Graph Laplacians and Nodal Domains

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Abstract

We investigate eigenvectors of a graph Laplacian and their nodal domains. We consider the adjacency, Laplacian, and generalized Laplacian (a symmetric matrix with non-positive off-diagonal elements) of a graph. The generalized Laplacian is also called a discrete Schrödinger operator. We associate a graph with a real vector. A nodal domain of a vector is a connected component of the maximal induced subgraph of the associated graph on which the vector does not change sign. A nodal domain is also called sign graph. The discrete analogue of Courant's nodal domain theorem provides upper bounds on the number of nodal domains of an eigenvector depending on the location of the corresponding eigenvalue in the spectrum. This bound is not sharp in general. We consider the problem of finding minimal and maximal numbers of nodal domains for some graph classes.

We present the relationship between nodal domains and hyperplane arrangements.

We consider a generalized Laplacian of a tree. We characterize for a tree: the maximal number of the strong nodal domains of an eigenvector corresponding to the k-th eigenvalue. We give an $O(n^2)$ time algorithm finding an eigenvector with maximum number of the strong nodal domains, which corresponds to the k-th eigenvalue. We show that to find an eigenvector of the k-th eigenvalue, which has minimum number of the strong nodal domains, is NP-complete.

For the Laplacian matrix of a hypercube, we show that each eigenvalue except the largest one has an eigenvector with two weak nodal domains. We also show that the first half of the eigenvalues have an eigenvector with two strong nodal domains. We give a lower bound for the number of nodal domains of eigenvectors belonging to the second largest eigenvalue.

We consider the Laplacian matrix of a cograph. A graph is called cograph if it has no path with four vertices as an induced subgraph. We give an algorithm for finding the minimum or maximum number of nodal domains of a cograph in $O(n^2)$ time. Finally we prove the conjecture that the rank of the adjacency matrix of a cograph is equal to the number of distinct nonzero columns of the adjacency matrix.

Zusammenfassung

Wir beschäftigen uns mit den Eigenvektoren von Graph-Laplace-Operatoren und ihren Knotengebieten. Wir betrachten Adjazenzmatrix, Laplacematrix und verallgemeinerte Laplacematrix (eine symetrische Matrix mit nichtpositiven nicht diagonal Elementen). Eine verallgemeinerte Laplacematrix heisst auch diskreter Schrödinger-Operator. Wir assoziieren einen Graphen mit einem Vektor. Ein Knotengebiet eines Vektors ist ein maximal zusammenhängender Teilgraph, auf dem der Vektor nicht das Vorzeichen wechselt. Ein Knotengebiet heisst auch ein Vorzeichengraph. Die diskrete Version von Courant's Knotengebiettheorem gibt eine obere Schranke für die Anzahl der Knotengebiete eines Eigenvektors in Abhängigkeit von der Lage des zugehörigen Eigenwertes im Spektrum an. Diese Schranke ist im allgemeinen nicht scharf. Wir betrachten minimale und maximale Anzahl an Knotengebieten für einigen Graphklassen.

Für eine verallgemeinerte Laplacematrix eines Baumes charakterisieren wir die maximale Anzahl an starken Knotengebieten eines Eigenvektors zum k-ten Eigenwert. Wir geben einen Algorithmus an, der einen Eigenvektor mit maximaler Anzahl an starken Knotengebieten in $O(n^2)$ Zeit findet. Wir zeigen, dass das Finden eines Eigenvektors zum k-ten Eigenwert mit minimaler Anzahl an starken Knotengebieten NP-vollständig ist.

Für die Laplacematrix eines Hyperwürfels zeigen wir, dass jeder Eigenwert (ausser dem grössten Eigenwert) einen Eigenvektor mit zwei schwachen Knotengebieten hat. Wir zeigen auch, dass für die erste Hälfte der Eigenwerte ein Eigenvektor mit zwei starken Knotengebieten existiert. Wir geben auch eine untere Schranke für die Anzahl an Knotengebieten des Eigenvektors des zweitgrössten Eigenwert an.

Wir berachten auch Laplacematrizen von Cographen. Wir geben einen Algorithmus an, der die minimale und maximale Anzahl der Knotengebiete in $O(n^2)$ Zeit findet. Wir beweisen, dass der Rang einer Adjazenzmatrix des Cographen gleich der Anzahl der paarweise verschiedenen Spalten ist.

CONTENTS

1. INTRODUCTION

The foundations of spectral graph theory were laid in the fifties and sixties of the last century. Since then, spectral methods have become standard techniques in (algebraic) graph theory. The eigenvalues of graphs, most often defined as the eigenvalues of the adjacency matrix, have received much attention over the last thirty years as a means of characterizing classes of graphs and for obtaining bounds on properties such as the diameter, girth, chromatic number, connectivity, etc. [5, 20, 21, 45, 47]. More recently, the interest has shifted somewhat from the adjacency spectrum to the spectrum of the closely related *graph Laplacian*, see e.g., [18, 50, 68, 69]. Again, the dominating part of the theory is concerned with the eigenvalues.

Kac [58] asked whether one could hear the shape of a drum. Consider an elastic plane membrane whose boundary is fixed. If small vibrations are induced in the membrane, it is not unreasonable to expect a point on its surface to move only vertically. If the effects of damping are ignored, the motion of the point is given (at least approximately) by a wave equation. By the assumption that the membrane is elastic and the vibrations are small, we get the classical solution of a Dirichlet problem which involves a countable sequence of eigenvalues (the human ear hears the spectrum, i.e., the frequencies of the tones, produced by the membrane). Kac's question is: Can nonisometric drums afford the same eigenvalues? The answer is: We can't hear the shape of a drum [48].

Fisher [38] considered the discrete analogue to Kac's problem. In his model the membrane consists a set of atoms which in the equilibrium state lie on the vertices of a regular lattice graph embedded in a plane. Each atom acts on its neighboring atoms by elastic forces. The discretization of the vibration of a membrane is the Laplacian matrix of the graph with its eigenvalues corresponding to the frequencies of the membrane. We also can't hear the discrete shape of a drum, because the eigenvalues of a graph don't determine the graph uniquely (see e.g., [21]).

The *eigenvectors* of graphs, on the other side, have received only sporadic attention on their own. Even the recent book on *Eigenspaces of Graphs* [22] contains only a few pages on the geometric properties of the eigenvectors which are mostly used as a convenient proof technique.

Eigenvectors of graphs have been used to design heuristics for some combinatorial optimization problems such as graph partitioning [52, 71, 72] and graph coloring [3]. Their application in graph drawing is discussed in [40, 49, 61, 70]. The cost functions of a number of prominent combinatorial optimization problems, among them the TSP, graph bi-partitioning, and certain spin glass models, are eigenfunctions of graphs associated with search heuristics for these problems [51, 55, 77]. This observation was one of the starting points of the algebraic theory of fitness landscapes which is reviewed in [73]. In this section we briefly review some of the applications of eigenvalues and eigenvectors of a graph.

The second smallest eigenvector of a Laplacian can be used for graph bipartitioning. By graph bipartition, we want to find a vertex separator S of a graph G such that S has few vertices and S disconnects $G - S$ into two parts A, B with nearly equal numbers of vertices. Pothen *et al.* [71] give the following heuristic method for the bipartition: Compute the second smallest eigenvector x of the Laplacian. Assign each vertex the value of its corresponding entry in x. Compute the median of elements of x. Bipartition the vertices as follows: the vertices whose values are less than or equal to the median form one part; the rest of the vertices form the other part. The quality of this heuristics is given by Guattery and Miller [52]. Alpert *et al.* [1] give a multiple eigenvector extension of this heuristics.

Eigenvectors can be used to obtain a coloring of a graph. Aspvall and Gilbert [3] used the sign pattern of an eigenvector of the adjacency matrix for a heuristics graph coloring algorithm. The following idea is used for this method. For a collection of eigenvectors, the vertices u and v belong to the same color class (partition) if and only if u and v have the same sign patterns of the collection (with the zero entries considered positive). We add new eigenvectors to the collection (if necessary) to get a valid coloring.

Eigenvectors are also used for graph drawing. An embedding of a graph in $\mathbb{R}^k$ is a map from vertices of a graph into $\mathbb{R}^k$, in other words an embedding consists of the positions of the vertices in an k-dimensional drawing of a graph. The second, third, and fourth (sometimes fifth) smallest eigenvectors of a Laplacian can be used for an embedding of a graph in $\mathbb{R}^3$. For a better embedding of fullerenes, the eigenvectors of the adjacency matrix are also used (see [49, 61]). Pisanski and Taylor [70] give a method for drawing a graph in any number of dimensions: Compute an orthonormal basis of eigenvectors $x^1, \ldots, x^n$ of the Laplacian matrix of a graph with n vertices. The eigenvectors $x^2, \ldots, x^{k+1}$ yields the columns of the embedding in $\mathbb{R}^k$ with minimum energy (energy is defined as the sum of the square of the Euclidean distance of two adjacent vertices).

Eigenvalues and eigenvectors have applications to chemistry. Accord-

ing to quantum theory, the properties of micro-objects (electrons, atoms, molecules) in a stationary state are described by wave functions Ψ, representing solutions of Schrödinger's equation $S\Psi = E\Psi$, in which S is the energy operator and E is the energy of the object under consideration. For a certain class of compounds of carbon and hydrogen, the conjugated hydrocarbons, the approximate solutions of the Schrödinger's equation are as follows. The skeleton of the molecule can be represented in a natural manner by a simple graph. The molecular orbitals are determined by approximation in quantum chemistry as an eigenvalue problem. The eigenvalues represent possible values for the energy of electrons, and the coordinates of the corresponding eigenvectors determine the molecular orbitals which are characterized by such energies. For details see, e.g., [79]. These approximations form the basis of the so-called *Hückel theory* [56]. In this way the task of determining molecular-orbital energies is reduced to the determination of the spectrum of the corresponding molecular graph. We refer to [4, 10, 79] for presentations of the chemical graph theory.

Maas [65] showed that the Laplacian eigenvalues of a graph determine the kinematic behavior of a liquid flowing through a system of communicating pipes. The second smallest eigenvalue determines the behavior of the flow.

Another application of graph eigenvectors is used in economics. Maslov [66] gives a simple measure of the level of financial globalization of a given country based on the analysis of cross-correlations between stock market indices in different countries and regions of the world. He studies the empirical correlation matrix (this matrix is symmetric, non-negative definite but in general it is not a graph Laplacian) of index price fluctuations in a large number of individual countries. The three largest eigenvalues and the corresponding eigenvectors are used for the observation of the influence of world index dynamics.

Organization of the Thesis

In chapter 2, we recall some notions from graph theory, linear algebra and complexity of algorithms. We give a brief introduction to the graph Laplacians that we use throughout this thesis.

Our main interest concerns the nodal domains, so chapter 3 gives an introduction to this topic. We associate a graph G with a real vector. A nodal domain of a vector is a connected components of the maximal induced subgraph of G on which vector does not change sign. The discrete analogue of Courant's nodal domain theorem and some other results are presented which were known before. Finally we present the relationship between nodal domains and hyperplane arrangements.

In particular, we investigate maximum or minimum number of nodal do-

mains of eigenvectors belonging to an eigenvalue of a graph Laplacian.

In chapter 4, the nodal domains of a tree is studied. We consider a generalized Laplacian of a tree. We characterize for a tree: the maximal number of the strong nodal domains of an eigenvector corresponding to an eigenvalue λ_k. We give an $O(n^2)$ time algorithm to find an eigenvector with maximum number of the strong nodal domains, which corresponds to an eigenvalue λ_k (see [6]). Finally we show that to find an eigenvector of an eigenvalue λ_k, which has minimum number of the strong nodal domains, is NP-complete (see [6]).

In chapter 5, the nodal domains of a hypercube is studied. We consider the Laplacian matrix of a hypercube. We show that each eigenvalue except the largest one has an eigenvector with two weak nodal domains. We also show that the first half of the eigenvalues have an eigenvector with two strong nodal domains (see [7]). Finally we give a lower bound for the number of nodal domains of eigenvectors belonging to the second largest eigenvalue (see [7]).

In chapter 6, the nodal domains of a cograph is studied. A graph $G = (V, E)$ is called cograph if G has no induced subgraph P_4. We consider the Laplacian matrix of a cograph. We give an algorithm that find the minimum or maximum number of nodal domains of a cograph in $O(|V| + |E|)$ time (see [8]). Finally we study the conjecture that the rank of the adjacency matrix $A(G)$ of a cograph G is equal to the number of distinct nonzero columns of $A(G)$. We prove this conjecture (see [8]).

In the last chapter we present some counterexamples and open problems on nodal domains.

2. GRAPH LAPLACIANS

2.1 Basic Definitions

In this section we recall some notions from graph theory, linear algebra and complexity of algorithms.

Graphs

We briefly give the terminology in graph theory needed in this thesis. For standard graph theoretical terms not defined here we refer to [29, 83].

A graph $G = (V, E)$ is a pair with V a nonempty finite set called the *vertices* and an *edge* set E, where an edge is an unordered pair of distinct vertices. We also use $V(G)$ and $E(G)$ to denote the vertex set and edge set of G, respectively. We denote the *cardinality* of a set S by $|S|$. An edge $e = uv$ connects the vertices u and v, and we say that u and v are *adjacent* or u is a *neighbor* of v.

Graphs as we have defined them above are sometimes referred to as *simple graphs*.

The number of neighbors of v is called the *degree* of v and denoted by d_v. If all the vertices of a graph G have the same degree k, then G is *k-regular*, or simply *regular*.

The *complement* G^c of a graph G has the same vertex set as G, where vertices u and v are adjacent in G^c if and only if they are not adjacent in G.

A graph is called *complete* if every pair of vertices are adjacent, and the complete graph with n vertices denoted by K_n.

A graph H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. A subgraph H of G is an *induced subgraph* if two vertices of $V(H)$ are adjacent if and only if the are adjacent in G. If $U \subseteq V(G)$, then $G[U]$ denotes the induced subgraph of G with vertex set U. If U is any set of vertices of G, we write $G - U$ for $G[V \setminus U]$. We write $G - v$ rather than $G - \{v\}$. For a subset F of $E(G)$ we write $G - F := (V, E \setminus F)$. Instead of $G - \{e\}$ we write $G - e$ and we say *deleting* edge e.

A *clique* is a subgraph that is complete. A set of vertices is *independent* if no two of its elements are adjacent.

A path with k vertices from u to v in a graph is a sequence of k distinct vertices starting with u and ending with v such that consecutive vertices are adjacent. We denote a path with k vertices by P_k. If there is a path between any two vertices of a graph G, then G is *connected*, otherwise *disconnected*. A maximal connected induced subgraph of G is called *(connected) component* of G.

A *cycle* is a connected graph where every vertex has exactly two neighbors. A graph containing no cycles is called a *forest*. A connected forest is called a *tree*.

A graph $G = (V, E)$ is called *k-partite* if V admits a partition into k classes such that vertices in the same partition class must not be adjacent. Instead of 2-partite one says usually *bipartite*. An k-partite graph in which every two vertices from different partition classes are adjacent is called *complete* and denoted by $K_{n_1,\ldots,n_k}$.

Let $e = uv$ be an edge of $G = (V, E)$. By G/e we denote the graph obtained from G by *contracting* the edge e into a new vertex v_e, which becomes adjacent to all the former neighbors of u and of v. We delete any multiple edges or loops.

A graph H that can be obtained from G by series of deletions and contractions of edges and deletions of isolated vertices is called a *minor* of G.

Linear Algebra

We recall the main results of the linear algebra of symmetric matrices over the real numbers, which is the basis for the subsequent chapters.

Let M be a real $n \times n$ matrix. An *eigenvalue* of M is a number λ satisfying $Mx = \lambda x$ for a nonzero vector x. Any such vector x is called an *eigenvector* of the matrix M belonging (affording, with) to the eigenvalue *lambda*. The space of all eigenvectors of M belonging to λ together with the null vector, is called the *eigenspace* of λ. The dimension of the eigenspace is called the *geometric multiplicity* of λ. If M is symmetric, the geometric multiplicity is equal to the multiplicity of λ as the root of the *characteristic polynomial* $\det(M - \lambda I)$ of M. The eigenvalues of a real symmetric matrix are real numbers. Let M be an $n \times n$ real symmetric matrix. Then $\mathbb{R}^n$ has an orthonormal basis consisting of eigenvectors of M.

The *spectrum* of a matrix is the list of its eigenvalues together with their multiplicities.

The *trace* of a square matrix A is the sum of the diagonal entries and is denoted by $tr(A)$. The trace of a square matrix is also equal to the sum of its eigenvalues. Therefore, $tr(L(G)) = \sum_{i=1}^{n} d_i = \sum_{i=1}^{n} \lambda_i$.

The *spectral radius* $\rho(A)$ of a matrix is the maximum of the absolute value of its eigenvalues.

Geršgorin Theorem. *Let M be an $n \times n$ matrix and let $r_i = \sum_{i \neq j} |M_{ij}|$, for $i = 1, \ldots, n$. Then every eigenvalue of M lies in at least one of the discs $|z - M_{ii}| \leq r_i$, for $i = 1, \ldots, n$ in the complex plane. Furthermore, if a union of k disks has no point in common with the remaining $n - k$ disks, then there are precisely k eigenvalues of M in this union.*

Algorithms and their Complexity

In the analysis of an algorithm, first of all we are interested in its *complexity*, which is measured by the number of elementary operations of an algorithm. The complexity of an algorithm depends on the size of its input. An algorithm is an $O(g(n))$ algorithm for some function $g(n)$ of its input size if the running time of its input size n never exceeds $cg(n)$ for some constant c and a positive integer n. An algorithm is a *polynomial* algorithm if $g(n)$ is a polynomial in n.

