{\|g-h\|} \end{aligned} \tag{260}$$

so that

$$\begin{aligned} \|Av_{2k}\| &\to \frac{\|Ag + Ah\|}{\|g+h\|} = \rho\frac{\|g-h\|}{\|g+h\|}, \\ \|Av_{2k+1}\| &\to \frac{\|Ag - Ah\|}{\|g-h\|} = \rho\frac{\|g+h\|}{\|g-h\|}. \end{aligned} \tag{261}$$

Since the limit of $\|Av_k\|$ exists we known that all subsequences converge to the same limit. By comparison of the limits of the two subsequences above, the theorem follows. ■

Although we may determine the spectral radius of A from Theorem 9.5 it is important to note that the sequence of the vectors v_k may not converge to a fixed vector at all. However, the following theorem shows that at least certain sums and differences of consecutive iterates do converge provided that $E_\rho \perp E_{-\rho}$.

Theorem 9.6. Let $E_\rho \perp E_{-\rho}$ with respect to the chosen norm.

1. If v has a nonzero component in $\mathrm{Ker}(A-\rho I)^n$, then the sequence $(v_k+v_{k+1})_{k\in\mathbb{N}_0}$ converges to an eigenvector for eigenvalue ρ.
2. If v has a nonzero component in $\mathrm{Ker}(A+\rho I)^n$, then the sequence $(v_{2k} - v_{2k+1})_{k\in\mathbb{N}_0}$ converges to an eigenvector for eigenvalue $-\rho$.

□

Proof. Again, we make use of equation (253). In this case the vectors g and h as defined in (252) are normalised and perpendicular eigenvectors for eigenvalues ρ and $-\rho$, respectively.

Consequently,

$$\|g-h\|^2 = (g-h)^2 = g^2 + h^2 = \|g+h\|^2. \qquad (262)$$

As the denominator in equation (253) converges to $\|g+h\|$, the assertion becomes obvious. ■

Corollary 9.7. Let $E_\rho \perp E_{-\rho}$ with respect to the chosen norm. Then the limit mentioned in Theorem 9.5 exists. □

Proof. Revisit the proof of Theorem 9.5 and observe that additionally $\|g-h\| = \|g+h\|$. ■

In the following, we will assume that A is symmetrical. Since then A is diagonisable over $\mathbb{R}$ we have mutually perpendicular eigenspaces (with respect to the standard inner product).

In consideration of equation (253) the following property of the power method applied to a symmetrical matrix is easy to see:

Theorem 9.8. Let $(v_k)_{k\in\mathbb{N}_0}$ be the iterates generated by Algorithm 9.1 for an initial vector v. If S is a matrix whose column vectors form a basis of the sum space of the eigenspaces belonging to all eigenvalues of A except those of largest modulus, then

$$\lim_{k\to\infty} \|S^T v_k\| = 0.$$

□

Moreover, we may state another may to determine the spectral radius of A from the sequence of the v_k:

Theorem 9.9. Let ρ be the spectral radius of A and assume that the Euklidean norm is used. Then

$$\lim_{k\to\infty} |v_k^T A v_k| = \rho. \tag{263}$$

□

Proof. This follows from the properties of the RAYLEIGH quotient and the fact that $\|v_k\| = 1$. ■

Now we turn our attention to graphs. Let us assume that A is the adjacency matrix of an undirected graph with at least one edge. Then A is diagonalisable and all its eigenvalues are real. Therefore, there exist at most two eigenvalues of largest modulus. But by Theorem 2.22 we know that $-\lambda_{max}$ is an eigenvalue of a connected graph if and only if it is bipartite.

We conclude that for non-bipartite graphs we can easily achieve convergence of the power method:

Theorem 9.10. Let G be a graph such that for each component of G with the same spectral radius the largest eigenvalue is only simple and that the component is non-bipartite. Choosing a vector v such that it is not perpendicular to $\mathrm{Eig}(\lambda_{max}; G)$, the iterates v_k generated by the power method 9.1 then converge to a normalised eigenvector v_∞ for the eigenvalue λ_{max} of A. The restriction of v_∞ to any component of G is either non-positive or non-negative. □

Proof. This follows directly from the previous theorems and the PERRON-FROBENIUS Theorem 2.7. ■

Corollary 9.11. Let $v \geq 0$. Then a vector $v_\infty \geq 0$ is obtained as a unique solution, provided that the power method converges. □

Theorem 9.12. Let G be a bipartite graph such that its largest eigenvalue is simple. Choose a vector v such that it is not perpendicular to $\mathrm{Eig}(\lambda_{max}; G)$, and compute iterates v_k using the power method 9.1.

Then the sequence $(w_k)_{k\in\mathbb{N}}$ with

$$w_k = v_k + v_{k-1}$$

converges to an eigenvector w_∞ for the eigenvalue λ_{max} of A. □

Proof. Assume $\lambda_1 \leq \ldots \leq \lambda_n$ and write v as in equation (244).

From equations (245) and (246) it follows directly that

$$\begin{aligned}\lim_{k\to\infty}\left\|\frac{1}{\lambda_{max}^{2k}}A^{2k}v_0-(\mu_1x_1+\mu_nx_n)\right\|&=0,\\ \lim_{k\to\infty}\left\|\frac{1}{\lambda_{max}^{2k+1}}A^{2k+1}v_0-(-\mu_1x_1+\mu_nx_n)\right\|&=0.\end{aligned} \tag{264}$$

We see that the subsequences of the even and odd iterates converge separately so that the sum sequence w_k converges to a multiple of x_n. ■

Alternatively, one may shift the spectrum of the adjacency matrix of G so that there is only one eigenvalue of largest modulus. One could then use the power method on $A+\varepsilon I$, $\varepsilon > 0$. But this only yields the largest eigenvalue of A, not a suitable eigenvector.

