Graph Laplacians, Nodal Domains, and Hyperplane Arrangements

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Abstract. Eigenvectors of the Laplacian of a graph G have received increasing attention in the recent past. Here we investigate their so-called nodal domains, i.e., the connected components of the maximal induced subgraphs of G on which an eigenvector ψ does not change sign. An analogue of Courant's nodal domain theorem provides upper bounds on the number of nodal domains depending on the location of ψ in the spectrum. This bound, however, is not sharp in general. In this contribution we consider the problem of computing minimal and maximal numbers of nodal domains for a particular graph. The class of Boolean Hypercubes is discussed in detail. We find that, despite the simplicity of this graph class, for which complete spectral information is available, the computations are still non-trivial. Nevertheless, we obtained some new results and a number of conjectures.

1. Introduction

The foundations of spectral graph theory were laid in the fifties and sixties. 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. [4, 13, 14, 33, 35]. More recently, the interest has shifted somewhat from the adjacency spectrum to the spectrum of the closely related *graph Laplacian*, see e.g., [12, 37, 48, 49]. Again, the dominating part of the theory is concerned with the eigenvalues.

The *eigenvectors* of graphs, however, have received only sporadic attention on their own. Even the recent book on *Eigenspaces of Graphs* [15] 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 [39, 51, 52] and graph coloring [3]. Their application in graph drawing is discussed in [53, 36, 45, 50]. 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 [38, 40, 56]. This observation was one of the starting points of the algebraic theory of fitness landscapes which is reviewed in [54]. In the latter context the Laplacian eigenvectors of the Boolean Hypercubes (binary Hamming Graphs, iterated cartesian product of K_2) are of particular interest.

2. Nodal Domain Theorems

Let $G(V, E)$ be a finite, connected, undirected graph, and denote its number of vertices by $N = |V|$. For standard graph-theoretical terms not defined here we refer to [58]. The entries of the adjacency matrix $\mathbf{A}$ are $\mathbf{A}_{xy} = 1$ if the vertices x and y are adjacent and 0 otherwise. The degree matrix $\mathbf{D}$ is diagonal with $\mathbf{D}_{xx}$ being the degree of vertex x. The Laplacian of G is the matrix

$$-\mathbf{\Delta} = \mathbf{D} - \mathbf{A} \tag{1}$$

The graph Laplacian is symmetric and non-negative definite. The constant vector $\mathbf{1} = (1, \ldots, 1)$ is the unique eigenvector with eigenvalue 0, $-\mathbf{\Delta}\mathbf{1} = 0$. The operator $\mathbf{\Delta}$ can be viewed as a proper discretization of the familiar Laplacian differential operator.

The graph Laplacian is a member of a larger class of symmetric matrices associated with G. Let $\mathbf{H}$ be a symmetric matrix with arbitrary diagonal elements, non-negative off-diagonal elements, and $\mathbf{H}_{xy} = \mathbf{H}_{yx} < 0$ if and only if $\{x, y\}$ is an edge in G. Such a matrix is called a *Schrödinger operator* associated with G, see e.g. [18]. Colin de Verdière's famous graph invariant μ is closely related to this class of operators [17].

Discrete Schrödinger operators and their eigenfuctions are of interest in simplified quantum mechanical models of organic molecules, the so-called Hückel model [41].

Now consider a function $f : V \to \mathbb{R}$ on $G(V, E)$. Such a function is called a *landscape* on G in [54]. A *strong nodal domain* of f is a maximal connected induced subgraph $G[W]$ of G with vertex set W such that $f(x)f(y) > 0$ for all $x, y \in W$. A *(weak) nodal domain* of f is a maximal connected induced subgraph $G[W]$ such that $f(x)f(y) \geq 0$ for all $x, y \in W$. A (strong or weak) nodal domain $G[W]$ is call *positive* (*negative*) if there is an $x \in W$ with $f(x) > 0$ ($f(x) < 0$). We write $\mathrm{WND}(f)$ and $\mathrm{SND}(f)$ for the number of weak and strong nodal domains, respectively. Obviously, $\mathrm{WND}(f) \leq \mathrm{SND}(f)$.