There are many interesting algorithmic problems concerning graphs for which no polynomial algorithm are known. Many of those problems belong to the class of *NP-complete* problems. For a detailed introduction to the class of NP-complete problems, see [43].

A problem is a *decision* problem if it requires the answer 'yes' or 'no'. A problem is understood as a family of instances. For example, we consider the *Hamilton cycle problem*: given a graph, decide whether or not it has a Hamilton cycle. Every graph provides an instance of this problem.

A decision problem S belongs to the complexity class P if and only if there exits a polynomial algorithm which, given any instance of S, produces answer 'yes' or 'no' such that the answer of the algorithm on input x is 'yes' if and only if x is a 'yes' instance for S.

A decision problem belongs to the complexity class *NP* if, for every 'yes' instance of the problem, there exists a short 'proof', called a *certificate*, of polynomial size such that, using the certificate, one can verify in polynomial time that the instance is indeed a 'yes' instance.

Given a pair of decision problems S, T, we say that S is *polynomially reducible* to T if there is a polynomial algorithm $\mathcal{A}$ that transforms an instance x of S into an instance $\mathcal{A}(x)$ of T such that the second instance has the same answer as the first one. That is, x is a 'yes' instance of S if and only if $\mathcal{A}(x)$ is a 'yes' instance of T.

A decision problem is *NP-hard* if all problems in NP can be polynomially reduced this problem. If the problem is NP-hard and also belongs to NP then it is *NP-complete*. Polynomial transformations are transitive. Hence, in order to prove that W is in NP-hard, it is sufficient to prove that there is some NP-complete problem which is polynomial reducible to W.

2.2 Graph Laplacians

There are various matrices that are associated with a graph. Here we introduce the adjacency, Laplacian and generalized Laplacian matrices of a graph.

Let $G = (V, E)$ be a simple graph with vertex set $V = \{1, \ldots, n\}$ and edge set E. The entries of the *adjacency matrix* $A(G)$ of G are $A_{uw} = 1$ if the vertices u and w are adjacent and 0 otherwise. The degree matrix $D(G)$ of G is diagonal with D_{vv} being the degree of vertex v. The *Laplacian matrix* of G is the matrix

$$L(G) = D(G) - A(G).$$

We also say graph Laplacian or Laplacian and we use L as shorthand for $L(G)$ when G is clear from the context or unimportant (analogously, A for $A(G)$). Similarly, we refer to the eigenvalues, eigenvectors etc. of G for the eigenvalues and eigenvectors and so on of the associated matrix of G. The graph Laplacian is symmetric.

The Laplacian $L(G)$ can be viewed as a proper discretization of the familiar Laplacian differential operator.

Now we show the basic fact that the graph Laplacian is non-negative definite (i.e., $x^t L(G)x \geq 0$ for vector x in $\mathbb{R}^n$). Let G be a graph with n vertices and x be a vector in $\mathbb{R}^n$).

$$\begin{aligned}
(Lx)_v &= d_v x_v - \sum_{vj \in E} x_j, \\
Lx &= (d_1 x_1 - \sum_{1j \in E} x_j, \ldots, d_n x_n - \sum_{nj \in E} x_j)^t, \text{ and} \\
x^t Lx &= \sum_{i=1}^{n} d_i x_i^2 - 2 \sum_{ij \in E} x_i x_j = \sum_{ij \in E} (x_i - x_j)^2 \geq 0.
\end{aligned}$$

If G is a connected graph with n vertices then the constant vector $e_n = (1, \ldots, 1)$ is the unique eigenvector with eigenvalue 0, $Le_n = 0$ (for a proof see Corollary 2.1). Each eigenvector x of $L(G)$, which is orthogonal to e_n, has at least two entries with opposite sign and of course $\sum_{i=1}^{n} x_i = 0$.

In particular, we are interesting in the eigenvectors of a Laplacian. Merris [67] considers several eigenvector principles for a Laplacian. We review here some of them.

Proposition 2.1. [67] *Let G be a graph with n vertices. If $0 \neq \lambda < n$ is an eigenvalue of $L(G)$, then any eigenvector affording λ takes the value 0 on every vertex of degree $n - 1$.*

Proof. Let v be a vertex of degree $n-1$. $(Lx)_v = (n-1)x_v - \sum_{i \neq v} x_i = \lambda x_v$, hence $nx_v = \lambda x_v$ and $x_v = 0$. □

Proposition 2.2. [67] *Let λ be an eigenvalue of $L(G)$ afforded by eigenvector x. If $x_u = x_v$, then λ is an eigenvalue of $L(G')$ afforded by x, where G' is the graph obtained from G by deleting or adding the edge $e = uv$ depending on whether or not $e = uv$ is an edge of G.*

Let $G = (V, E)$ be a graph. Fix a nonempty subset W of V. Delete all the vertices in $V \setminus W$ that are not adjacent to a vertex of W. Then remove any remaining edges that are not incident with a vertex of W. The resulting graph is called *reduced graph* $G\{W\}$.

Proposition 2.3. [67] *Let $G = (V, E)$ be a graph. Fix a nonempty subset W of V. Suppose x is an eigenvector of the reduced graph $G\{W\}$ that affords λ and is supported by W in the sense that if $x_u \neq 0$, then $u \in W$. Then the extension $x' = (x, 0)$ is an eigenvector of G affording λ.*

Proposition 2.4. [67] *Let G be a graph with n vertices and x an eigenvector affording λ. Let N_v be the set of neighbors of v. Suppose $x_u = x_v = 0$, where $N_u \cap N_v = \emptyset$. Let G' be the graph on $n-1$ vertices obtained by coalescing u and v into a single vertex, which is adjacent in G' precisely to those vertices that are adjacent in G to u or to v. The vector obtained from x by deleting uth coordinate of x is an eigenvector of G' affording λ.*

If G is a regular graph, then the eigenvalues of the Laplacian are determined by the eigenvalues of the adjacency matrix.

Proposition 2.5. *Let G be a k-regular graph. If the adjacency matrix $A(G)$ has eigenvalues $\lambda_1, \ldots, \lambda_n$, then the Laplacian $L(G)$ has eigenvalues $k - \lambda_1, \ldots, k - \lambda_n$.*

Proof. If G is k-regular, then $L(G) = D(G) - A(G) = kI - A$. Thus every eigenvector of A with eigenvalue λ is an eigenvector of $L(G)$ with eigenvalue $k - \lambda$. □

The next well-known result describes the relation between the Laplacian spectrum of G and the Laplacian spectrum of its complement G^c. The matrix J is the $n \times n$ matrix each of whose entries is 1.

Proposition 2.6. *If G is a graph with n vertices, x is orthogonal to e_n and x is an eigenvector of $L(G)$ with eigenvalue λ, then x is an eigenvector of $L(G^c)$ with eigenvalue $n - \lambda$.*

Proof. We start observing that $L(G) + L(G^c) = nI - J$ and $Jx = 0$. Then,

$$nx = (nI - J)x = L(G)x + L(G^c) = \lambda x + L(G^c)x.$$

Therefore, $L(G^c)x = (n - \lambda)x$. □

Let A be an $n \times n$ real matrix. The *underlying directed graph* of A has vertex set $\{1, \ldots, n\}$, with an arc from vertex u to vertex w if and only if $A_{uw} \neq 0$. (Note that this directed graph may have loops). A square matrix is *irreducible* if its underlying graph is strongly connected (i.e., any two vertices u, s can be joined by a directed path).

Perron-Frobenius Theorem. *Let A be a real nonnegative $n \times n$ matrix whose underlying directed graph is strongly connected. Then*

(i) $\rho(A)$ is a single eigenvalue of A. If x is an eigenvector for ρ, then no entries of x are zero, and all have the same sign.

(ii) Let A_1 be a real nonnegative $n \times n$ matrix such that $A - A_1$ is nonnegative. Then $\rho(A_1) \leq \rho(A)$, with equality if and only if $A_1 = A$.

There are many generalized Laplacians associated with each graph, which at first glance seem only tenuously related.

Chung [18] defined a general and normalized form of the Laplacian matrix, which is consistent with the eigenvalues in spectral geometry and in stochastic processes. She defined the Laplacian matrix as follows:

$$M_{uv} = \begin{cases} 1 & \text{if } u = v \text{ and } d_v \neq 0, \\ -\frac{1}{\sqrt{d_u d_v}} & \text{if } u \text{ and v are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

Another graph Laplacian comes from quantum mechanics. The approximations of Schrödinger's equation give the following eigenvalue problem for organic molecules (see for details, e.g., [79]).

$$Hx = (\alpha - \lambda)x, \quad H = (\beta - \lambda\sigma)A,$$

where A is the adjacency matrix of the graph representing the organic molecule, and α, β, σ are constants which are assumed to be known. The matrix H is also called *Hückel matrix*. These approximations form the basis of the so-called *Hückel theory* [56].

Fiedler [35] considers a more general matrix for a tree. He called a real symmetric $n \times n$ matrix M *acyclic* if for any mutually distinct indices $k_1, \ldots, k_s$ $(s \geq 3)$ the equality $M_{k_1 k_2} M_{k_2 k_3} \cdots M_{k_s k_1} = 0$ is fulfilled.

We generalize the Laplacian matrix of a graph as follows. Let G be a graph with n vertices. We call a symmetric matrix M a *generalized Laplacian* of G if $M_{uw} < 0$ when uw is an edge of G and $M_{uw} = 0$ when u and w are distinct and not adjacent. There are no constraints on the diagonal entries of M. The ordinary Laplacian is a generalized Laplacian, and if A is the adjacency matrix of G, then $-A$ is a generalized Laplacian. A generalized Laplacian matrix is also called a *discrete Schrödinger operator* associated with G, see e.g. [25]. Colin de Verdière's famous graph invariant μ is closely related to this class of operators [24].

The generalized Laplacian $M(G)$ can be viewed as a linear operator on the space of a function $f: V(G) \to \mathbb{R}$ which satisfies

$$Mf(v) = M_{vv}f(v) - \sum_{vu \in E(G)} M_{vu}f(u).$$

We consider the smallest eigenvalue λ_1 of a generalized Laplacian of G.

Corollary 2.1. *Let G be a connected graph with a generalized Laplacian M. If G is connected, then the smallest eigenvalue λ_1 of M is simple and the corresponding eigenvector can be taken to have all entries positive.*

Proof. If M is a generalized Laplacian of G, then for any c, the matrix $M - cI$ is a generalized Laplacian of G with the same eigenvectors as M. We choose a constant c such that all diagonal entries of $M - cI$ are nonpositive. By Perron-Frobenius Theorem, the largest eigenvalue of $-M + cI$ is simple and the associated eigenvector may be taken to have only positive entries. □

3. NODAL DOMAINS

In the previous chapter we have seen that by the Perron-Frobenius Theorem the eigenvector of the first eigenvalue λ_1 have all entries positive for a generalized Laplacian matrix M of a connected graph G. In this chapter we see that something similar holds for eigenvectors belonging to the other eigenvalues of M. We investigate nodal domains of an eigenvector, i.e., the connected components of the maximal induced subgraph of G on which an eigenvector does not change sign. The analogue of Courant's nodal domain theorem provides upper bounds on the number of nodal domains depending on the location of the eigenvalue in the spectrum.

3.1 Nodal Domains

We associate a graph $G = (V, E)$ with vertex set $V = \{1, \ldots, n\}$ vertices with a real vector $x = (x_1, \ldots, x_n)$. A *positive (negative) strong nodal domain* is a maximal connected induced subgraph of G on vertices $i \in V$ with $x_i > 0$ ($x_i < 0$). Analogously, a *positive (negative) weak nodal domain* is a maximal connected induced subgraph of G on vertices $i \in V$ with $x_i \geq 0$ ($x_i \leq 0$). Let $\mathrm{SND}(x)$ denote the number of strong nodal domains of the vector x and $\mathrm{WND}(x)$ the number of weak nodal domains of the vector x. Obviously, $\mathrm{WND}(x) \leq \mathrm{SND}(x)$. A strong or weak nodal domain is also called *sign graph* (see [23]). E.g., for the graph G in Fig. 3.1 with vector x, the vector x has two positive and three negative strong nodal domains, respectively. The vector x has also one positive and two negative weak nodal domains, respectively. Hence $\mathrm{SND}(x) = 5$ and $\mathrm{WND}(x) = 3$.

In other words, we consider a function $f : V \to \mathbb{R}$ on $G = (V, E)$. Such a function is called a *landscape* on G in [73]. A strong nodal domain (weak nodal domain) of f is a maximal connected induced subgraph $G[W]$ of G with vertex set W such that $f(u)f(v) > 0$ ($f(u)f(v) \geq 0$) for all $u, v \in W$.

By the definition of weak nodal domains, each zero vertex belongs to exactly one weak positive nodal domain and exactly one weak negative nodal domain. If two different weak nodal domains S_1, S_2 of a vector overlap, then they must have opposite signs except zero vertices.

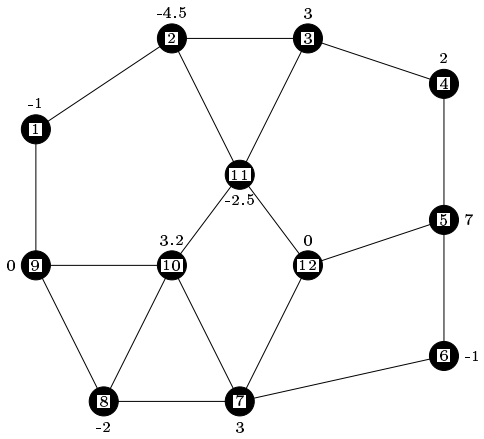

Fig. 3.1: The strong and weak nodal domains of the vector $x = (-1, -4.5, 3, 2, 7, -1, 3, -2, 0, 3.2, -2.5, 0)$

For a graph G, it is easy to see that the number of strong nodal domains is at most the number of vertices of the induced bipartite subgraph of G with maximum number of vertices. To find such an induced bipartite subgraph of G is a well known NP-complete problem (see, e.g., [43]).
Similarly, there exists an upper bound for weak nodal domains of an arbitrary vector.

Proposition 3.1. [63] *Let $G = (V, E)$ be a connected graph and $G^* = (V^*, E^*)$ be a bipartite minor with a maximum number of vertices of G such that edges are only contracted in G and multiple edges and loops are deleted in the resulting graph, if necessary. Then* $\mathrm{WND}(x) \leq |V^*|$*, for any real vector x.*

Proof. By contraction all edges uv for which $x_u, x_v \geq 0$ and all edges uv with $x_u, x_v \leq 0$ we get a bipartite minor of G. Thus every weak positive nodal domain and every strong negative nodal domain of x collapses in to a single vertex. This minor is bipartite and the result follows, since G^* is bipartite minor with maximum vertices. □

We remark that finding maximal bipartite minors is also an NP-complete problem[1]. The upper bound according to maximal bipartite minor does not hold for strong nodal domains. For the graph in Fig. 3.2 the eigenvector $(1, -1, 0, 1, -1)$ has four strong nodal domains, but maximum bipartite minor has at most three vertices.

[1] I thank H. Müller for this note.

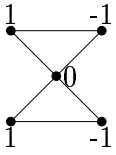

Fig. 3.2: A counterexample to the maximum bipartite minor

Instead of arbitrary vectors let us now consider the nodal domains of an eigenvector of a generalized Laplacian.

Proposition 3.2. *Let M be a generalized Laplacian of a graph G and let x be an eigenvector of M. Then any vertex v with $x_v = 0$ either has all neighbors u with $x_u = 0$, or has two neighbors u and w with $x_u > 0$ and $x_w < 0$.*

Proof. Let v be a vertex with $x_v = 0$. Then

$$(Mx)_v = M_{vv}x_v + \sum_{vu \in E(G)} M_{vu}x_u = \sum_{vu \in E(G)} M_{vu}x_u = 0$$

Since $M_{vu} < 0$ when v is adjacent to u, either $x_u = 0$ for all vertices adjacent to v, or the sum has both positive and negative terms. □

We say two different strong (weak) nodal domains S_1, S_2 of a vector are *adjacent* if there exit vertices $v_1 \in S_1, v_2 \in S_2$ such that $v_1v_2 \in E(G)$. By the definition, if two different strong (weak) nodal domains are adjacent, then they have opposite signs.

Proposition 3.3. [23] *Let x be an eigenvector of a generalized Laplacian $M(G)$. Suppose S_1, S_2 are adjacent weak nodal domains of x. There is a pair of vertices v_1, v_2 such that $v_1 \in S_1$, and $v_2 \in S_2 \setminus S_1$ and v_1v_2 is an edge of G.*

We focus our attention on the k-th eigenvalue λ_l of a generalized Laplacian M, and suppose that it has multiplicity r, so that

$$\lambda_1 \leq \cdots \leq \lambda_{k-1} < \lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+r-1} < \lambda_{k+r} \leq \cdots \leq \lambda_n.$$

Throughout this manuscript we assume that the eigenvalues are numbered in non-decreasing order.

Theorem 3.1. Discrete Nodal Domain Theorem [23]
Let M be a generalized Laplacian of a connected graph with n vertices. Then any eigenvector x corresponding to eigenvalue λ_k with multiplicity r has at most $k + r - 1$ strong nodal domains and at most k weak nodal domains. It means $\mathrm{SND}(x) \leq k + r - 1$ *and* $\mathrm{WND}(x) \leq k$.