We can now prove the initially mentioned theorem by T. H. Wei and also state correct prerequisites:

Theorem 9.13. [44] Let G be connected and non-bipartite. Let $N_k(i)$ denote the number of all walks of length k starting from vertex x_i. Then for $k \to \infty$ the vector

$$s_k = \frac{1}{\sum_{j=1}^{n} N_k(j)} \cdot (N_k(1), N_k(2), \ldots, N_k(n))^T, \quad k \in \mathbb{N},$$

converges to a positive eigenvector for the largest eigenvalue of G. □

Proof. Choose the norm

$$\|(x_1,\ldots,x_n)^T\| = \sum_{j=1}^{n} |x_j|. \tag{265}$$

If A is the adjacency matrix of G we have precisely (cf. Theorem 2.11)

$$s_k = \frac{A^k \mathbb{1}}{\|A^k \mathbb{1}\|} \tag{266}$$

and therefore $v_k = s_k$ if we apply the power method for the initial vector $v = \mathbb{1}$. To prove convergence of the iteration it suffices to show that $\mathbb{1}$ is not perpendicular to $\mathrm{Eig}(\lambda_{max}; G)$. By Theorem 2.7 we know that

$$\mathrm{Eig}(\lambda_{max}; G) = \mathrm{Span}\{z\} \tag{267}$$

for some vector $z > 0$. But $\mathbb{1}^T z = 0$ is impossible since $z > 0$ and $\mathbb{1} > 0$. ■

If G is regular we see that all s_k are identical and eigenvectors for the degree of regularity. In this case, Theorem 9.13 is valid even if G is bipartite.

The results of this section can be extended to directed graphs. For strongly connected digraphs it is known that their maximum eigenvalue is simple since they have irreducible adjacency matrices so that Theorem 2.7 can be applied. For the convergence of the power method (provided that the initial vector is chosen suitably) we need to ensure that there is only one eigenvalue of largest modulus.

Theorem 9.14. Let G be a strongly connected digraph. Then λ_{max} is the only eigenvalue of largest modulus if and only if there exists a number $k \in \mathbb{N}$ such that between any pair of (not necessarily distinct) vertices of G there exists a directed walk of length k from the first vertex to the second. □

Proof. Let A be the adjacency matrix of G. Since G is strongly connected the matrix A is nonnegative and irreducible. But according to [16] the matrix A is primitive (i.e. it has only one eigenvalue of largest modulus) if and only if $A^k > 0$ for some $k \in \mathbb{N}$. The result now follows from Theorem 2.11. ■

10 Conclusion

In the previous chapters a number of interesting structural results have been obtained. However, some questions remain unanswered and may possibly be the starting point of future research. One strong conjecture is 6.26, which claims that for $1 \leq d \leq \frac{n}{2}$ every eigenvalue $\lambda \notin \{-2, -1, 0\}$ of $P_n^{(d)}$ is simple. The techniques used for $\frac{n}{2} < d < n-1$ cannot be applied any more since they rely on the fact that there exist at least two vertices that are adjacent to all other vertices.

The second interesting open topic is the existence of simple bases for certain eigenspaces. For a simply singular forest we have shown that its kernel can be spanned by a vector with entries only from $\{0, 1, -1\}$. Conjecture 4.10 states that this is probably true for every singular forest. A similar claim is made for distance powers $C_n^{(d)}$ of circuits (cf. Conjecture 8.18).

A List of Figures

B List of Tables

C Symbols

$\alpha(G)$	independence number of G
$\delta(G)$	minumum degree of graph G
$\Delta(G)$	maximum degree of graph G
$\gamma_G(v)$	degree of vertex v in graph G
$\mu(x;G)$	matching polynomial of graph G
$\chi_A(x)$	characteristic polynomial of matrix A
$\chi(x;G)$	characteristic polynomial of graph G
$\chi(G)$	chromatic number of graph G
$\omega(G)$	size of a maximum clique of G
$\mathrm{d}(x,y)$	distance of vertices x,y in graph G
e_i	i-th standard unit vector
$m(G,k)$	number of matchings of size k in graph G
$\mathrm{rk}\,A$	rank of matrix A
A^T	transpose of matrix A
A^{-1}	inverse matrix of A
A^*	adjugate of matrix A
$\mathbb{1}_n$	all-ones vector of size n
C_n	cicuit with n vertices
$J_{k,l}$	all-ones matrix of size $k \times l$
$E(G)$	edge set of graph G
E_λ	eigenspace for eigenvalue λ of the given graph
$\mathrm{Eig}(\lambda;G)$	eigenspace for eigenvalue λ of graph G
$\overline{E}_\lambda$	eigenspace for eigenvalue λ of the complement of the given graph
$G^{(k)}$	k-th distance power of graph G
I_n	identity matrix of size $n \times n$
$\mathrm{Im}\,A$	image of the endomorphism defined by matrix A
$\mathrm{Ker}\,A$	kernel (null space) of the endomorphism defined by matrix A
K_n	complete graph with n vertices
L_k	all-ones lower triangular matrix of size $k \times k$
$\tilde{L}_k$	all-ones strictly lower triangular matrix of size $k \times k$
$L(G)$	line graph of graph G
$N_G(v)$	neighbourhood of vertex v in graph G
$N_{k,l}$	all-zero matrix of size $k \times l$
P_{ij}	unique path between two vertices of a tree
P_n	path with n vertices
U_k	all-ones upper triangular matrix of size $k \times k$
$\tilde{U}_k$	all-ones strictly upper triangular matrix of size $k \times k$
$V(G)$	vertex set of graph G

D References

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