Theorem 1. Discrete Nodal Domain Theorem [16]
Let $\mathbf{H}$ *be a Schrödinger operator of* G *with eigensystem* $\mathbf{H}\phi_k = \lambda_k\phi_k$, $1 \leq k \leq N$ *and suppose the eigenvalues* λ_k *are arranged in non-decreasing order*

$$0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_N$$

and have multiplicities m_k. *Then* ϕ_k *has at most* $\mathrm{WND}(\phi_k) = k$ *weak nodal domains and at most* $\mathrm{SND}(\phi_k) = k + m_k - 1$ *strong nodal domains.*

This is the graph version of Courant's celebrated Nodal Domain Theorem for Riemannian manifolds, see e.g. [10, 11]. Various versions of the nodal domain theorem and partial proofs were obtained independently by different authors [18, 24, 32, 52, 59], beginning with the work of M. Fiedler who proved the following two results that are corollaries of the nodal domain theorem:

Corollary 1. [27, 28] *The eigenvector* ψ_2 *to the smallest non-zero eigenvalue of any connected graph* $G(V, E)$ *has* $\mathrm{WND}(\psi_2) = 2$ *weak nodal domains.*

Corollary 2. [29] *The eigenvector* ψ_k *has at most* $k-1$ *positive weak nodal domains for* $k > 1$.

The eigenvector ψ_2 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:

$$\lambda_2 \leq \mathbf{v}(G) \leq \mathbf{e}(G) \tag{2}$$

A general method for obtaining asymptotic isoperimetric inequalities for families of graphs based on λ_2 is developed is described in [1]. A Cheeger like inequality has been shown in, e.g., [19].

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 [46] but so far no sharp upper bounds are available, see e.g. [2, 43, 44, 47]. For graphs the situation is similar. There only exist improved upper bounds for trees, see [6], and for cographs and threshold graphs, see [5]. 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 [26]: A vector ξ is called a *Faria vector*, if ξ has only two non-zero elements $\xi(x) = -\xi(y) = 1$.

Proposition 1. *A Faria vector ξ is an eigenvector of the Laplacian of the graph G if and only if x and y are* twins*, i.e., if every vertex $v \notin \{x, y\}$ is either adjacent to both x and y or to neither one of them.*

We refer to [8] 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.

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

Theorem 2. [55] *Let $G(V_1 \cup V_2, E)$ be a connected bipartite graph with $N = |V_1 \cup V_2|$ vertices and let $\mathbf{H}$ be any Schrödinger operator on G. Then there is a unique eigenvector ψ_N to the largest eigenvalue of $\mathbf{H}$. The eigenvector ψ_N is positive on V_1 and negative on V_2 or* vice versa *and hence satisfies* $\mathrm{WND}(\psi_N) = \mathrm{SND}(\psi_N) = N$.

Theorem 2 generalizes an analogous result for the the smallest eigenvalue of the adjacency matrix $\mathbf{A}$ [3].

In the case of degenerate eigenvalues the situation becomes even more difficult because the number of nodal domains may vary considerably depending on which vector from the m_k-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 ψ_k?
What is the minimal number of nodal domains of ψ_k?
What is the maximal number of nodal domains of ψ_k?

Given a fixed tree T and an eigenvalue λ_k, $2 < k < N$, the problem of finding an eigenvector ψ_k with the minimal number of nodal domains is NP-complete, i.e., really hard to solve [6].

3. 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 the number of nodal domains may vary considerably depending on which vector from the m_k-dimensional eigenspace of λ_k is chosen. To handle this situation we choose an orthonormal basis $u_1, \ldots, u_{m_k}$ for the eigenspace of λ_k ($\cong \mathbb{R}^{m_k}$). Every eigenvector ψ to the eigenvalue λ_k is then given by

$$\psi(x) = \sum_{j=1}^{m_k} a_j \, u_j(x) = \langle a, u(x) \rangle \tag{3}$$

where $a = (a_1, \ldots, a_{m_k})$, and $u(x) = (u_1(x), \ldots, u_{m_k}(x))$ is the vector that contains the values of the basis at the vertex x. Notice that if $\mathbf{U}$ is the matrix containing the basis vectors u_j as its columns then $u(x)$ forms the x-th row of $\mathbf{U}$.