Sketch of the proof. Let x be an eigenvector of λ_k and x has m strong nodal domains S_i, $i = 1, \ldots, m$. We define m vectors y^i, $i = 1, \ldots, m$ such that $y^i_j = x_j$ if $v_j \in S_i$, and $y^i_j = 0$ otherwise. Thus $x = \sum_{i=1}^m y^i$. Now we form a new vector $z = \sum_{i=1}^m c_i y^i$. Since y^i are not identically to zero and are disjoint, their span has dimension m. It follows that there exist nonzero real coefficients c_i, $i = 1, \ldots, m$ such that z is nonzero and is orthogonal to the first $m-1$ eigenvectors of M (i.e., eigenvectors belonging to the eigenvalues $\lambda_1, \ldots, \lambda_{m-1}$). Without loss of generality we can take $z^t z = 1$. By the minmax theorem and using straightforward algebra (for details see [23]), we get

$$z^t M z \geq \lambda_m \tag{3.1}$$

and

$$z^t M z - \lambda_k = -\frac{1}{2} \sum_{i,j=1}^{m} (c_i - c_j)^2 {y^i}^t M y^j. \tag{3.2}$$

A term ${y^i}^t M y^j$ is nonzero only if y^i and y^j correspond to adjacent nodal domains. The adjacent nodal domains have opposite signs and they are disjoint. Therefore ${y^i}^t M y^j > 0$. Thus Equation (3.2) gives $y^t M y - \lambda_k \leq 0$. This combined with (3.1) states that $\lambda_m \leq \lambda_k$. Therefore we have $m \leq k + r - 1$, i.e., $\mathrm{SND}(x) \leq k + r - 1$.

For the proof of the weak nodal domain theorem we use a continuation result for the coefficients c_i, which is a discrete analogue of the unique continuation principle for eigenfunctions.

Suppose that x has $s \geq k$ weak nodal domains W_i, $i = 1, \ldots, s$. We choose c_i, $i = 1, \ldots, s$, not all zero, to make z orthogonal to the first $s-1$ eigenvectors of M as we did above. If two weak nodal domains W_i and W_j are adjacent, then $c_i = c_j$ (for details see [23]).
Suppose $s > k$. Since G is connected, W_1 must be adjacent to at least one other nodal domain, which we label W_2. Then $c_1 = c_2$. If $s \geq 3$, one of W_1 and W_2 must be adjacent to one of the remaining nodal domains, say W_3, otherwise G is not connected. Therefore $c_1 = c_2 = c_3$. In $s-1$ steps we conclude that $c_s = c_{s-1} = \cdots = c_1$. Hence $z = c_1 x$. This is a contradiction to the claim that z is orthogonal to the first $s-1$ eigenvector. Therefore $s \leq k$. □

This is the graph version of Courant's celebrated Nodal Domain Theorem for Riemannian manifolds, see e.g. [15, 17]. Various versions of the nodal domain theorem for graphs and partial proofs were obtained independently by different authors [25, 31, 41, 72, 80], beginning with the work of M. Fiedler

who proved the following two results that are corollaries of the nodal domain theorem:

Corollary 3.1. [34, 35] *The eigenvector x affording to the smallest non-zero eigenvalue of any connected graph has* $\mathrm{WND}(x) = 2$ *weak nodal domains.*

Corollary 3.2. [36] *The eigenvector affording λ_k has at most $k-1$ positive weak nodal domains for $k > 1$.*

The eigenvector affording the second eigenvalue is often called a *Fiedler vector* of G. The associated eigenvalue λ_2 is the *algebraic connectivity* of G, which is closely related to the vertex and edge connectivities of G:

$$\lambda_2 \leq \mathbf{v}(G) \leq \mathbf{e}(G)$$

As for manifolds, the nodal domain theorem for graphs does not provide a sharp inequality for all graphs. For manifolds equality for every eigenvalue holds only in dimension one, i.e. for a string. For spheres with the standard metric a sharp lower bound on the number of nodal domains exists [62] but so far no sharp upper bounds are available, see e.g. [2, 59, 60, 64]. For graphs the situation is similar. There only exist improved upper bounds for trees, cographs, and hypercubes. In coming chapters we look at the nodal domains for trees, hypercubes, and cographs. These results show that the "Courant bounds" are not sharp on non-trivial graph classes.

The number of nodal domains can be much smaller than the bound obtained from the Nodal Domain Theorem. An example are the so-called Faria vectors [33]: A vector x is called a *Faria vector*, if x has only two non-zero elements $x_u = -x_v = 1$. Two vertices u and v are called *twins* if every vertex $w \notin \{u, v\}$ is either adjacent to both u and v or to neither one of them.

Proposition 3.4. *A Faria vector x is an eigenvector of the Laplacian of the graph G if and only if u and v are twins or they are twins except the edge uv.*

Proof. It is easy to see from $(L(G))_v$. □

We refer to [11] for a more detailed discussion of twin vertices. Obviously, Faria vectors exist for arbitrarily large graphs if there is a vertex that is adjacent to at least two vertices of degree 1.

Proposition 3.5. *If a graph with n vertices has a vertex v with degree $n-1$, then each eigenvector of an eigenvalue $\lambda \neq 0$ of Laplacian has two weak nodal domains.*

Proof. Let v be a vertex of G with degree $n-1$. By Proposition 2.1 $x_v = 0$, for eigenvector x of eigenvalue $\lambda \neq 0$. □

Proposition 3.6. *Let x and y be eigenvectors affording eigenvalue λ of $L(G)$ and $L(H)$, respectively. Let Z_G and Z_H be the vertices with $x_v = 0$ and $y_u = 0$, respectively. If we add some edges between Z_G and Z_H, then $z = (x, y)$ is an eigenvector affording eigenvalue λ of the new graph G'. Of course* $\mathrm{SND}(z) = \mathrm{SND}(x) + \mathrm{SND}(y)$.

Proof. It is easy to see from $(L(G')z)_v$. □

Research on the sign properties of the eigenvectors goes back to the research of tridiagonal matrices with negative off-diagonals (see e.g., [42]).

Lower bounds are unknown with the exception of the trivial bound $\mathrm{SND}(x) \geq 2$ for λ_k, $k > 1$, and the following result on the largest eigenvalue of a bipartite graph.

Theorem 3.2. [74] *Let $G = (V_1 \cup V_2, E)$ be a connected bipartite graph with $n = |V_1 \cup V_2|$ vertices and let M be a generalized Laplacian of G. Then there is an eigenvector x to the largest eigenvalue of M, such that x is positive on V_1 and negative on V_2 or* vice versa *and hence satisfies* $\mathrm{WND}(x) = \mathrm{SND}(x) = n$.

Theorem 3.2 generalizes an analogous result for the the smallest eigenvalue of the adjacency matrix $A(G)$ [3].

By Proposition 2.6 and Corollary 2.1, the largest eigenvalue of the Laplacian matrix is simple for a connected bipartite graph. In general, this is not the case for generalized Laplacian.

The upper bound for the number strong nodal domains is the number of vertices of maximum induced bipartite subgraph. Now we show that this upper bound also holds for some generalized Laplacian.

Theorem 3.3. *Let G be a connected graph and H be the maximum induced bipartite subgraph of G, then there exits a generalized Laplacian $M(G)$ such that $M(G)$ has an eigenvector x with $|V(H)|$ strong nodal domains.*

Proof. Let H be the maximum induced bipartite subgraph of G with components $C_1, \ldots, C_k$ and let R be the remaining vertices of G. Let $M_1, \ldots, M_k$ be the generalized Laplacians of $C_1, \ldots, C_k$ such that diagonal elements of M_i are positive. By Theorem 3.2 the largest eigenvalue $\lambda(M_i)$ of M_i has an eigenvector x^i with $\mathrm{SND}(x^i) = |V(C_i)|$. Eigenvalues $\lambda(M_i)$ are positive, since $\mathrm{tr}(M_i) > 0$. Without loss of generality, $\lambda(M_i) = b_i \lambda(M_1)$, for $i = 1, \ldots, k$.

The generalized Laplacian of G has the following form:

$$M = \begin{pmatrix} M_1 & 0 & \cdots & 0 & A_1^t \\ 0 & 1/b_2 M_2 & 0 & 0 & A_2^t \\ 0 & 0 & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 1/b_k M_k & A_k^t \\ A_1 & \cdots & \cdots & A_k & M_R \end{pmatrix}$$

Each vertex v of R has two neighbors u, w in one of C_i such that x_u^i and x_w^i have opposite sign, otherwise we get a new bipartite graph with more vertices then H. Thus we can choose $A_1, \ldots, A_k$ such that $A_1 x^1 + \cdots + A_k x^k = 0$. Now we show that the vector $x = (x^i, \ldots, x^k, 0)^t$ is an eigenvector of M, where $x_v = 0$ for every vertex v of R.

$$Mx = (M_1 x^1, \ldots, M_k x^k, A_1 x^1 + \cdots + A_k x^k)^t = \lambda(M_1)(x^1, \ldots, x^k, 0)^t$$

□

One of the open questions is to find a similar result for the weak nodal domains with respect to the maximum bipartite minor.

Question 3.1. *Let F be a maximum bipartite minor of a graph G as defined in Proposition 3.1. Is there a generalized Laplacian matrix $M(G)$ such that an eigenvector of $M(G)$ has $|V(F)|$ weak nodal domains?*

In the case of degenerate eigenvalues the situation for nodal domains becomes even more difficult because the number of nodal domains may vary considerably depending on which vector from the r-dimensional eigenspace of λ_k is chosen.

Hence, given a fixed graph $G = (V, E)$ and an eigenvalue λ_k three questions immediately arise:
What is the "typical" number of nodal domains of a corresponding eigenvector x?
What is the minimal number of nodal domains of x?
What is the maximal number of nodal domains of x?

3.2 Nodal Domains and Hyperplane Arrangements

It is easy to compute the number of nodal domains for a given eigenvector. Thus it is no problem to compute the possible number of nodal domains, when all eigenvalues are simple. The situation changes completely in the case of degenerate eigenvalues because then the number of nodal domains may vary

considerably depending on which vector from the r-dimensional eigenspace of λ_k is chosen. To handle this situation we choose an orthonormal basis $u^1, \ldots, u^r$ for the eigenspace of λ_k. Every eigenvector x to the eigenvalue λ_k is then given by

$$x_v = \sum_{j=1}^{r} a_j \, u_v^j = \langle a, u(v) \rangle$$

where $a = (a_1, \ldots, a_r)$, and $u(v) = (u_v^1, \ldots, u_v^r)$ is the vector that contains the values of the basis at the vertex v. The term $\langle a, u(v) \rangle = a^t u(v)$ is the inner product. Notice that if U is the matrix containing the basis vectors u^j as its columns then $u(v)$ forms the v-th row of U.

The convex hull of the vectors $u(v)$, for $v \in V$, forms a polytope in $\mathbb{R}^r$, which is called the *eigenpolytope* of the graph, see e.g. [14, 46].

It is obvious that the number of nodal domains only depends on the signs of the eigenvector on each vertex. There is a one-to-one relation between the eigenvector x and its "coordinate vector" a. The sign at vertex v is given by the sign of $\langle a, u(v) \rangle$. The set of eigenvectors that vanish on vertex v corresponds to the set

$$H_v = \{a \in \mathbb{R}^r : \langle a, u(v) \rangle = 0\}$$

which is either a hyperplane through the origin in $\mathbb{R}^r$ or, if $u(v) = 0$, $H_v = \mathbb{R}^r$. The set of all proper hyperplanes forms a *hyperplane arrangement*

$$\mathcal{H} = \{H_v | v \in V\}$$

in $\mathbb{R}^r$, see e.g. [32, 84]. The union of all these hyperplanes creates a *cellular complex* in $\mathbb{R}^r$ or (if we look at normalized eigenvectors) in the sphere S^{r-1}. A cellular complex consists of disjoint cells, where each cell is either homeomorphic to an open disc $D_d = \{a \in \mathbb{R}^d : ||a||_2 < 1\}$ or a single point. In the former case we say that the cell has dimension d and the cell is called a *d-cell*. In the latter case we have a *0-cell*. Additionally, a cellular complex satisfies the following properties: (i) The union of all cells is the entire space $\mathbb{R}^r$ (or S^{r-1}); (ii) The boundary of a d-cell consists of the union of cells of dimension less than d.

Each of the hyperplanes H_v splits the $\mathbb{R}^r$ into three pieces: the hyperplane H_v itself and the two open half-spaces $\{a \in \mathbb{R}^r | \langle a, u(v) \rangle > 0\}$ and $\{a \in \mathbb{R}^r | \langle a, u(v) \rangle < 0\}$. Hence, for each vector $a \in \mathbb{R}^r$ we may introduce the *covector* or *position vector* c_a. The coordinate $c_a(v)$ is the sign of $\langle a, u(v) \rangle$. The covector c_a is constant in each cell of the cellular complex and it uniquely determines each cell. Moreover, it corresponds to the sign pattern of the associated eigenvector. The co-vectors represent an oriented matroid [9]. Finding

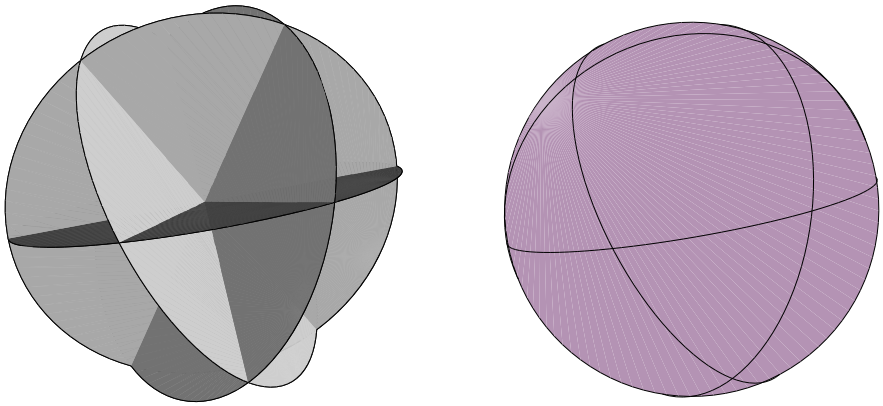

Fig. 3.3: Hyperplane arrangement (l.h.s.) and the corresponding cells on the sphere (r.h.s.) of eigenvalue 4 for the hypercube K_2^3. We have $r = 3$ and $|V(G)| = 8$. The vectors $u(v)$ are given by the eight vectors $(\pm 1, \pm 1, \pm 1)$. Due to symmetry we only have the following cells

dim	shape	SND	WND
2	rectangle	4	4
2	triangle	3	3
1	edge	4	3
0	point	3	2

on the sphere S^2. This is easily checked using `Mathematica`.

all possible values for the number of nodal domains is equivalent to finding all cells of this complex. However the number of cells explodes with the number of vertices and the multiplicity r of the eigenvalue. Using a general upper bound for hyperplane arrangements [32] we have the asymptotic behavior

$$\text{number of } d\text{-cells} \sim |V(G)|^r. \tag{3.3}$$

An exact and sharp upper bound is given, e.g., in [32].

The following observations will simplify our task. Assume that we go along a path within a cell towards its boundary. As long as we stay inside the cell nothing happens and the number of nodal domains remains unchanged. But if we reach the boundary the eigenvector vanishes on some (but at least one) of the non-zero vertices whereas all other remain unchanged. This has two consequences.

If we look at weak nodal domains, then their number is either decreasing or remains constant, since zero vertices do not separate weak nodal domains. So we have to look at 0-cells if we want to minimize $\mathrm{WND}(x)$ and to cells of highest dimension if we want to maximize $\mathrm{WND}(x)$, for the eigenvector x of

λ_k.

If we look at strong nodal domains the situation is much more complicated. Because then zeros separate nodal domains, and SND(x) may increase. However, if the eigenvector vanishes on too many vertices when we reach the boundary, it might happen that nodal domains disappear which decreases SND(x). This happens for example with some eigenvectors to the second eigenvalue of stars (connected graphs where all but one vertex have degree 1), or more generally with some eigenvectors to eigenvalues where Faria vectors exist. Figure 3.3 illustrates the situation.

Because of equ.(3.3) it is in practice impossible to calculate all cells of a hyperplane arrangement for any reasonably sized graph. We have therefore devised a *hillclimbing algorithm* to search for the minimum (or maximum) number of strong (or weak) nodal domains. This algorithm is based on the above observations, moving from a cell to neighboring cells in search of an improved number of nodal domains.

Briefly, the algorithm works as follows. Starting from some random point a in the hyperplane arrangement with corresponding eigenvector $x_v = \langle a, u(v)\rangle$. Pick a second random point a' and move into the direction of this second point until a boundary in the cellular complex is crossed (i.e., at least one of the coordinates of the position vector has changed sign and a neighboring cell is entered). To this end we define $\delta(v) = \frac{\langle a,u(v)\rangle}{\langle a',u(v)\rangle}$, and find the vertices v_1 and v_2 such that $\delta(v_1)$ is smallest with $\delta(v) > 0$ and $\delta(v_2)$ is smallest with $\delta(v) > \delta(v_1)$. Then set $\delta = (\delta(v_1) + \delta(v_2))/2$ and move from a to $a^* = a - \delta\, a'$, with corresponding eigenvector $x'_v = \langle a', u(v)\rangle$. If the number of (strong) nodal domains of this new cell is less than or equal to that of the cell that was moved from, accept this move (i.e., make the new point the current one). Otherwise, return to the original point (i.e., do not update the current point). Now repeat this sequence of picking a random second point, moving towards it from the current point until a cellular boundary is crossed, and determining whether the move is accepted or not, until some stopping criterion is reached.