The convex hull of the vectors $u(x)$, for $x \in V$, forms a polytope in $\mathbb{R}^{m_k}$, which is called the *eigenpolytope* of the graph, see e.g. [9, 34].

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 ψ and its "coordinate vector" a. The sign at vertex x is given by the sign of $\langle a, u(x)\rangle$. The set of eigenvectors that vanish on vertex x corresponds to the set

$$H_x = \{a \in \mathbb{R}^{m_k} \colon \langle a, u(x)\rangle = 0\} \tag{4}$$

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

$$\mathcal{H} = \{H_x | x \in V\} \tag{5}$$

in $\mathbb{R}^{m_k}$, see e.g. [25, 61]. The union of all these hyperplanes creates a *cellular complex* in $\mathbb{R}^{m_k}$ or (if we look at normalized eigenvectors) in the sphere S^{m_k-1}. A cellular complex consists of disjoint cells, where each cell is either homeomorphic to an open disc $D_d = \{a \in \mathbb{R}^d \colon ||a||_2 < 1\}$ 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 $\mathbb{R}^{m_k}$ (or S^{m_k-1}); (ii) The boundary of a d-cell consists of the union of cells of dimension less than d.

Each of the hyperplanes H_x splits the $\mathbb{R}^{m_k}$ into three pieces: the hyperplane H_x itself and the two open half-spaces $\{a \in \mathbb{R}^{m_k} | \langle a, u(x)\rangle > 0\}$ and $\{a \in \mathbb{R}^{m_k} | \langle a, u(x)\rangle < 0\}$. Hence, for each vector $a \in \mathbb{R}^{m_k}$ we may introduce the *covector* or *position vector* c_a with coordinates

$$c_a(x) = \operatorname{sgn}\langle a, u(x)\rangle \tag{6}$$

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 [7]. Finding 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 m_k of the eigenvalue. Using a general upper bound for hyperplane arrangements [25] we have the asymptotic behavior

$$\text{number of } d\text{-cells} \sim N^{m_k} \tag{7}$$

An exact and sharp upper bound is given, e.g., in [25].

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

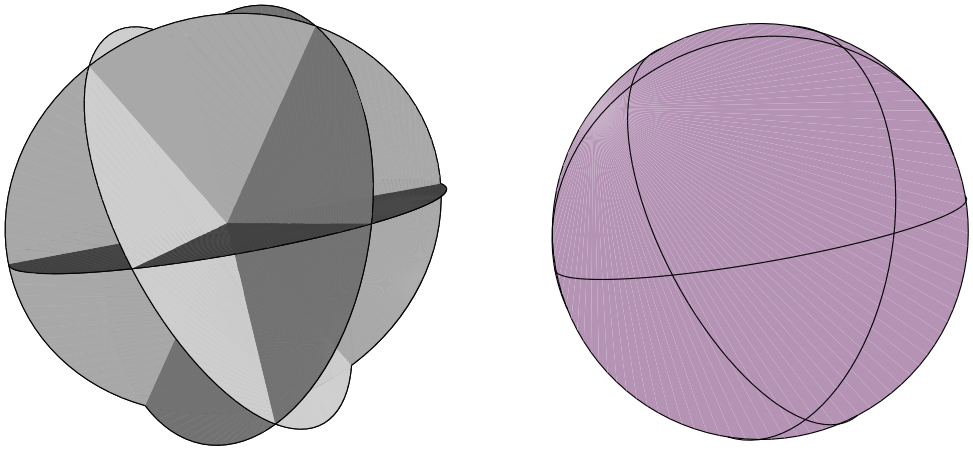

Figure 1. Hyperplane arrangement (l.h.s.) and the correponding cells on the sphere (r.h.s.) of eigenvalue 4 for the cube K_2^3. We have $m_k = 3$ and $N = 8$. The vectors $u(x)$ are given by the eight vectors $(\pm 1, \pm 1, \pm 1)$. Due to symmetry we only have the following cells

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`.

at 0-cells if we want to minimize $\mathrm{WND}(\psi_k)$ and to cells of highest dimension if we want to maximize $\mathrm{WND}(\psi_k)$.

If we look at strong nodal domains the situation is much more complicated. Because then zeros separate nodal domains, and $\mathrm{SND}(\psi_k)$ 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 $\mathrm{SND}(\psi_k)$. 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 1 illustrates the situation.

Because of equ.(7) 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) 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 $\psi(x) = \langle a, u(x)\rangle$. 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 $\delta(x) = \frac{\langle a,u(x)\rangle}{\langle a',u(x)\rangle}$, and find the vertices x_1 and x_2 such that $\delta(x_1)$ is smallest with $\delta(x) > 0$ and $\delta(x_2)$ is smallest with $\delta(x) > \delta(x_1)$. Then set $\delta = (\delta(x_1) + \delta(x_2))/2$ and move from a to $a^* = a - \delta\, a'$, with corresponding eigenvector $\psi'(x) = \langle a', u(x)\rangle$. 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 M 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 M 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.

4. Boolean Hypercubes

The hypercube K_2^n is the graph with vertex set $V = \{(x_1, x_2, \ldots, x_n) | x_i = \pm 1\}$ and edges connecting two vertices that differ in a single coordinate, i.e., $\{x, y\} \in E$ iff $x_i = y_i$ for all but one index j for which we then have $x_j = -y_j$. The number n of coordinates is usually called the *dimension* of K_2^n. The graph has $N = 2^n$ vertices and $|E| = n2^{n-1}$ edges.

Given two non-empty graphs $G = (V_G, E_G)$ and $H = (V_H, E_H)$ the Cartesian product $G \square H$ has vertex set $V_G \times V_H$ and $(x_1, x_2)(y_1, y_2)$ is an edge in $E_{G \square H}$ iff either $x_2 = y_2$ and $x_1 y_1 \in E_G$ or if $x_1 = y_1$ and $x_2 y_2 \in E_H$, see e.g. [42]. It is not hard to verify that the hypercube 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* [30, 60]

$$\varphi_I(x) = \prod_{k \in I} x_k \tag{8}$$

Table 1. Upper bounds on the number of strong and weak nodal domains as function of n and $p = |I|$ as given in equ.(13).

$p=$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
n	$s_{n,p}$														
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	$w_{n,p}$														
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

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

$$-\mathbf{\Delta}\varphi_I = 2|I|\varphi_I \tag{9}$$

and the orthogonality relation

$$\langle \varphi_I, \varphi_J \rangle = \sum_{x \in V} \varphi_I(x)\varphi_J(x) = \delta_{I,J}|V| \tag{10}$$

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:

$$\varphi'_I(x; x_{n+1}) = \varphi_I(x) \qquad \text{and} \qquad \varphi'_{I\cup\{x_n\}}(x; x_{n+1}) = x_{n+1}\,\varphi_I(x) \tag{11}$$

It is sometime more convenient to write equ.(11) as a tensor product:

$$\varphi'_I = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \varphi_I \qquad \text{and} \qquad \varphi'_{I\cup\{n+1\}} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \varphi_I \tag{12}$$

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. [14, 23].

Equ.(11) of course holds for any eigenvector ϕ of K_2^n with eigenvalue $2p$: The vector $\phi^+ = \binom{1}{1} \otimes \phi$ is an eigenvector of K_2^{n+1} with eigenvalue $2p$, while $\phi^- = \binom{1}{-1} \otimes \phi$ is an eigenvector of K_2^{n+1} with eigenvalue $2(p+1)$.