Notice that the algorithm also accepts neutral moves, i.e., moves to neighboring cells that have an equal number of nodal domains. This way, getting stuck in the middle of some plateau is avoided. Since it is not obvious with this "random move" algorithm when a local optimum is reached, we terminate the search when the number R of moves without improvement exceeds a user-defined upper bound.

In practice, one wants to avoid moving back to the cell out of which a move was just made. This can be easily achieved by either explicitly excluding this cell from consideration when calculating δ for the next step, or by multiplying

the randomly picked a' with -1 if it turns out that it causes a move back into the previously visited cell. We use the latter solution in our implementation of the algorithm.

Obviously this algorithm can be used for maximizing the number of nodal domains as well. The maximum number R of unproductive moves and the probability distribution from which the random vectors a and a' are sampled are parameters of the algorithm.

It must be noted here that this algorithm only deals with coordinate vectors in cells of highest dimension correctly, i.e., the corresponding eigenvectors have no vanishing vertices (except those vertices where all eigenvectors to the given eigenvalue vanish). It can be adopted such that it also including searching on cells of lower dimension. However, there are some difficult numerical problems that require sophisticated methods from computational geometry for their solution.

We have made use of this algorithm in Chapter 5 to get an idea of possible numbers of nodal domains of a hypercube.

4. NODAL DOMAINS OF A TREE

In general it is unknown, whether the upper bound relating to the order of the eigenvalues is sharp for an arbitrary graph. Moreover, no method is known to construct an eigenvector to the eigenvalue λ_k with maximal or minimal number of the strong (or weak) nodal domains. In this chapter we characterize for a tree: the maximal number of the strong nodal domains of an eigenvector corresponding to an eigenvalue λ_k. We give an $O(n^2)$ time algorithm to find an eigenvector with maximum number of the strong nodal domains, which corresponds to an eigenvalue λ_k. We show that to find an eigenvector of an eigenvalue λ_k, which has minimum number of the strong nodal domains, is NP-complete.

Gantmacher and Krein [42] show that Discrete Nodal Domain theorem is sharp for paths.

Proposition 4.1. [42] *Let M be a generalized Laplacian matrix of a path. The eigenvalues of M are all simple, and the eigenvector belonging to the eigenvalue λ_k has exactly k strong nodal domains and exactly k weak nodal domains.*

4.1 The Maximal Number of Nodal Domains of a Tree

In the following we say that y is a *λ-eigenvector* (of A) if $Ay = \lambda y$.

We begin with a special simple case.

Theorem 4.1. *Let G be a tree and let M be a generalized Laplacian of G. If y is a λ_k-eigenvector without a vanishing coordinate, then λ_k is simple and y has exactly* $\mathrm{SND}(y) = k$ *strong nodal domains.*

The following lemma plays an important role in the proof of the Theorem 4.1.

Lemma 4.1. [35] *Let M be a generalized Laplacian of a tree. If y is a λ_k-eigenvector without a vanishing coordinate, then λ_k is simple and there are exactly $n - k$ edges ij, for which $M_{ij}y_iy_j < 0$.*

Proof of Theorem 4.1. By Lemma 4.1, λ_k is simple and there are exactly $n-k$ edges ij, for which y_i and y_j have the same sign. Note that $M_{ij}y_iy_j < 0$ if and only if i and j are adjacent and y_i and y_j have the same sign. We divide V in three disjoint sets in the following way:
$P = \{i \in V \ : \ y_i > 0, \text{ and there is an edge } ij \in E, \text{ s.t. } y_j > 0\}$,
$S = \{i \in V \ : \ y_i < 0, \text{ and there is an edge } ij \in E, \text{ s.t. } y_j < 0\}$. C is the set of remaining vertices. The induced subgraphs $G[P]$ and $G[S]$ are forests. Let p and s are the number of components of $G[P]$ and $G[S]$, respectively. $G[P]$ and $G[S]$ have $|P|-p$ edges and $|S|-s$ edges, respectively. Since $\{P, S, C\}$ is a partition of V and using Lemma 4.1, we see $|P|-p+|S|-s = n-k$. Now we show that $\mathrm{SND}(y) = k$. Let i and j be vertices of C. If y_i and y_j have the same sign, then i and j are not adjacent. Let $C_- = \{i \in C \ : \ y_i < 0\}$ and $C_+ = \{i \in C \ : \ y_i > 0\}$. By the definition of P and S, there exist no edges between C_- and S and no edges between C_+ and P, respectively. Consequently the number of strong nodal domains of y is equal to $|C|+p+s$. Thus

$$\mathrm{SND}(y) = |C| + p + s = n - |P| - |S| + |P| + |S| - n + k = k.$$

□

Remark. We remark that by Theorems 3.2 and 4.1, the largest eigenvalue of a generalized Laplacian of a tree is simple.

Next we consider eigenvectors of trees with vanishing coordinates.
Let $G = (V, E)$ be a connected graph, and let M be a generalized Laplacian of G. Let Z be a subset of V, let $G_1, \ldots, G_m$ be the components of $G - Z$ and let $M_1, \ldots, M_m$ be generalized Laplacians of $G_1, \ldots, G_m$. We say $(M_1, \ldots, M_m, A_Z)$ is a *rearrangement of* M, if we rearrange the matrix M with permutation similarity operations in the following way:

$$M = \begin{pmatrix} M_1 & M_{12} & \cdots & M_{1Z} \\ \vdots & \ddots & \cdots & \vdots \\ M_{m1} & \cdots & M_m & M_{mZ} \\ M_{Z1} & \cdots & M_{Zm} & M_Z \end{pmatrix}$$

Theorem 4.2. *Let G be a tree with n vertices and let M be a generalized Laplacian of G. Let λ be an eigenvalue of M with multiplicity $r \geq 2$. Then there exists a rearrangement $(M_1, \ldots, M_m, M_Z)$ of M such that the following statements hold:*

(i) λ is a simple eigenvalue of $M_1, \ldots, M_m$. The matrix M_j has a λ-eigenvector without vanishing coordinates, for $j = 1, \ldots, m$.

(ii) *Let $k_1, \ldots, k_m$ be the positions of λ in the spectra of $M_1, \ldots, M_m$ in non-decreasing order. Then the number of strong nodal domains of an eigenvector of λ is at most $k_1 + \cdots + k_m$,*

(iii) *There exists an eigenvector of λ with $k_1 + \cdots + k_m$ strong nodal domains. Such an eigenvector can be found in $O(n^2)$ time.*

For the proof of Theorem 4.2 we need the following two Lemmas. We shall prove Lemma 4.3 after the proof of Theorem 4.2.

Lemma 4.2. [35] *Each eigenvector corresponding to a multiple eigenvalue of a generalized Laplacian of a tree has at least one vanishing coordinate.*

We remark that Fiedler [35] proved the results of Lemmas 4.1 and 4.2 for a more general matrix of a tree.

Lemma 4.3. *Let $x^1, \ldots, x^k$ be linearly independent vectors in $\mathbb{R}^n$ and $k < n$. If all linear combinations of $x^1, \ldots, x^k$ have a vanishing coordinate, then the vectors $x^1, \ldots, x^k$ have a common vanishing coordinate.*

Proof of Theorem 4.2. Let λ be an eigenvalue of M with multiplicity $r \geq 2$. Let $y^1, \ldots, y^r$ be linearly independent λ-eigenvectors. Let Z be the set of all common vanishing coordinates of $y^1, \ldots, y^r$. By lemmas 4.2 and 4.3, Z is not empty and the choice of $y^1, \ldots, y^r$ has no influence on Z. The graph $G - Z$ is a forest with components $T_1, \ldots, T_m$. Let $M_1, \ldots, M_m$ be generalized Laplacians of $T_1, \ldots, T_m$. According to the rearrangement $(M_1, \ldots, M_m, M_Z)$ the matrix M has the following form:

$$M = \begin{pmatrix} M_1 & 0 & \cdots & 0 & M_{1Z} \\ 0 & M_2 & \cdots & 0 & M_{2Z} \\ 0 & \cdots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & M_m & M_{mZ} \\ M_{Z1} & \cdots & \cdots & M_{Zm} & M_Z \end{pmatrix}$$

(i) We write each eigenvector y of λ as $y = (y_{T_1}, \ldots, y_{T_m}, 0, \ldots, 0)$, where y_{T_j} denotes the coordinates of eigenvector y belonging to the tree T_j. By the definition of Z, the coordinates of eigenvector y belonging to Z are equal to zero. Thus the vector My has the following form:

$$My = (M_1 y_{T_1}, \ldots, M_m y_{T_m}, *, \ldots, *) = (\lambda y_{T_1}, \ldots, \lambda y_{T_m}, 0, \ldots, 0) = \lambda y$$

for each λ-eigenvector y. Therefore λ is an eigenvalue of the matrices $M_1, \ldots, M_m$.

Now we prove that λ is a simple eigenvalue of M_j and the matrix M_j has a λ-eigenvector without vanishing coordinates, for $j = 1, \ldots, m$.
We show that the number of linearly independent vectors of $y^1_{T_j}, \ldots, y^r_{T_j}$ is equal to one, for $j = 1, \ldots, m$. Note that $y^1_{T_j}, \ldots, y^r_{T_j}$ are the restrictions of the eigenvectors $y^1, \ldots, y^r$ to the subtree T_j. Assume that there are linearly independent vectors $y^1_{T_j}, \ldots, y^h_{T_j}$, $h \geq 2$. Then the vectors $y^1_{T_j}, \ldots, y^h_{T_j}$ are linearly independent λ-eigenvectors of M_j. By Lemmas 4.2 and 4.3 the vectors $y^1_{T_j}, \ldots, y^h_{T_j}$ have a common vanishing coordinate. Hence $y^1_{T_j}, \ldots, y^r_{T_j}$ have a common vanishing coordinate, a contradiction to the definition of Z.
We denote by b_j the only one linearly independent vector of $y^1_{T_j}, \ldots, y^r_{T_j}$, for $j = 1, \ldots, m$. The vector b_j is a λ-eigenvector of M_j, for $j = 1, \ldots, m$. The eigenvector b_j has no vanishing coordinate, for $j = 1, \ldots, m$. We suppose that b_j has a vanishing coordinate. Then $y^1_{T_j}, \ldots, y^r_{T_j}$ have a common vanishing coordinate, a contradiction to the definition of Z.

(*ii*) Let $k_1, \ldots, k_m$ be the positions of λ in the spectrum of $M_1, \ldots, M_m$ in non-decreasing order. The number of strong nodal domains of an eigenvector $y = (\beta_1 b_1, \ldots, \beta_l b_m, 0, \ldots, 0)$ is equal to the sum of the number of strong nodal domains of $\beta_1 b_1, \ldots, \beta_m b_m$. By Theorem 4.1, $\mathrm{SND}(b_j) = k_j$, for $j = 1, \ldots, m$. Therefore, $\mathrm{SND}(y) \leq k_1 + \cdots + k_m$.

(*iii*) Now we construct an eigenvector x of λ with $\mathrm{SND}(x) = k_1 + \cdots + k_m$ in following way: By the definition of b_j, the linearly independent eigenvectors $y^1, \ldots, y^r$ are of the form $y^i = (\beta_{i1} b_1, \ldots, \beta_{im} b_m, 0, \ldots, 0)$, for $i = 1, \ldots, r$, where the coefficients $\beta_{i1}, \ldots, \beta_{im}$ are real numbers.

$x := y^1$;
for $i = 2, \ldots, r$ **do**
  $x := x + \alpha_i y^i$,
  choose α_i: $\alpha_i \neq 0$ and $\alpha_i \notin \{-\frac{x_j}{y^i_j} : y^i_j \neq 0,\ j = 1, \ldots, n\}$.

After this iteration we obtain $x = (\beta'_1 b_1, \ldots, \beta'_m b_m, 0, \ldots, 0)$. The coefficients $\beta'_1, \ldots, \beta'_m$ are nonzero numbers. Assume that there exists a $\beta'_j = 0$. By the choice of α_i, then all $\beta_{1j}, \ldots, \beta_{rj}$ are equal to zero. This is a contradiction to the definition of Z. Therefore, $\mathrm{SND}(x) = \mathrm{SND}(\beta'_1 b_1) + \cdots + \mathrm{SND}(\beta'_m b_m) = k_1 + \cdots + k_m$. It is easy to see that we need $O(n^2)$ operations to find an eigenvector x with $\mathrm{SND}(x) = k_1 + \cdots + k_m$ from an arbitrary eigensystem of M. □

Finally, we complete the eigenvalues of a tree.

Corollary 4.1. *By Theorem 4.2, if we replace the multiple eigenvalue λ by the simple eigenvalue λ with an eigenvector y, which has at least one vanishing coordinate, then the statements of Theorem 4.2 also hold.*

Proof of Lemma 4.3. Let $x^1, \ldots, x^k$ be linearly independent vectors in $\mathbb{R}^n$, $k < n$ such that all linear combinations of $x^1, \ldots, x^k$ have a vanishing coordinate. We prove that the vectors $x^1, \ldots, x^k$ have a common vanishing coordinate.
If $k = 1$, this is trivial. Let $k \geq 2$. Let y be a linear combination of $x^1, \ldots, x^{k-1}$. Let $Z_y = \{j \ : \ y_j = x^k_j = 0\}$. Without loss of generality let the first d coordinates of x^k be zero and all others elements of x^k be nonzero.
Claim 1: y and x^k have a common vanishing coordinate, i.e. Z_y is not empty. Suppose that y and x^k have no common vanishing coordinate. Then the first d elements of y are nonzero. Now we construct a new vector $t = y + \beta x^k$. We choose β in the following way: $\beta \neq 0$ and $\beta \neq \frac{-y_i}{x^k_i}$, for $i = d+1, \ldots, n$. Then t has no vanishing coordinate. This is a contradiction.
Claim 2: If u and y are linear combinations of $x^1, \ldots, x^{k-1}$, then $Z_u \cap Z_y \neq \emptyset$. Suppose that there exists u and y, such that $Z_u \cap Z_y = \emptyset$. By claim 1, Z_u and Z_y are not empty. Without loss of generality, the first d elements of u and y are look like: $u = (0, \ldots, 0, \pm, \ldots, \pm)$, $y = (\pm, \ldots, \pm, 0, \ldots, 0, \pm, \ldots, \pm)$. Now we construct a new vector $t = u + \beta y$. We choose β such that: $\beta \neq 0$ and $\beta \neq \frac{-u_i}{y_i}$, for $i = 1, \ldots, d$ and y_i are nonzero. Then t and x^k have no common zero coordinate. This is a contradiction to claim 1.

Now we define new vectors y^i in the following way:
$y^1 = x^1$, $y^i = y^{i-1} + \alpha_i x^i$, for $i = 2, \ldots, k-1$. We choose α_i such that:
$\alpha_i \neq 0$ and $\alpha_i \neq -\frac{y^{i-1}_j}{x^i_j}$, for all x^i_j nonzero elements, for $j = 1, \ldots, d$.
Claim 3: Z_{y^i} is not empty and $Z_{y^i} = Z_{x^1} \cap \cdots \cap Z_{x^i}$, for $i = 1, \ldots, k-1$.
By Claim 1, Z_{y^i} is not empty. We prove the other argument with induction on i. For $i = 1$, $y^1 = x^1$. By Claim 1, x^1 and x^k have a common zero coordinate. We suppose that the claim holds for $y^1, \ldots, y^{i-1}$. Now we show that it holds for $y^i = y^{i-1} + \alpha_i x^i$. We choose α_i as defined. By Claim 2, $Z_{y^{i-1}} \cap Z_{x^i} \neq \emptyset$. By the choice of α_i, $y^i_j = 0$ if and only if $j \in Z_{y^{i-1}}$ and $j \in Z_{x^i}$. It means that $j \in Z_{y^{i-1}} \cap Z_{x^i}$. By induction $Z_{y^{i-1}} = Z_{x^1} \cap \cdots \cap Z_{x^{i-1}}$. Then $j \in Z_{x^1} \cap \cdots \cap Z_{x^{i-1}} \cap Z^i_x$.

By Claim 3, $Z_{y^{k-1}}$ is not empty and $Z_{y^{k-1}} = Z_{x^1} \cap \cdots \cap Z_{x^{k-1}}$. Therefore $x^1, \ldots, x^k$ have a common vanishing coordinate. □

We remark that to find the minimum (or maximum) number of weak nodal domains of a tree is an open problem.

4.2 The Minimal Number of Nodal Domains

In this section we show that the following problem is NP-complete.
MINIMUM NUMBER OF NODAL DOMAINS
Instance: An $n \times n$ matrix M, where M is a generalized Laplacian of a tree, an eigenvalue λ of M with multiplicity $r \geq 2$.
Question: Find an eigenvector y of λ such that the number of strong nodal domains of y is minimal.