It follows immediately from Theorem 1 that an eigenvector ξ with eigenvalue $2p$ has at most

$$\mathrm{SND}(\xi) \leq s_{n,p} = \sum_{k=0}^{p} \binom{n}{k} \qquad \text{and} \qquad \mathrm{WND}(\xi) \leq w_{n,p} = 1 + \sum_{k=0}^{p-1} \binom{n}{k} \tag{13}$$

strong and weak nodal domains, respectively. Numerical values are listed in Table 1.

We can use the recursive construction of the Walsh functions in equ.(11) to obtain bounds on the number of nodal domains. The following technical result will be used repeatedly:

Lemma 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

$$\partial W = \big\{ y \in V \setminus W \,|\, \exists x \in W : \{x, y\} \in E \big\}$$

We write $(W, x_{n+1}) = \{x' \in K_2^{n+1} \,|\, x' = (x, x_{n+1}),\, x \in W\}$ 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 $\partial(W, x_{n+1}) = (\partial W, x_{n+1}) \cup (W, -x_{n+1})$.
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 x with $f(x) = 0$. Then there exists a weak negative nodal domain Q that also contains x. Then $(P, +1)$ and $(Q, -1)$ are weak positive nodal domains that are connected by the vertices $(x, +1) \in (P, +1)$ and $(x, -1) \in (Q, -1)$, 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. 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 $\{\psi | -\mathbf{\Delta}\xi = \lambda_k \xi\}$ we want to

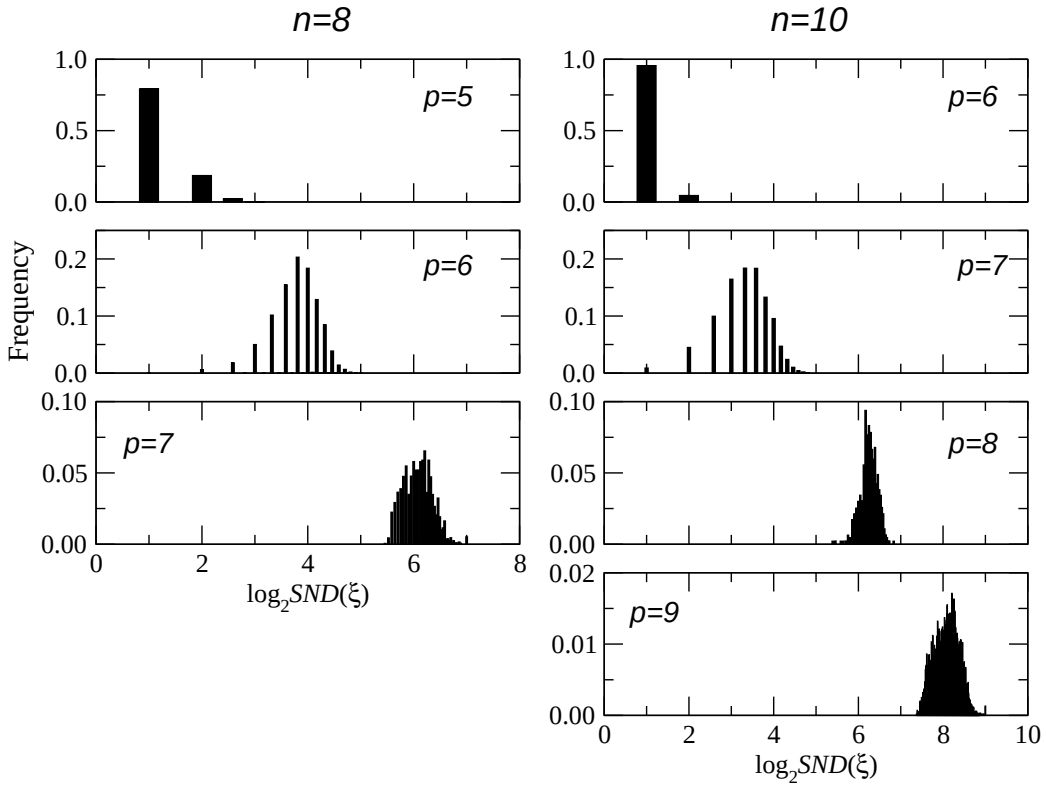

Figure 2. Distribution of $SND(\psi)$ with Walsh coefficients a_I, $|I| = p$ drawn independently from a Gaussian distribution.

consider. Since we have

$$\xi(x) = \sum_{I:|I|=p} a_I \varphi_I(x) \tag{14}$$

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.(14) defines Derrida's p-spin models [20, 21] which form an important and well-studied class of spin glasses which also play an important role in the theory of fitness landscapes [57].