Let M be a generalized Laplacian of a tree and λ is an eigenvalue of M with multiplicity $r \geq 2$. In Theorem 4.2 we proved that linearly independent eigenvectors $y^1, \ldots, y^r$ of λ have common vanishing coordinates Z and $y^i = (\beta_{i1}b_1, \ldots, \beta_{im}b_m, 0, \ldots, 0)$, for $i = 1, \ldots, r$, where $b_1, \ldots, b_m$ are vectors without vanishing coordinates and $\beta_{i1}, \ldots, \beta_{im}$ are real numbers. m is the number of components of $G - Z$.
Let $B = (\beta_{ij})$, $i = 1, \ldots, m$, $j = 1, \ldots, r$. Then an eigenvector y of λ has the following form: $y = ((Bx)_1 b_1, \ldots, (Bx)_m b_m, 0, \ldots, 0)$, where $x = (x_1, \ldots, x_r)$ is a real vector. Let $k_1, \ldots, k_m$ be the number of strong nodal domains of $b_1, \ldots, b_m$, respectively. Now we define new variables $c_i(x)$, $i = 1, \ldots, m$ as follows:

$$c_i(x) = \begin{cases} 0, & \text{if} \quad (Bx)_i = 0, \\ 1, & \text{if} \quad (Bx)_i \neq 0. \end{cases}$$

Then $\mathrm{SND}(y) = k_1 c_1(x) + \cdots + k_m c_m(x)$. Therefore MINIMUM NUMBER OF NODAL DOMAINS is equivalent to the following minimization problem:

$$\begin{aligned} &\textbf{min } k_1 c_1(x) + \cdots + k_l c_l(x) \\ &\quad x = (x_1, \ldots, x_r) \text{ is a nonzero real vector.} \end{aligned}$$

Consequently the decision problem of MINIMUM NUMBER OF NODAL DOMAINS is the following problem:
MIN(SND)
Instance: An $(m \times r)$ matrix B with real entries, positive integers $k_1, \ldots, k_m$ and a positive integer s.
Question: Is there a nonzero rational vector $x = (x_1, \ldots, x_r)$, such that $k_1 c_1(x) + \cdots + k_m c_m(x) \leq s$?

Lemma 4.4. *The $(m \times r)$ matrix B of decision problem* MIN(SND) *can be arbitrary large.*

Proof. The required example is constructed from the following result by Faria [33]. Let p be the number of vertices of G with degree one. Let q be the number of vertices, which are adjacent to a vertex with degree one. Then

$\lambda = 1$ is an eigenvalue of the Laplacian $L(G)$ with multiplicity $r \geq p - q$. We consider a binary tree with n vertices and $n/2$ endvertices. Therefore $\lambda = 1$ is an eigenvalue of $L(G)$ with multiplicity $r \geq n/4$. It is straightforward to show that m is at least the number of endvertices. Thus $m \geq n/2$. □

Now we show that MIN(SND) is NP-complete. For the proof we give another NP-complete problem. Let $x = (x_1 \ldots, x_n)$ be a real vector. We denote by $support(x)$, the number of nonzero elements of x.
MINIMUM SUPPORT
Instance: An $(m \times r)$ matrix B with rational entries, a positive integer s.
Question: Is there a nonzero rational vector $x = (x_1, \ldots, x_r)$ such that $support(Bx) \leq s$?

Lemma 4.5. MINIMUM SUPPORT *is* NP-complete.

Theorem 4.3. *The decision problem* MIN(SND) *is* NP-complete.

Proof. It is easy to see that MIN(SND) is in NP. We reduce MINIMUM SUPPORT to MIN(SND) in following way. We choose $k_1 = \cdots = k_m = 1$. The matrix B is the same matrix. We have the bound s. We assume that there is a vector x such that $c_1(x) + \cdots + c_m(x) \leq s$. By the definition of $c_1(x), \ldots, c_m(x)$, the inequality $c_1(x) + \cdots + c_m(x) \leq s$ holds if and only if $support(Bx) \leq s$. Therefore we have the solution of MINIMUM SUPPORT. Thus MIN(SND) is NP-complete. □

Proof of Lemma 4.5. It is easy to see that MINIMUM SUPPORT is in NP. The following problem is NP-complete:
ONE-IN-THREE
Instance: Set X with n elements and a subset T of $X \times X \times X$.
Question: Is there a subset Y of X, such that each triple $t = (t_1, t_2, t_3)$ in T has exactly one element in Y ?
ONE-IN-THREE is a variant of [LO4] in Garey and Johnson [43] page 259. We reduce ONE-IN-THREE to MINIMUM SUPPORT in following way. For each element of X we give a variable x_i, for $i = 1, \ldots, n$. We add a new variable x_{n+1}. We introduce rows $x_i + x_{n+1}$ and $x_i - x_{n+1}$ in the matrix B, for $i = 1, \ldots, n$. For each triple $t = (t_i, t_j, t_k)$ in T we introduce the row $x_i + x_j + x_k + x_{n+1}$, $n + 1$ times in B. We set the bound $s = n$. We assume that $support(Bx) \leq n$. Then each variable x_i is equal to x_{n+1} or $-x_{n+1}$, for $i = 1, \ldots, n$ and each expression $x_i + x_j + x_k + x_{n+1}$ is equal to zero. Otherwise $support(Bx) > n$. Now we put the variables $x_i = x_{n+1}$ in Y. It is easy to see that each triple $t = (t_1, t_2, t_3)$ in T has exactly one element in Y if and only if $x_i + x_j + x_k + x_{n+1}$ is equal to zero. Therefore we have the solution of ONE-IN-THREE. Thus MINIMUM SUPPORT is NP-complete. □

5. BOOLEAN HYPERCUBES

In this chapter we study the nodal domains of boolean hypercubes. They are special *graph products*. Given two non-empty graphs $G = (V, E)$ and $H = (W, F)$ the Cartesian product $G\Box H$ has vertex set $V \times W$ and $(x_1, x_2)(y_1, y_2)$ is an edge in $E(G\Box H)$ iff either $x_2 = y_2$ and $x_1y_1 \in E(G)$ or if $x_1 = y_1$ and $x_2y_2 \in H(E)$. One may view $G\Box H$ as the graph obtained from G replacing each of its vertices of with a copy of H and each of its edges with $|V(H)|$ edges joining corresponding vertices of H in the two copies. The graph product is a commutative, associative binary operation on graphs, see e.g. [57].

The *Kronecker product*, also known as *tensor product* or *direct product*, of two matrices A and B of sizes $m \times n$ and $s \times t$, respectively, is the $ms \times nt$ partitioned matrix

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix}$$

Let G and H be graphs with n, s vertices, respectively. The Laplacian matrix $L(G\Box H) = L(G)\otimes I_s + I_n \otimes L(H)$. If x is an eigenvector of $L(G)$ affording the eigenvalue λ and y an eigenvector of $L(H)$ affording the eigenvalue μ, then $x \otimes y$ is an eigenvector of $L(G\Box H)$ affording the eigenvalue $\lambda + \mu$. Therefore the eigenvalues of $L(G\Box H)$ is the multiset of sum of the eigenvalues of $L(G)$ and $L(H)$, see e.g. [67]. By the definitions of $G\Box H$ and Kronecker product,

$$\mathrm{SND}(x \otimes y) \leq \mathrm{SND}(x)\mathrm{SND}(y).$$

The hypercube K_2^n is the graph with vertex set $V = \{(v_1, v_2, \ldots, v_n) | v_i = \pm 1\}$ and edges connecting two vertices that differ in a single coordinate, i.e., $uv \in E$ iff $u_i = v_i$ for all but one index j for which we then have $u_j = -v_j$. The number n of coordinates is usually called the *dimension* of K_2^n. The graph has $|V| = 2^n$ vertices and $|E| = n2^{n-1}$ edges. It is not hard to verify that the hypercube is a bipartite graph and it is is equivalently defined as n-fold Cartesian product of K_2, the graph consisting of a single edge and its two end vertices.

The *Walsh functions* [37, 81]

$$\varphi_I(v) = \prod_{k \in I} v_k$$

where $I \subseteq \{1, 2, \ldots, n\}$ are a complete set of eigenvectors of the Laplacian of the hypercube. These functions satisfy the eigenvalue equation

$$L\varphi_I = 2|I|\varphi_I$$

and the orthogonality relation

$$\langle \varphi_I, \varphi_J \rangle = \sum_{v \in V} \varphi_I(v)\varphi_J(v) = \delta_{I,J}|V|$$

Thus there are $m = \binom{n}{|I|}$ eigenvectors with eigenvalue $2|I|$. It is customary to call $p = |I|$ the order of the Walsh function φ_I.

The Walsh functions satisfy the following important recursion w.r.t. the number n of coordinates:

$$\varphi'_I(v; v_{n+1}) = \varphi_I(v) \qquad \text{and} \qquad \varphi'_{I \cup \{v_n\}}(v; v_{n+1}) = v_{n+1}\,\varphi_I(v) \tag{5.1}$$

It is sometime more convenient to write equ.(5.1) as a tensor product:

$$\varphi'_I = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \varphi_I \qquad \text{and} \qquad \varphi'_{I \cup \{n+1\}} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \varphi_I$$

Clearly, $\varphi'_{I \cup \{n+1\}}$ is an eigenvector of K_2^{n+1} with eigenvalues $2(|I| + 1)$. It follows that all Walsh functions can be obtained recursively in this way. For more details and further applications of this construction see e.g. [21, 30].

Equ.(5.1) of course holds for any eigenvector x of K_2^n with eigenvalue $2p$: The vector $x^+ = \binom{1}{1} \otimes x$ is an eigenvector of K_2^{n+1} with eigenvalue $2p$, while $x^- = \binom{1}{-1} \otimes x$ is an eigenvector of K_2^{n+1} with eigenvalue $2(p + 1)$.

It follows immediately from Theorem 3.1 that an eigenvector x with eigenvalue $2p$ has at most

$$\mathrm{SND}(x) \leq \mathrm{SND}_{n,p} = \sum_{k=0}^{p} \binom{n}{k}, \;\; \mathrm{WND}(x) \leq \mathrm{WND}_{n,p} = 1 + \sum_{k=0}^{p-1} \binom{n}{k} \tag{5.2}$$

strong and weak nodal domains, respectively. Numerical values are listed in Table 5.1.

We can use the recursive construction of the Walsh functions in equ.(5.1) to obtain bounds on the number of nodal domains. The following technical result will be used repeatedly:

Tab. 5.1: Upper bounds on the number of strong and weak nodal domains as function of n and $p = |I|$ as given in equ.(5.2).

$p=$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
n	$\mathrm{SND}_{n,p}$														
2	1	3	4												
3	1	4	7	8											
4	1	5	11	15	16										
5	1	6	16	26	31	32									
6	1	7	22	42	57	63	64								
7	1	8	29	64	99	120	127	128							
8	1	9	37	93	163	219	247	255	256						
9	1	10	46	130	256	382	466	502	511	512					
10	1	11	56	176	386	638	848	968	1013	1023	1024				
11	1	12	67	232	562	1024	1486	1816	1981	2036	2047	2048			
12	1	13	79	299	794	1586	2510	3302	3797	4017	4083	4095	4096		
13	1	14	92	378	1093	2380	4096	5812	7099	7814	8100	8178	8191	8192	
14	1	15	106	470	1471	3473	6476	9908	12911	14913	15914	16278	16369	16383	16384
n	$\mathrm{WND}_{n,p}$														
2	1	2	4												
3	1	2	5	8											
4	1	2	6	12	16										
5	1	2	7	17	27	32									
6	1	2	8	23	43	58	64								
7	1	2	9	30	65	100	121	128							
8	1	2	10	38	94	164	220	248	256						
9	1	2	11	47	131	257	383	467	503	512					
10	1	2	12	57	177	387	639	849	969	1014	1024				
11	1	2	13	68	233	563	1025	1487	1817	1982	2037	2048			
12	1	2	14	80	300	795	1587	2511	3303	3798	4018	4084	4096		
13	1	2	15	93	379	1094	2381	4097	5813	7100	7815	8101	8179	8192	
14	1	2	16	107	471	1472	3474	6477	9909	12912	14914	15915	16279	16370	16384

Lemma 5.1. *Let f be any vector on K_2^n and let $f^+ = \binom{1}{1} \otimes f$ and $f^- = \binom{1}{-1} \otimes f$ be vectors on K_2^{n+1}. Then $WND(f^+) = WND(f)$, $SND(f^+) = SND(f)$, $WND(f^-) \leq 2\, WND(f)$, and $SND(f^-) = 2\, SND(f)$.*

Proof. Let W be a connected vertex subset of K_2^n and denote its boundary by

$$\partial W = \{u \in V \setminus W \,|\, \exists v \in W : uv \in E\}$$

We write $(W, v_{n+1}) = \{v' \in K_2^{n+1} \,|\, v' = (v, v_{n+1}),\, v \in W\}$ and $W' = (W, +1) \cup (W, -1)$. Clearly, W' is connected and its boundary is $\partial W' = (\partial W, +1) \cup (\partial W, -1)$. Furthermore $(\partial W, +1) \cap (\partial W, -1) = \emptyset$ and $\partial(W, v_{n+1}) = (\partial W, v_{n+1}) \cup (W, -v_{n+1})$.

Now let P be a positive strong nodal domain of f. Then f^+ is positive on both $(P, +1)$ and $(P, -1)$ and hence on P', while f^+ is non-positive on $\partial P'$, i.e., P' is a positive strong nodal domain of f^+, and consequently $\mathrm{SND}(f^+) = \mathrm{SND}(f)$. The same argument works analogously for weak nodal domains.

If P is a strong positive nodal domain of f then $f^-((P, +1)) > 0$, $f^-((P, -1)) < 0$, $f^-((\partial P, +1)) \leq 0$, $f^-((\partial P, -1)) \geq 0$. It follows immediately that $(P, +1)$ is a strong positive nodal domain while $(P, -1)$ is a strong negative nodal domain. Hence $\mathrm{SND}(f^-) = 2\,\mathrm{SND}(f)$.

Finally, suppose P is a weak positive nodal domain. Then analogously to the case of strong nodal domains we find $\mathrm{WND}(f^-) \leq 2\,\mathrm{WND}(f)$. However it might happen that P contains a vertex v with $f(v) = 0$. Then there exists

a weak negative nodal domain Q that also contains v. Then $(P,+1)$ and $(Q,-1)$ are weak positive nodal domains that are connected by the vertices $(v,+1) \in (P,+1)$ and $(v,-1) \in (Q,-1)$, since $f^-((P,+1)) = f^-((Q,-1)) = 0$. Thus $\mathrm{WND}(f^-) < 2\,\mathrm{WND}(f)$. □

Remark. The same results also holds for the Cartesian product of an arbitrary graph with K_2.

5.1 The Typical Number of Nodal Domains

In order to define more what we mean by the "typical number of nodal domains" we must be precise about which vectors in the eigenspace $\{x|Lx = \lambda_k x\}$ we want to consider. Since we have

$$x_v = \sum_{I:|I|=p} a_I \varphi_I(v) \tag{5.3}$$

for hypercubes this amounts to specifying a distribution of the coefficients a_I.

From a physics point of view it is most natural to assume that a_I are independent identically distributed Gaussian random variables. In this case equ.(5.3) defines Derrida's p-spin models [26, 27] which form an important and well-studied class of spin glasses which also play an important role in the theory of fitness landscapes [78].

If we use the hyperplane arrangement described above we might be interested in the volume of the cells that correspond to a given number of nodal domains. Computing this volume is very hard to compute, but it can be done approximately using Monte Carlo integration (see e.g. [39]). For this purpose the coefficient vectors are sampled from a uniform distribution on the corresponding sphere.

Fortunately these two pictures are equivalent. Normalizing random vectors that follow a multivariate Gaussian law (as in the first approach) gives uniformly distributed points on the sphere (see e.g. [28]).

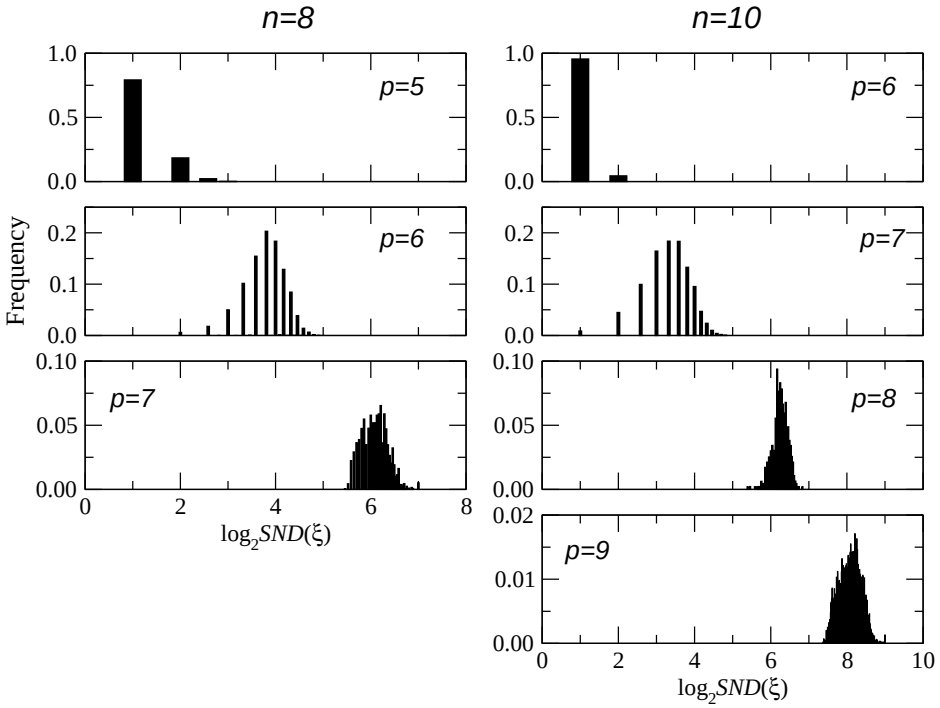

Fig. 5.1: Distribution of $SND(\xi)$ with Walsh coefficients a_I, $|I| = p$ drawn independently from a Gaussian distribution.