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. [31]). For this purpose the coefficent 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. [22]).

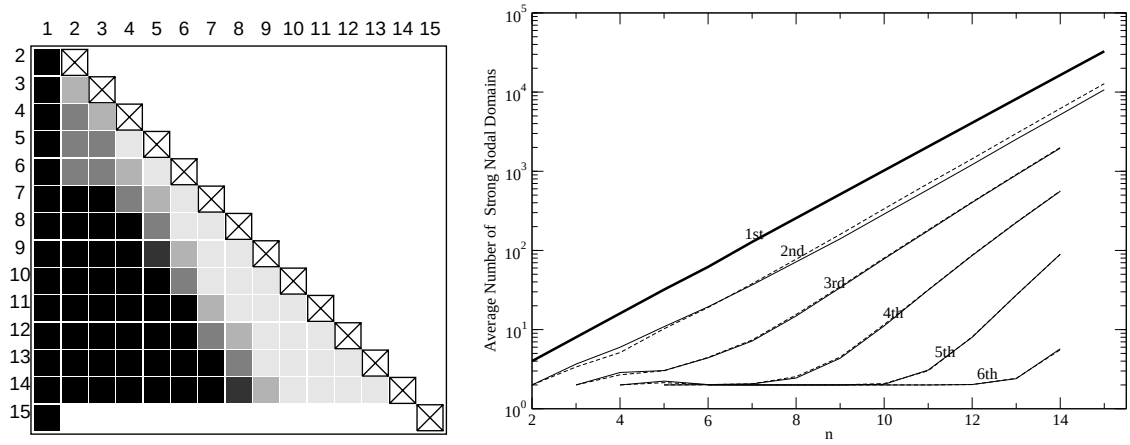

Figure 3. Average number of nodal domains for the eigenvectors of the hypercubes with $n = 2$ to 15 as a function of p. The l.h.s. panel gives an overview of the numerical survey. Black squares denote (n, p)-pairs for which all of the 1000 randomly generated instances had exactly 2 nodal domains, ⊠ denotes 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.

6. The Minimal Number of Nodal Domains

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

Theorem 3. *For all* $1 \leq p \leq n-1$ *there is an eigenvector* ϕ *of the Boolean Hypercube with eigenvalue* $\lambda = 2p$ *such that* $\mathrm{WND}(\phi) = 2$.

Proof. We will proceed by induction. The hypercube K_2^2 is a cycle with four vertices. It is straightforward to check that $\phi_1^{(2)} = (0, 1, 0, -1)$ is an eigenvector with eigenvalue $\lambda = 2$ and $\mathrm{WND}(\phi_1^{(2)}) = 2$.

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

$$\begin{aligned} \phi_p^{(n+1)} &= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \phi_p^{(n)} = \left(\phi_p^{(n)}\right)^+ \quad \text{for } p \leq n-1 \\ \phi_n^{(n+1)} &= \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \phi_{n-1}^{(n)} = \left(\phi_{n-1}^{(n)}\right)^- \end{aligned} \tag{15}$$

where we use the notation of Lemma 1. Recall from the discussion in section 4 that $\phi_p^{(n+1)}$ is an eigenvector of K_2^{n+1} with eigenvalue $2p$. By Lemma 1 we find for $p \leq n$, $\mathrm{WND}(\phi_p^{(n+1)}) = \mathrm{WND}(\phi_p^{(n)}) = 2$, where the second equality holds by assumption of induction.
Now consider $\phi_{n-1}^{(n)}$. Assume by induction that $\mathrm{WND}(\phi_{n-1}^{(n)}) = 2$. For an arbitrary vector f we write $V_0(f)$, $V_+(f)$ and $V_-(f)$ for the sets of vertices x where $f(x) = 0$, $f(x) > 0$, and $f(x) < 0$, respectively. Let V_0^+ be a copy of $V_0(\phi_{n-1}^{(n)})$ in K_2^{n+1} with coordinate $x_{n+1} = +1$ while V_0^- is the copy with $x_{n+1} = -1$. The sets V_+^+, V_+^-,

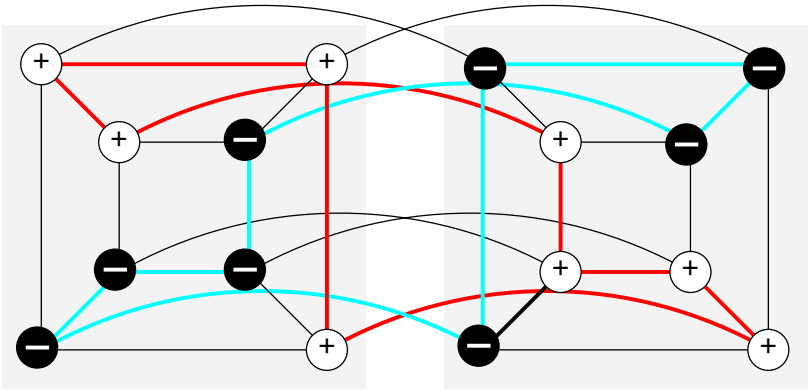

Figure 4. The sign pattern of the eigenvector θ_4.

V_-^+, and V_-^- are defined analogously. We have $V_0(\phi_n^{(n+1)}) = V_0^+ \cup V_0^-$, $V_+(\phi_n^{(n+1)}) = V_+^+ \cup V_-^-$ and $V_-(\phi_n^{(n+1)}) = V_-^+ \cup V_+^-$.

By induction hypothesis $V_+(\phi_{n-1}^{(n)}) \cup V_0(\phi_{n-1}^{(n)})$ and $V_-(\phi_{n-1}^{(n)}) \cup V_0(\phi_{n-1}^{(n)})$ 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

$$\begin{aligned} V_+(\phi_n^{(n+1)}) \cup V_0(\phi_n^{(n+1)}) &= V_+^+ \cup V_0^+ \cup V_0^- \cup V_-^- \\ V_-(\phi_n^{(n+1)}) \cup V_0(\phi_n^{(n+1)}) &= V_-^+ \cup V_0^+ \cup V_0^- \cup V_+^- \end{aligned} \tag{16}$$

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

The eigenvector to the highest eigenvalue (which is simple) always has N nodal domains (see Thm. 2).

For strong nodal domain theorems the situtation is much more complicated (see Tab. 2). We can obtain at least a partial result.

Theorem 4. *For all $1 \le p \le n/2$ there is an eigenvector ϕ of the Boolean Hypercube with eigenvalue $\lambda = 2p$ such that $\mathrm{SND}(\phi) = 2$.*

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

Suppose $\xi(x) \in \{-1, 1\}$ for all $x \in V$ and $\sum_{x \in V} \xi(x) = 0$, i.e., half of the vertices have value $+1$, the others -1. Such a vector ξ is an eigenvector of the Laplacian with eigenvalue n if and only if for each vertex $x \in V$ half of its neighbors $y \in \partial\{x\}$ have $\xi(y) = +1$ and the other half satisfies $\xi(y) = +1$. Figure 4 shows that such a vector θ_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 $(x, +1)$ according to $\mathcal{X}$ and the vertices $(x, +1)$ according to $\mathcal{Y}$, see Fig. 4. We write $-\mathcal{X}$ for the pattern with reversed signs.