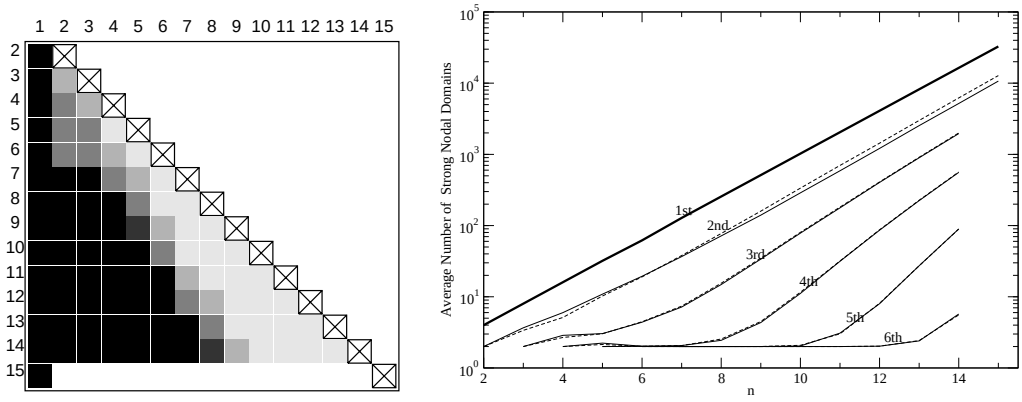

Fig. 5.2: Average number of nodal domains for the eigenvectors of the hypercubes with $n = 2$ to 15 as a function of p. The l.h.s. panel gives an overview of the numerical survey. Black squares denote (n, p)-pairs for which all of the 1000 randomly generated instances had exactly 2 nodal domains, ⊠ denotes the 2^n nodal domains for $p = n$ and the gray boxes scale denote average numbers of strong nodal domains in the ranges $2-3$, $3-10$, and larger 10.
The r.h.s. panel displays the k-th largest eigenvectors as a function of n. Note that the largest eigenvalue is unique and has the maximally possible number of $|V| = 2^n$ strong nodal domains.

5.2 The Minimal Number of Nodal Domains

In the case of weak nodal domains the situation is remarkably simple as the following result shows:

Theorem 5.1. *For all $1 \leq p \leq n-1$ there is an eigenvector x of the Boolean Hypercube with eigenvalue $\lambda = 2p$ such that* $\mathrm{WND}(x) = 2$.

Proof. We will proceed by induction. The hypercube K_2^2 is a cycle with four vertices. It is straightforward to check that $x_1^{(2)} = (0, 1, 0, -1)$ is an eigenvector with eigenvalue $\lambda = 2$ and $\mathrm{WND}(x_1^{(2)}) = 2$.

We construct eigenvectors of K_2^n recursively, for $n \geq 3$:

$$x_p^{(n+1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes x_p^{(n)} = \left(x_p^{(n)}\right)^+ \quad \text{for } p \leq n-1 \tag{5.4}$$

$$x_n^{(n+1)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes x_{n-1}^{(n)} = \left(x_{n-1}^{(n)}\right)^- \tag{5.5}$$

where we use the notation of Lemma 5.1. We recall that $x_p^{(n+1)}$ is an eigenvector of K_2^{n+1} with eigenvalue $2p$. By Lemma 5.1 we find for $p \leq n$, $\mathrm{WND}(x_p^{(n+1)}) = \mathrm{WND}(x_p^{(n)}) = 2$, where the second equality holds by assumption of induction.
Now consider $x_{n-1}^{(n)}$. Assume by induction that $\mathrm{WND}(x_{n-1}^{(n)}) = 2$. For an arbitrary vector f we write $V_0(f)$, $V_+(f)$ and $V_-(f)$ for the sets of vertices v where $f(v) = 0$, $f(v) > 0$, and $f(v) < 0$, respectively. Let V_0^+ be a copy of $V_0(x_{n-1}^{(n)})$ in K_2^{n+1} with coordinate $v_{n+1} = +1$ while V_0^- is the copy with $v_{n+1} = -1$. The sets V_+^+, V_+^-, V_-^+, and V_-^- are defined analogously. We have $V_0(x_n^{(n+1)}) = V_0^+ \cup V_0^-$, $V_+(x_n^{(n+1)}) = V_+^+ \cup V_-^-$ and $V_-(x_n^{(n+1)}) = V_-^+ \cup V_+^-$.

By induction hypothesis $V_+(x_{n-1}^{(n)}) \cup V_0(x_{n-1}^{(n)})$ and $V_-(x_{n-1}^{(n)}) \cup V_0(x_{n-1}^{(n)})$ are connected, thus the sets $V_+^+ \cup V_0^+$, $V_-^+ \cup V_0^+$, $V_+^- \cup V_0^-$, and $V_-^- \cup V_0^-$ are also connected. For each vertex in V_0^+ there is a neighboring vertex in V_0^- and *vice versa*, hence

$$\begin{aligned} V_+(x_n^{(n+1)}) \cup V_0(x_n^{(n+1)}) &= V_+^+ \cup V_0^+ \cup V_0^- \cup V_-^- \\ V_-(x_n^{(n+1)}) \cup V_0(x_n^{(n+1)}) &= V_-^+ \cup V_0^+ \cup V_0^- \cup V_+^- \end{aligned}$$

are connected sets, i.e., $\mathrm{WND}(x_n^{(n+1)}) = 2$. □

The eigenvector to the highest eigenvalue (which is simple) always has $|V|$ nodal domains, hence a hypercube is a bipartite graph and by Theorem 3.2.

For strong nodal domain theorems the situation is much more complicated (see Tab. 5.2). We can obtain at least a partial result.

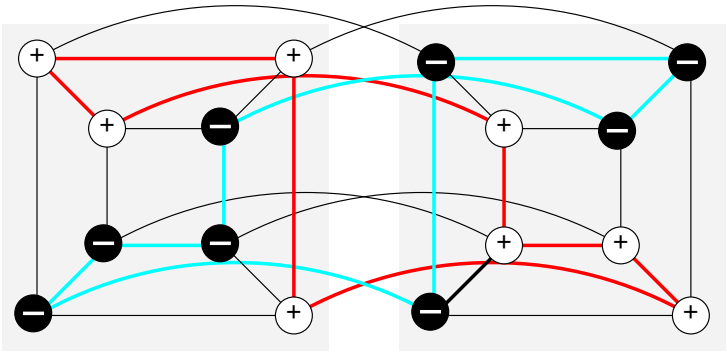

Fig. 5.3: The sign pattern of the eigenvector $x^{(4)}$.

Theorem 5.2. *For all* $1 \leq p \leq n/2$ *there is an eigenvector* x *of the Boolean Hypercube with eigenvalue* $\lambda = 2p$ *such that* $\mathrm{SND}(x) = 2$.

Proof. We will recursively construct eigenvectors $x^{(n)}$ for even n with eigenvalue n and $\mathrm{SND}(x^{(n)}) = 2$.

Suppose $y_v \in \{-1, 1\}$ for all $v \in V$ and $\sum_{v \in V} y_v = 0$, i.e., half of the vertices have value $+1$, the others -1. Such a vector y is an eigenvector of the Laplacian with eigenvalue n if and only if for each vertex $v \in V$ half of its neighbors u have $y_u = +1$ and the other half satisfies $y_u = +1$. Figure 5.3 shows that such a vector $x^{(4)}$ exists on K_2^4.

The following notation will be convenient. A *sign pattern* $\mathcal{X}$ is a map $V \to \{+, -\}$ that assign a sign to each vertex of the hypercube. Given two sign-patterns $\mathcal{X}$ and $\mathcal{Y}$ on K_2^n we obtain the sign pattern $\mathcal{X}|\mathcal{Y}$ on $K_2^{n+1} = K_2^n \square K_2$ by labeling the vertices $(v, +1)$ according to $\mathcal{X}$ and the vertices $(v, +1)$ according to $\mathcal{Y}$, see Fig. 5.3. We write $-\mathcal{X}$ for the pattern with reversed signs.

Let us call a sign pattern $\mathcal{Z}$ on K_2^n *admissible* if:

(i) There is a product decomposition $K_2^n = K_2^{n-1} \square K_2$ with sign patterns $\mathcal{X}$ and $\mathcal{Y}$ on each of the two copies of K_2^{n-1} that have half of their vertices labeled $+$;

(ii) The subgraph Γ_+^n of K_2^n induced by $+$labeled vertices of $\mathcal{X}|\mathcal{Y}$ is $n/2$-regular. Of course the same holds for the subgraph Γ_-^n induced by $+$labeled vertices.

Fig. 5.3 shows that the sign pattern of $x^{(4)}$ is admissible.

From $(\mathcal{X}|\mathcal{Y})$ we construct the sign pattern

$$\mathcal{X}^*|\mathcal{Y}^* = ((\mathcal{X}|\mathcal{Y})|(\mathcal{Y}|\mathcal{X})) \;\Big|\; ((-\mathcal{Y}|-\mathcal{X})|(-\mathcal{X}|-\mathcal{Y})) \tag{5.6}$$

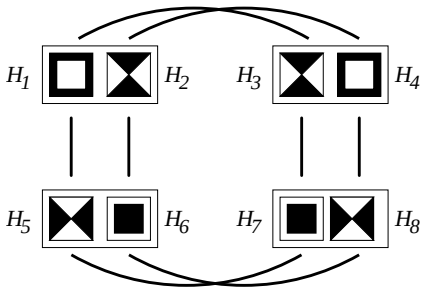

Fig. 5.4: The sign pattern on K_2^{n+2} is built up from the sign sign patterns $\mathcal{X}$ and $\mathcal{Y}$ on two copies K_2^{n-1} that together form a K_2^n. The negative patterns $-\mathcal{X}$ and $-\mathcal{Y}$ are shown with black and white exchanged.

on K_2^{n+2}, which is composed of eight copies of K_2^{n-1} labeled H_1 through H_8 as in Fig. 5.4. Each of the four copies K_2^n labeled H_1H_2, H_3H_4, H_5H_6, and H_7H_8 has either the sign pattern $\mathcal{X}|\mathcal{Y}$ or the sign pattern $-\mathcal{X}|-\mathcal{Y}$ and hence is admissible. Furthermore both $(\mathcal{X}|\mathcal{Y})|(\mathcal{Y}|\mathcal{X})$ and $(-\mathcal{Y}|-\mathcal{X})|(-\mathcal{X}|-\mathcal{Y})$ have half of their vertices labeled $+$.

Now fix an arbitrary vertex v of H_1 and consider its neighbors v' and v'' in H_3 and H_5, respectively. These neighbors are of course uniquely defined. Since H_3 has sign pattern $\mathcal{Y}$ while H_5 has sign pattern $-\mathcal{Y}$ we conclude that v' and v'' must have the opposite sign, and hence v has $n/2+1 = (n+2)/2$ positive neighbors. The same argument can be made for any vertex in each of the $n-1$ dimensional cubes. Thus the subgraph Γ_+^{n+2} of K_2^{n+2} induced by the $+$labeled vertices is $(n+2)/2$-regular. Therefore $\mathcal{X}^*|\mathcal{Y}^*$ is an admissible sign pattern on K_2^{n+2} and the corresponding vector $x^{(n+2)}$ is a Laplacian eigenvector with eigenvalue $n+2$.

Next we show that Γ_+^{n+2} and Γ_+^{n+2} are connected. Again we proceed by induction. The sign pattern of $x^{(4)}$ in Fig. 5.3 is such that there are edges with all four sign combinations $++$, $+-$, $-+$, and $--$ between the two copies of K_2^3 with the sign patterns $\mathcal{X}$ and $\mathcal{Y}$, i.e., Γ_+^4 and Γ_-^4 are connected.

Now assume that edges with all sign combinations between $\mathcal{X}$ and $\mathcal{Y}$ on K_2^n. Then edges with all sign combinations exist also between $\mathcal{X}$ and $-\mathcal{Y}$ on, say, the cube (H_1, H_3) and between $-\mathcal{X}$ and $\mathcal{Y}$ on (H_5, H_7). It follows that Γ_+^{n+2} and Γ_-^{n+2} are connected, and we see that $\mathrm{SND}(x^{(n+2)}) = 2$.

Finally we construct for each $p \leq n/2$ the vector

$$y_p^{(n)} = \begin{cases} x^{(n)} & \text{if} \quad p = n/2 \\ \binom{1}{1} \otimes y_p^{(n-1)} & \text{if} \quad p < n/2 \end{cases}$$

We know that $y_p^{(n)}$ is an eigenvector with eigenvalue p by construction.

Furthermore, Lemma 5.1 implies that $\mathrm{SND}(y_p^{(n)}) = \mathrm{SND}(y_p^{(n-1)}) = \ldots = \mathrm{SND}(y_p^{(2p)}) = \mathrm{SND}(x^{(2p)}) = 2$. □

Remark. In general, if we find a partition (A, B) of $K_2^n = (A, B)$ with $|A| = |B|$ such that the induced subgraphs $G[A]$ and $G[B]$ are connected and k-regular, then the eigenvalue $\lambda = 2(n-k)$ has an eigenvector x with $SND(x) = 2$. This can be constructed by setting $x_v = 1$ for $v \in A$ and $x_v = -1$ for $v \in B$. In the proof of Theorem 5.2 we have found such a partition for $k = n/2$. Whether such a partition exists for $3 \leq k < n/2$ is an open problem.

From an extensive numerical survey we conclude that probably a much stronger result than Theorem 5.2 holds:

Conjecture 5.1. *For all $1 \leq p \leq n-2$ there is an eigenvector x of the Boolean Hypercube with eigenvalue $\lambda = 2p$ such that* $\mathrm{SND}(x) = 2$.

For the second largest eigenvalue we can find a lower bound:

Theorem 5.3. *For every eigenvector y of the Hypercube K_2^n, $n \geq 3$, with eigenvalue $\lambda = 2(n-1)$ we have* $\mathrm{SND}(y) \geq n$.

Proof. In order to prove this theorem we first need the following technical result:

Lemma 5.2. *Let x be a Laplacian eigenvector to the eigenvalue $2(n-1)$ that satisfies $x_v \neq 0$ for all $v \in V$ and that has positive coefficients $a_I \geq 0$ for all I with $|I| = n-1$ in its Walsh expansion equ.(5.3) and define $x'_v = x_v \varphi_{\{1,\ldots,n\}}(v) = x_v \prod_{i=1}^{n} v_i$. Then:*

(1) $x' = \sum_{I,|I|=n-1} v_{i_I} a_I$, where i_I is the unique coordinate not contained in I.

(2) x' is monotonically decreasing on every path of length n from $\mathbf{1} = (1,\ldots,1)$ to $-\mathbf{1} = (-1,\ldots,-1)$.

(3) For every path of length n from $\mathbf{1}$ to $-\mathbf{1}$ there is exactly one edge where x does not change sign.

Remark. x' is an eigenvector to eigenvalue 2.

Tab. 5.2: Upper and Lower Bounds on the number of nodal domains as functions of n and p found by numerical experiments using hillclimbing algorithm.

$p=$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
n	Upper Bounds on Minimal Number of Strong Nodal Domain													
2	2	4												
3	2	3	8											
4	2	2	4	16										
5	2	2	2	8	32									
6	2	2	2	2	14	64								
7	2	2	2	2	2	24	128							
8	2	2	2	2	2	2	44	256						
9	2	2	2	2	2	2	2	84	512					
10	2	2	2	2	2	2	2	2	160	1024				
11	2	2	2	2	2	2	2	2	2	314	2048			
12	2	2	2	2	2	2	2	2	2	2	620	4096		
13	2											1280	8192	
14	2												2446	16384
n	Lower Bounds on Maximal Number of Weak Nodal Domain[†]													
2	2	4												
3	2	4	8											
4	2	4	8	16										
5	2	4	**10**	16	32									
6	2	4	*8*	**18**	32	64								
7	2	4	*4*	*15*	**34**	64	128							
8	2	*2*			*12*	*57*	128	256						
9	2						*72*	**261**	512					

[†] Numbers in **bold** are bounds that are better then Corollary 5.1. Entries in *italics* are numerical value that are known to be underestimates because of Lemma 5.1.

Proof of Lemma 5.2. (1) From the definition we obtain

$$x'_v = x_v \prod_{j=1}^{n} v_j = \sum_{I,|I|=n-1} a_I \, \varphi_I(v) \prod_{j=1}^{n} x_j = \sum_{I,|I|=n-1} a_I \prod_{k\in I} v_k \prod_{j=1}^{n} v_j$$
$$= \sum_{I,|I|=n-1} a_I \, v_{i_I} \prod_{k=1}^{n} v_k \prod_{j=1}^{n} v_j = \sum_{I,|I|=n-1} v_{i_I} \, a_I \, .$$

(2) On any path from $\mathbf{1}$ to $-\mathbf{1}$ the number of negative coordinates of v is strictly increasing. The result follows since $a_k \geq 0$ by assumption.
(3) By (2) there is exactly one edge e in every such path where x' changes sign. Since $\prod_{j=1}^{n} v_j$ has alternating signs on every path, the sign of $x_v = x'_v \prod_{j=1}^{n} v_j$ changes except along the edge e. □

First assume that y does not vanish on any vertex. Then using Lemma 5.2 it is easy to show that for every path of length n from the absolute maximum of y to its antipodal point, y changes sign exactly $(n-1)$ times. Since every such path is isometric in K_2^n, vertices of the same sign that are not adjacent in this path cannot belong to the same nodal domain. Thus such a path intersects exactly n (different) nodal domains and the proposition follows.
If $y_v = 0$ for some vertex $v \in V$ then we can use the same idea as in the proof of Lemma 5.2. However we find on this path (at most) one vertex v where y vanishes. Now on each edge of this path y either changes sign or joins v with a vertex of positive of negative sign. Again the result follows. □

Our experiments show that this bound is not sharp, see Table 5.2.

5.3 The Maximal Number of Nodal Domains

Much less can be said on the maximal number of nodal domains a function of p. It follows from Lemma 5.1 that the maximum number of strong nodal domains (listed in the lower part of Table 5.2) must be non-decreasing with n for fixed p. A hypercube is a bipartite graph and by the trivial consequence of Theorem 3.2 we have therefore

Corollary 5.1. *The eigenvalue $2p$ has an associated eigenvector x with at least $\mathrm{SND}(x) \geq \mathrm{WND}(x) \geq 2^p$ nodal domains for all $n \geq p$.*

For reasons that we do not fully understand maximizing the number of nodal domains on a given eigenspace seems to be much harder than minimizing.

5.4 Open Questions

We suspect that the bounds in Tab. 5.2 for the minimum number of strong nodal domains for the 2nd largest eigenvalue are sharp at least for $n \leq 10$. However, the sequence 2, 3, 4, 8, 14, 24, 44, 84, 160, ... does not appear to be a known integer sequence.

A direct computational approach for the maximum number of strong nodal domains fails because we would have to compute all cells of dimension 0; this is not only numerically difficult but the number of 0-cells is also too large. A completely different approach is therefore required.

The difference in difficulty between minimizing and maximizing the number of nodal domains deserves an explanation.

It would be interesting to know whether the lower bound $\mathrm{WND}(x) = 2$ for almost all eigenvectors is sharp for e.g. for all expander graphs.

6. COGRAPHS

In the previous chapters we see that it is not always easy to find the maximum or minimum number of nodal domains. In this chapter we see that this problem is easy for cographs.

A graph G is called *cograph* if G has no induced subgraph P_4. Cographs arise in many disparate areas of mathematics and computer science. In this chapter we consider the Laplacian and adjacency matrices of cographs. We characterize the number of nodal domains of cographs with respect to the Laplacian matrix, and the rank of the adjacency matrix of a cograph.

6.1 Nodal Domains of a Cograph

Cographs have several characterizations. The following tree representation with join and disjoint union operations is more suitable for our purpose.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs on disjoint sets of r and s vertices, respectively. Their *disjoint union* $G_1 + G_2$ is the graph $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$, and their *join* $G_1 * G_2$ is the graph on $n = r + s$ vertices obtained from $G_1 + G_2$ by inserting new edges from each vertex of G_1 to each vertex of G_2.

Lemma 6.1. [19] *To each cograph $G = (V, E)$, one can associate a unique rooted tree T, called the cotree of G. Each leaf node of T corresponds to a (unique) vertex of V. Each internal node is labeled with a $*$ or a $+$. Children of nodes labeled with $+$ are labeled with $*$, and vice versa. It is possible to associate a cograph with each node of the cotree T. Leaf nodes correspond to the cograph with the one vertex they represent. Internal nodes labeled with $*(+)$ correspond to the join (disjoint union) of the cographs, corresponding to the children of the node (see Fig. 6.1). G equals the cograph corresponding with the root of T. Cographs can be in $O(|V| + |E|)$ time recognized, and in the same time the corresponding cotree can be built.*

It means that each cograph G is the disjoint union of two disjoint cographs G_1 and G_2, $G = G_1 + G_2$ or G is the join of two disjoint cographs G_1 and G_2, $G = G_1 * G_2$.

The following Lemma invites to look for the nodal domains of cographs.

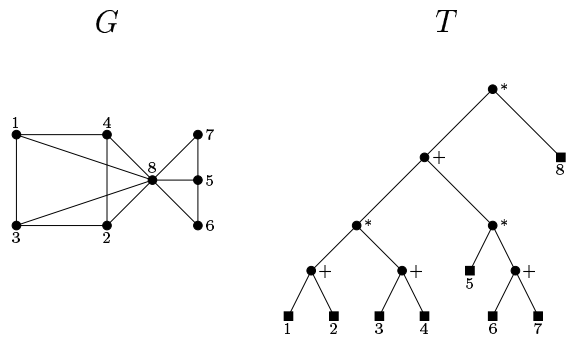

Fig. 6.1: The cograph G and the cotree T of G

Lemma 6.2. [67] *Let G_1 and G_2 be graphs on disjoint sets of r and s vertices, respectively. If $\mu_1 \leq \cdots \leq \mu_r$ and $\nu_1 \leq \cdots \leq \nu_s$ are eigenvalues of Laplacian of G_1 and G_2, respectively. Then the eigenvalues of $G_1 * G_2$ are $n = r + s$; $\mu_2 + s, \ldots, \mu_r + s$; $\nu_2 + r, \ldots, \nu_s + r$; and 0. Suppose y is an eigenvector of G_1 that is orthogonal to e_r. Extend y to $G_1 * G_2$ by defining it to be zero on $V(G_2)$. If y affords the eigenvalue μ, the extension of y is an eigenvector of $G_1 * G_2$ affording $\mu + s$. Similarly an eigenvector of G_2 affording ν extends to an eigenvector of $G_1 * G_2$ affording $\nu + r$. The eigenvalue $\lambda = r + s$ corresponds to an eigenvector whose value is $-s$ on each of the r vertices of G_1 and r on each of the s vertices of G_2. Finally, the trivial eigenvalue is afforded by e_{r+s}.*

Obviously, the eigenvalues of the Laplacian $L(G_1 + G_2)$ are the union of eigenvalues of $L(G_1)$ and $L(G_2)$ (respecting multiplicity). It follows from Lemmas 6.1 and 6.2 that the Laplacian eigenvalues of a cograph are integers and easy to compute from its cotree.

Let T be a rooted tree and let v be a node of T. A *subtree at v* is the induced tree by v and all descendants of v. Similarly, a *subtree of v* is the subtree at one of the children of v.

Theorem 6.1. *For each eigenvalue of the Laplacian of a cograph $G = (V, E)$ we can find an eigenvector with maximum or minimum number of strong nodal domains in $O(|V| + |E|)$ time.*

Proof. By Lemma 6.1 a cograph G has a unique cotree T. Let v be a node of the cotree T with subtrees $T_1, \ldots, T_k$ and $G_1, \ldots, G_k$ the respective cographs.

Let G_v be the cograph corresponding with v as root. Now we show that the number of strong nodal domains of G_v can be expressed in terms of the number of strong nodal domains of $G_1, \ldots, G_k$. Let $\mathrm{MaxND}(\lambda)$ and $\mathrm{MinND}(\lambda)$ be eigenvectors of the eigenvalue λ with maximum and minimum number of strong nodal domains, respectively.

If v has the label $+$ (disjoint union), then the eigenvalues of G_v are the union of eigenvalues of $G_1, \ldots, G_k$. Let $x^1, \ldots, x^k$ be the eigenvectors of λ with maximum number of strong nodal domains. Then $x = (x^1, \ldots, x^k)$ is the eigenvector of λ of cograph G_v with maximum number of strong nodal domains and $\mathrm{SND}(x) = \sum_{i=1}^{n} \mathrm{SND}(x^i)$. Similarly let $y^1, \ldots, y^k$ be the eigenvectors of λ with minimum number of nodal domains. Then $y = (0, \ldots, 0, y^i, 0, \ldots, 0)$ is the eigenvector of λ and $\mathrm{MinND}(\lambda) = \min\{\mathrm{SND}(y^1), \ldots, \mathrm{SND}(y^k)\}$.

If v has the label $*$ (join operation), then an easy induction gives that the eigenvalues of G_v are $|V(G_v)|$ and $\lambda_{G_i} + \sum_{j \neq i} |V(G_j)|$, where $\lambda_{G_i} > 0$ is an eigenvalue of G_i for $i = 1, \ldots, k$. By Lemma 6.2 the extension $(0, \ldots, 0, x^i, 0, \ldots, 0)$ of the eigenvector x^i of λ_{G_i} is an eigenvector of $\mu = \lambda_{G_i} + \sum_{j \neq i} |V(G_j)|$. The eigenvectors $\{(0, \ldots, 0, x^{i_1}, 0, \ldots, 0), \ldots, (0, \ldots, 0, x^{i_p}, 0, \ldots, 0)\}$ span the eigenspace of $\mu \neq |V(G_v)|$ with respect to the choice of the basis of $\lambda_{G_{i_1}}, \ldots, \lambda_{G_{i_p}}$, where $\mu = \lambda_{G_{i_1}} + \sum_{j \neq i_1} |V(G_j)| = \cdots = \lambda_{G_{i_p}} + \sum_{j \neq i_p} |V(G_j)|$. The eigenvectors $x^{i_1}, \ldots, x^{i_p}$ have at least two vertices with opposite sign. By join operation all linear combinations of $(0, \ldots, 0, x^{i_1}, 0, \ldots, 0), \ldots, (0, \ldots, 0, x^{i_p}, 0, \ldots, 0)$ have two nodal domains. Therefore $\mathrm{MaxND}(\mu) = \max\{\mathrm{MaxND}(\lambda_{G_{i_1}}), \ldots, \mathrm{MaxND}(\lambda_{G_{i_p}})\}$. Similarly, $\mathrm{MinND}(\mu) = 2$ for $p \geq 2$ and $\mathrm{MinND}(\mu) = \mathrm{MinND}(\lambda_{G_{i_1}})$ for $p = 1$. For the eigenvalue $\mu = |V(G_v)|$ by Lemma 6.1 the children of the node v are labeled with $+$. Therefore each of the graphs $G_1, \ldots, G_k$ is either not connected or a single vertex. Let $c_1, \ldots, c_k$ be the number of connected components of $G_1, \ldots, G_k$. By Lemma 6.2 it is easy to see that $\mathrm{MaxND}(\mu) = \max\{c_1, \ldots, c_k\} + 1$ when the node v has more than two children and $\mathrm{MaxND}(\mu) = c_1 + c_2$ when v has two children.

We have shown that it is enough to build the cotree of a cograph to find $\mathrm{MaxND}(\lambda)$ or $\mathrm{MinND}(\lambda)$. By Lemma 6.1 we can build the cotree of $G = (V, E)$ in $O(|V| + |E|)$ time. □

Corollary 6.1. *The Laplacian eigenvalues of a complete k-partite graph $K_{n_1,\ldots,n_k}$ with $n_1 \geq \cdots \geq n_k$ are 0; $n = n_1 + \cdots + n_k$; and $n - n_i$, for $i = 1, \ldots, k$. The maximum number of nodal domains of eigenvalues n and $n - n_i$ are equal to $n_1 + n_2$ and n_i, respectively. The minimum number of nodal domains of all eigenvalues are equal to two.*

Corollary 6.2. *Let G be a connected cograph with n vertices. Every eigenvec-*

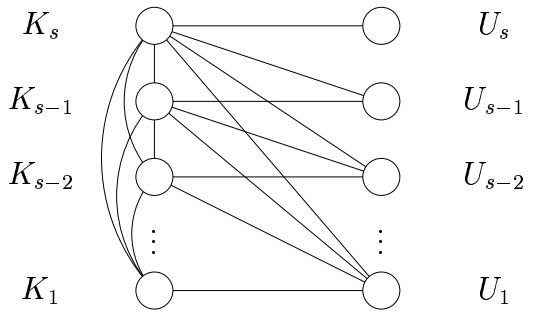

Fig. 6.2: The typical structure of a threshold graph. A line between cells K_i and U_j indicates that each vertex in K_i is adjacent to each vertex of U_j.

tor affording the eigenvalue $0 < \lambda \neq n$ *of the Laplacian* $L(G)$ *has* $\mathrm{WND}(x) = 2$ *weak nodal domains.*

For the $\mathrm{WND}(x)$ of an eigenvector x of $\lambda = n$, see the Proof of Theorem 6.1.

For an important subclass of cographs, namely threshold graphs, we can directly compute the number of nodal domains without using Theorem 6.1. A graph $G = (V, E)$ is called as a *threshold graph*, if G does not contain one of the three forbidden induced subgraph graphs, $K_2 + K_2$, C_4, or P_4. Another useful characterization of threshold graph is the following.

Lemma 6.3. [16] *G is a connected threshold graph if and only if $G = (K, U)$, where K is a complete graph with a partition of non empty cliques $K_1, \ldots, K_s$ and U is an independent set with a partition of non empty independent sets $U_1, \ldots, U_s$. All vertices of K_i are adjacent with all vertices of U_h, for $1 \leq h \leq i$ and for $i = 1, \ldots, s$. (see Fig. 6.2)*

In the next section we use this lemma to characterize the rank of a cograph.

By Lemmas 6.2 and 6.3 the Laplacian eigenvalues of a threshold graph are obtained easily by induction; for a similar procedure see [53].

Corollary 6.3. *Let $G = (K, U)$ be a connected threshold graph with the partitions K_i and U_i, for $i = 1, \ldots, s$. The eigenvalues of the Laplacian $L(G)$ are 0; $\sum_{i=1}^{h} |U_i| + \sum_{j=1}^{s} |K_j|$ for $h = 1, \ldots, s$; $\sum_{j=h}^{s} |K_j|$ for $h = 2, \ldots, s$; $\sum_{j=1}^{s} |K_j|$ when $|U_1| \geq 2$. The bounds for the number of strong nodal domains are:*

(i) If $\lambda = \sum_{i=1}^{h} |U_i| + \sum_{j=1}^{s} |K_j|$, *then*

1. $2 \leq \mathrm{SND}(x) \leq |U_h| + 2$ *when* $h \geq 2$,
2. $2 \leq \mathrm{SND}(x) \leq |U_1| + 1$ *when* $h = 1$.

(ii) If $\lambda = \sum_{j=h}^{s} |K_j|$, *then*

1. $2 \leq \mathrm{SND}(x) \leq |U_h| + 1$ *when* $h \geq 2$,
2. $\mathrm{SND}(x) \leq |U_1|$ *when* $h = 1$ *and* $|U_1| \geq 2$.

These bounds on $\mathrm{SND}(x)$ *are sharp. The special case* $G = K_n$ *is trivial.*

6.2 The Rank of a Cograph

In this section we prove the following conjecture of T. Sillke about the rank of cographs [76]: The rank of the adjacency matrix $A(G)$ of a cograph G is equal to the number of distinct nonzero columns of $A(G)$.

First we characterize cographs G, where all columns of $A(G)$ are different. We prove that adjacency matrices of such cographs have also full rank.

By Lemma 6.1 we know that each cograph G has an associated rooted cotree T. It is easy to see that we can get a new tree T' from T such that the leaf nodes of T' correspond to the set of threshold graphs. We look the *threshold maximal* tree T' with leaf nodes $B_1, \ldots, B_s$, that means T' has no internal node with children B_i and B_j such that the corresponding cograph of $B_i * B_j$ $(B_i + B_j)$ is a set of threshold graphs (see Fig. 6.3). We call T' as *threshold cotree* of G.

Proposition 6.1. *Let* $G = (V, E)$ *be a cograph and* T *its (threshold) cotree* T. *Let* v *be a node of* T *and* L *the subtree at* v. *Let* F *be vertices of* G *which correspond to leaf nodes of* L. *Then the vertices of* F *have same neighbors in* $V - F$ *(we say also outside of* F *or outside of the subtree* L*).*

Proof. It is easy to see by induction from leaves to the root. □

Lemma 6.4. *Let* G *be cograph and* $A(G)$ *its adjacency matrix. All columns of* $A(G)$ *are distinct and nonzero if and only if* G *has a threshold cotree* T *with leaves* $B_1, \ldots, B_s$, *where* B_j *are a set of threshold graphs and it holds:*

(i) Each independent set U_i *of a threshold graph of* B_j *has at most one vertex.*

(ii) All internal nodes of T *with label* $+$ *have at most one subtree* L *such that the corresponding cograph of* L *has at most one isolated vertex.*

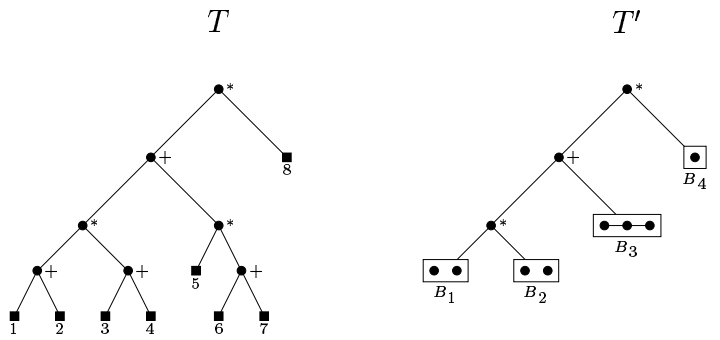

Fig. 6.3: The cotree T and the threshold cotree T' from T with leaves $B_1, \ldots, B_4$.

Proof. Let all columns of $A(G)$ be distinct and nonzero. Let T be a threshold cotree of G with leaves $B_1, \ldots, B_s$. B_j are set of threshold graphs. We assume that B_j has a threshold graph with $|U_i| \geq 2$. By Proposition 6.1 all vertices of U_i have the same neighbors. Therefore the columns of vertices of U_i are equal, a contradiction. Let v be an internal node of T and v has at least two subtrees with corresponding cographs with isolated vertices. By Proposition 6.1, the corresponding vertices of these isolated vertices have the same neighbors outside of these subtrees. Therefore their columns are equal. The sufficiency part is easy to see by induction from leaves to the root. □

Theorem 6.2. *Let $G = (V, E)$ be a cograph and let $A(G)$ be its adjacency matrix. The rank of $A(G)$ is equal to the number of distinct nonzero columns of $A(G)$.*

Proof. We show by induction on the number of vertices of G. The case $|V(G)| \leq 2$ is trivial. We assume that the assertion holds for $|V(G)| \leq n-1$. We first consider the case that $A(G)$ has at least two equal columns. Without loss of generality we may assume that $A(G) = [a_1, ..., a_{n-2}, a_{n-1}, a_n = a_{n-1}]$, where a_i are the columns of the $A(G)$ and the last two columns are equal. Then $\text{rank}(A(G)) = \text{rank}(A(G - v_n))$. $G - v_n$ is a cograph and by induction hypothesis, $\text{rank}(A(G - v_n))$ is equal to the number of distinct nonzero columns of the $A(G - v_n)$.

It remains to consider the case that all columns of $A(G)$ are different and nonzero. This is the main part of the proof. We show that if all columns of $A(G)$ are different, then all columns of $A(G)$ are linearly independent. Let $\alpha_1, \ldots, \alpha_n$ be the coefficient of columns $a_1, \ldots, a_n$ such that $\sum_{i=1}^{n} \alpha_i a_i = 0$.

We have to show $\alpha_1 = \cdots = \alpha_n = 0$. Let T be the threshold cotree of G with leaves $B_1, \ldots, B_s$. The B_j are the set of threshold graphs. By Lemma 6.4, each independent set U_i of a threshold graph of B_j has at most one vertex, i.e. the adjacency matrix of such a threshold graph has the form

	K_1	K_2	$\cdots$	K_s	U_1	U_2	$\cdots$	U_s
K_1	$A(K_1)$	1	$\cdots$	1	1	0	$\cdots$	0
K_2	1	$A(K_2)$	1	1	1	1	0	0
$\vdots$	1	1	$\ddots$	1	1	1	$\ddots$	0
K_s	1	$\cdots$	1	$A(K_s)$	1	$\cdots$	$\cdots$	1
U_1	1	1	$\cdots$	1	0	0	$\cdots$	0
U_2	0	1	$\cdots$	1	0	0	$\cdots$	0
$\vdots$	0	0	$\ddots$	1	$\vdots$	$\vdots$	$\ddots$	$\vdots$
U_s	0	$\cdots$	0	1	0	$\cdots$	$\cdots$	0

Claim: Let v be the node of the threshold cotree T and L be the subtree at v. Let $a_1, \ldots, a_k$ be the columns of vertices of corresponding cograph of the subtree L. It exists a coefficient α_h, where $1 \leq h \leq k$ such that α_j are either $\alpha_j = c_j \alpha_h$, $c_j > 0$ or $\alpha_j = 0$ for $j = 1, \ldots, k$.

Before we prove the claim, let us apply the claim to the root of the threshold cotree T. Then $\alpha_j = c_j \alpha_h$, $c_j > 0$ or $\alpha_j = 0$ for $j = 1, \ldots, n$. From the row of an arbitrary vertex x of the cograph G, we have

$$\sum_{xj \in E(G)} \alpha_j = \alpha_h \sum_{xj \in E(G)} c_j = 0, \text{ then } \alpha_h = 0.$$

Hence all coefficients are equal to zero. Therefore all columns of $A(G)$ are linearly independent.

We prove the claim by induction from leaves to the root of T. Let H be one of the threshold graphs of the leaf B_j (for $A(H)$ see above). By Lemma 6.3, $H = (K, U)$ and K_i are cliques and U_i are independent sets for $i = 1, \ldots, s$. It is easy to show that the coefficients of the vertices of the clique K_i are equal for $i = 1, \ldots, s$. By Proposition 6.1 each vertex of threshold graph H has the same neighbors outside of H. Let R_H be the sum of the coefficient of these neighbors. By using the row belonging to U_s the coefficients of $K_1, \ldots, K_{s-1}$ are zero. By the rows belonging to $U_{s-1}, \ldots, U_1$, the coefficients $\alpha_{U_1} = \cdots = \alpha_{U_{s-1}} = 0$. By one of the rows of K_s and U_s we get $\alpha_{U_s} = \alpha_{K_s}$ where α_{K_s} is the coefficient of each vertex of K_s, since

$$\alpha_{K_s}(|K_s| - 1) + \alpha_{U_s} + R_H = 0 = \alpha_{K_s}|K_s| + R_H.$$

Therefore we are finished for each threshold graph of B_j. By Proposition 6.1 each threshold graph of B_j has the same neighbors outside of B_j. Hence we are also finished for the leaves B_j. Let us now consider an internal node v of T. Let L_1 and L_2 be the subtrees of v and G_1 and G_2 the corresponding cographs (we argue analogously to more subtrees). Let $a_1, \ldots, a_{k-1}$ and $a_k, \ldots, a_r$ be the columns of corresponding vertices of the cographs of L_1 and L_2, respectively. By induction hypothesis, $\alpha_i = b_i\alpha_h$, $b_i > 0$ or $\alpha_i = 0$ for $i = 1, \ldots, k-1$, where $1 \leq h \leq k-1$ and $\alpha_j = c_j\alpha_m$, $c_j > 0$ or $\alpha_j = 0$ for $j = k, \ldots, r$, where $k \leq p \leq r$. Then $\sum_{i=1}^{k-1} \alpha_i = \alpha_1 \sum_{i=1}^{k-1} b_i$ and $\sum_{j=k}^{r} \alpha_j = \alpha_k \sum_{j=k}^{r} c_j$. By Proposition 6.1 all vertices of the corresponding cographs of L_1 and L_2 have the same neighbors outside of $L_1 \cup L_2$ and let R be the sum of the coefficients of these neighbors. If v has the label $*$, we look at the rows of the vertices h and p and obtain

$$\sum_{hi \in E(G_1)} b_i\alpha_h + \sum_{j=k}^{r} c_j\alpha_p + R = 0 = \sum_{pj \in E(G_2)} c_j\alpha_p + \sum_{i=1}^{k-1} b_i\alpha_h + R.$$

If v has the label $+$, then G_1 and G_2 are connected. We look at the rows y and z such that $yh \in E(G_1)$ and $zp \in E(G_2)$ (otherwise $\alpha_1 = 0$ or $\alpha_k = 0$) and we have

$$\sum_{yi \in E(G_1)} b_i\alpha_h + R = 0 = \sum_{zj \in E(G_2)} c_j\alpha_p + R.$$

For both labels $*$ and $+$ it follows that $\alpha_1 = c\alpha_k$ and $c > 0$, and hence induction is complete. □

During the final stages of the preparation of this manuscript we became aware that G.F. Royle [75] has recently found a quite different proof for Sillke's conjecture. Royle's proof is based on properties of the characteristic polynomials, while we exploit here the structure of cographs with respect to cotree and threshold graphs.

7. OPEN PROBLEMS AND COUNTEREXAMPLES

Traditionally, there are more open problems in graph theory than answers. We follow this tradition. We present miscellaneous results, negative results and open problems. We hope that presenting counterexamples and negative results prevent unnecessary repetitions and show where intuitions lead to wrong assumptions.

We have seen that the nodal domains of multiple eigenvalues are difficult to handle, therefore we desire for simple eigenvalues of a Laplacian.

Question 7.1. [54] *Which graphs have only simple (Laplacian) eigenvalues?*

For the Laplacian $L(G)$, by Proposition 3.4 such a graph has neither twins u, v nor twins except the edge uv. By Geršgorin Theorem, we can always choose the diagonal elements of a generalized Laplacian $M(G)$ such that $M(G)$ has always simple eigenvalues[1]. It is also interesting to consider the influence of these choices of diagonal elements to the number of nodal domains. If we combine the choice of diagonal elements and Theorem 3.3, maybe it is possible to get good heuristics for finding an induced bipartite subgraph with maximum vertices.

On the other hand, there exists no closed relation between the number of nodal domains and the induced bipartite subgraph with maximum vertices of G ($\mathrm{MIB}(G)$) with respect to the Laplacian matrix. Let $\mathrm{SND}_L(G)$ be the number of strong nodal domains of an eigenvector of the Laplacian $L(G)$ with maximum number of strong nodal domains. $\mathrm{SND}_L(G)$ can be far from $\mathrm{MIB}(G)$, e.g., we take a path P_{2n} and two new vertices u and v. We add the edges between u and the first n vertices of P_{2n} and add the edges between v and the last n vertices of P_{2n}, finally add the edge uv, see the graph G in Fig. 7.1. For the graph G in Fig. 7.1 it holds $\mathrm{SND}_L(G) \leq n + 2$, but $\mathrm{MIB}(G) = 2n - 2$.

If graph H is a minor of G, then $\mathrm{MIB}(H) \leq \mathrm{MIB}(G)$. However, this is not the case for the number of nodal domains. It can happen that $\mathrm{SND}_L(H) > \mathrm{SND}_L(G)$. For example, if we contract the edge uv of graph G in Fig. 7.1, then $\mathrm{SND}_L(G/uv) = 2n > \mathrm{SND}_L(G)$.

[1] I thank P. Spellucci for this note.

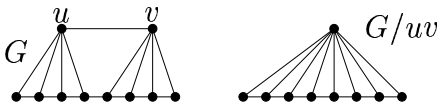

Fig. 7.1: An example for $\mathrm{MIB}(G) \gg \mathrm{SND}_L(G) \ll \mathrm{SND}_L(G/e)$

For the cartesian graph product $G\Box H$, the elementary observation $\mathrm{SND}(z) \leq \mathrm{SND}(x) \cdot \mathrm{SND}(y)$ holds, when $z = x \otimes y$. This upper bound does not hold for all eigenvectors of λ. The graph $K_2\Box G$ in Fig. 7.2 is a counterexample for such a bound. K_2 has the eigenvalues $\beta = 0$ and $\beta = 2$ with eigenvectors $(1, 1)$ and $(1, -1)$, respectively. G has the eigenvalues $\mu = 1$ with multiplicity two with the eigenspace of $(0, 0, 0, 0, 1, -1, 0)$ and $(0, 0, 0, 0, 0, 1, -1)$. $\mathrm{SND}(x) \leq 3$, for each eigenvector x of $\mu = 1$. G has also the simple eigenvalue $\mu = 3$ with the eigenvector $(1, -1, 0, 0, 0, 0, 0)$. Therefore $K_2\Box G$ has the eigenvalue $\lambda = 3$ with multiplicity three. $\mathrm{SND}(z) \leq 6$, for each eigenvector $z = x \otimes y$ affording $\lambda = 3$. However, the eigenvector $s = (1, -1, 0, 0, 2, -1, -1, 1, -1, 0, 0, -2, 1, 1)$ affording $\lambda = 3$ has eight strong nodal domains.

It can be of interest to characterize the graph products such that the elementary upper bound holds.

Question 7.2. *For which graphs G, H,*

$$\mathrm{SND}_L(G\Box H) \leq \mathrm{SND}_L(G) \cdot \mathrm{SND}_L(H)?$$

We conjecture that it holds if the Discrete Nodal Domain Theory is sharp for the eigenvalues of G and H. Specially, we conjecture that it holds for $P_k\Box P_l$.

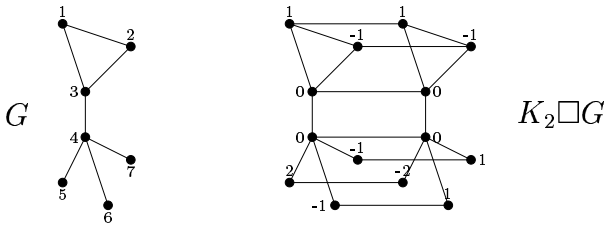

Fig. 7.2: A counterexample to $\mathrm{SND}_L(G\Box H) \leq \mathrm{SND}_L(G)\mathrm{SND}_L(H)$

In chapter 6 we have seen that a cograph has a tree representation. Chordal graphs also have tree representation. A graph is a *chordal graph* if it has no induced cycles larger than triangles. A tree T is a *clique tree* of a graph G if there is a bijection between $V(T)$ and the maximal cliques of G

such that for each vertex v of $V(G)$ the cliques containing v induce a subtree of T (see Fig. 7.3).

Theorem 7.1. [82, 44, 13] *A graph is a chordal graph if and only if it has a clique tree.*

It seems that the tree representation of a chordal graph G give an lower bound on the maximum number of nodal domains.

Conjecture 7.1. *Let G be a connected chordal graph and T be the clique tree of G. Then* $\mathrm{SND}_L(G) \geq |V(T)| + 1$.

This lower bound is not sharp, e.g., the graph G in Fig. 7.3 has more strong nodal domains than the number of vertices of its clique tree.

The vector $x = (1, -1, 0, 1, -1)$ is an eigenvector affording $\lambda = 3$, for the graph G in Fig. 7.3. By Proposition 3.6 H is the k-bundle of G (see Fig. 7.3) has an eigenvector with $4k$ strong nodal domains and the clique tree of k-bundle of G has $3k - 1$ vertices.

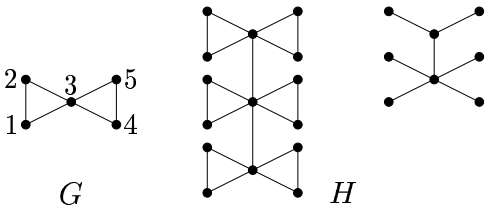

Fig. 7.3: The graph G, H is the 3-bundle of G, and clique tree of H

In chapters 5 and 6 we have seen that we can easily deal with eigenvectors with respect to graph product and the join operation.

Question 7.3. *Which graph operations are suitable for eigenvectors of (generalized) Laplacian of graphs?*

It is also interesting to find out, for which graphs the Discrete Nodal Domain Theory is sharp at least for two non-trivial eigenvalues or for all eigenvalues. In chapter 4 we see that it is sharp for paths and for some specific simple eigenvalues of a tree. Similarly, for which graphs do the eigenvectors of λ_k with multiplicity r have at most k strong nodal domains? The trivial example is a complete graph. After some numerical experiments it seems reasonable to expect that Andrásfai graphs are another example. The *Andrásfai graph* has the vertex set $V\{1, \ldots, 3n - 1\}$, for $n \geq 1$. The vertex 1 is adjacent the vertices congruent to 2 modulo 3. Let A, B, C be the set of

vertices congruent to 0 modulo 3, congruent to 2 modulo 3 and congruent to 1 modulo 3, respectively. The vertex 1 is adjacent to the vertices congruent to 2 modulo 3. For other vertices $a \in A, b \in B, c \in C$ hold: $ab \in E$ iff $b < a$, $ac \in E$ iff $a < c$, and $ab \in E$ iff $c < b$ (see for another definition of Andrásfai graph [47]). For example, the Andrásfai graph with five vertices is C_5, see Fig. 7.4 for the Andrásfai graph with eight vertices.

Conjecture 7.2. *Let λ_k be an eigenvalue of Laplacian of an Andrásfai graph. Then the eigenvectors of λ_k with multiplicity r has at most k strong nodal domains.*

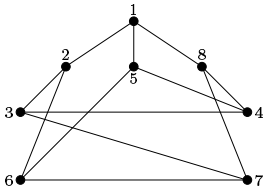

Fig. 7.4: The Andrásfai graph with eight vertices

Till now we look at the nodal domains of the (generalized) Laplacian of a graph. Another aspect is to give for each vertex of a graph a sign $\{+, -, 0\}$. The resulting nodal domains are nodal domains which we want and try to find a generalized Laplacian with desired nodal domains. This problem is an eigenvalue problem of *sign-solvable linear systems*. We refer to [12] for sign-solvable systems.

Question 7.4. *Let G be a graph and S be a sign pattern of the vertices of G. Can we find a generalized Laplacian $M(G)$ such that $M(G)$ has an eigenvector x with the same sign pattern as S?*

GLOSSARY OF SYMBOLS

$\|S\|$	cardinality of set S
$\langle x, y\rangle$	inner product of x and y
$A(G)$	adjacency matrix of G
$A \otimes B$	Kronecker product of two matrices
d_v	degree of vertex v
$D(G)$	degree matrix of G
e_n	constant vector $(1, \ldots, 1)$ of lengt n
$E(G)$	edge set of G
$G[U]$	induced subgraph of G with vertex set U
G^c	complement of graph G
$G - e$	deletion of edge e
$G - v$	deletion of vertex v
G/e	contraction of edge e
$G\{W\}$	reduced graph
$G \square H$	Cartesian product of two graphs
$G + H$	disjoint union of two graphs
$G * H$	join of two graphs
I	identity matrix
J	matrix of all ones
K_n	complete graph with n vertices
$K_{n_1,\ldots,n_k}$	complete k-partite graph
K_2^n	n dimensional hypercube
$L(G)$	Laplacian matrix of G
$M(G)$	generalized Laplacian matrix of G
P_k	path with k vertices
$\mathrm{SND}(x)$	number of strong nodal domains of vector x
$tr(A)$	trace of matrix A
uv	edge with incident vertices u and v
$V(G)$	vertex set of G
$\mathrm{WND}(x)$	number of weak nodal domains of vector x
$\rho(A)$	spectral radius of matrix A
$\varphi_I(v)$	Walsh function

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List of Publications

1. T. Bıyıkoğlu. A discrete nodal domain theorem for trees. *Lin. Alg. Appl.*, 360:197–205, 2003.

2. T. Bıyıkoğlu. A counterexample to a conjecture of Erdos *Discrete Math.*, 250:231–232, 2002.

3. T. Bıyıkoğlu. Degree sequences of Halin graphs and forcibly cograph-graphic sequences. *Ars Comb.* to appear.

4. T. Bıyıkoğlu, W. Hordijk, J. Leydold, T. Pisanski, and P.F. Stadler. Graph Laplacians, Nodal Domain, and Hyperplane Arrangements. submitted.

5. T. Bıyıkoğlu. Rank and Number of Nodal Domains of Cographs. submitted.