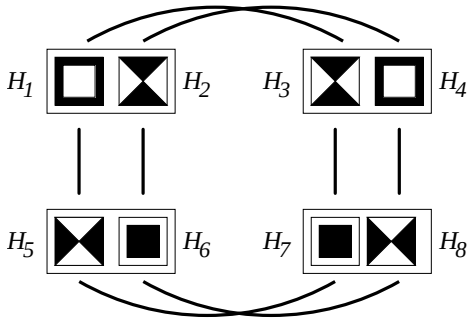

Figure 5. The sign pattern on K_2^{n+2} is built up from the sign sign patterns $\mathcal{X}$ and $\mathcal{Y}$ on two copies K_2^{n-1} that together form a K_2^n. The negative patterns $-\mathcal{X}$ and $-\mathcal{Y}$ are shown with black and white exchanged.

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

(i) There is a product decomposition $K_2^n = K_2^{n-1} \Box K_2$ 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. 4 shows that the sign pattern of θ_4 is admissible.

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

$$\mathcal{X}^*|\mathcal{Y}^* = \big((\mathcal{X}|\mathcal{Y})\big|(\mathcal{Y}|\mathcal{X})\big) \;\Big|\; \big((-\mathcal{Y}|-\mathcal{X})\big|(-\mathcal{X}|-\mathcal{Y})\big) \tag{17}$$

on K_2^{n+2}, which is composed of eight copies of K_2^{n-1} labelled H_1 through H_8 as in Fig. 5. 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 θ_{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 θ_4 in Fig. 4 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

Table 2. Upper and Lower Bounds on the number of nodal domains as functions of n and p found by numerical experiments.

$p=$	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 3. Entries in *italics* are numerical value that are known to be underestimates because of Lemma 1.

(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 $\mathrm{SND}(\theta_{n+2}) = 2$.

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

$$\phi_p^{(n)} = \begin{cases} \theta_n & \text{if} \quad p = n/2 \\ \binom{1}{1} \otimes \phi_p^{(n-1)} & \text{if} \quad p < n/2 \end{cases} \tag{18}$$

We know that $\phi_p^{(n)}$ is an eigenvector with eigenvalue p by construction. Furthermore, Lemma 1 implies that $\mathrm{SND}(\phi_p^{(n)}) = \mathrm{SND}(\phi_p^{(n-1)}) = \cdots = \mathrm{SND}(\phi_p^{(2p)}) = \mathrm{SND}(\theta_{2p}) = 2$. □

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 ψ with $SND(\psi) = 2$. This can be constructed by setting $\psi(x) = 1$ for $x \in A$ and $\psi(x) = -1$ for $x \in B$. In the proof of Theorem 4 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 4 holds:

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

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

Theorem 5. *For every eigenvector ψ of the Hypercube K_2^n, $n \geq 3$, with eigenvalue $\lambda = 2(n-1)$ we have* $\mathrm{SND}(\psi) \geq n$.

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

Lemma 2. *Let ϑ be a Laplacian eigenvector to the eigenvalue $2(n-1)$ that satisfies $\vartheta(x) \neq 0$ for all $x \in V$ and that has positive coefficients $a_I \geq 0$ for all I with $|I| = n-1$ in its Walsh expansion equ.(14) and define $\widehat{\vartheta}(x) = \vartheta(x)\varphi_{\{1,\ldots,n\}}(x) = \vartheta(x)\prod_{i=1}^{n} x_i$. Then:*

(1) *$\widehat{\vartheta}(x) = \sum_{I,|I|=n-1} x_{i_I} a_I$, where i_I is the unique coordinate not contained in I.*
(2) *$\widehat{\vartheta}$ 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 ϑ does not change sign.*

Remark. $\widehat{\vartheta}(x)$ is an eigenvector to eigenvalue 2.

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

$$\widehat{\vartheta}(x) = \vartheta(x)\prod_{j=1}^{n} x_j = \sum_{I,|I|=n-1} a_I\,\varphi_I(x)\prod_{j=1}^{n} x_j = \sum_{I,|I|=n-1} a_I \prod_{k\in I} x_k \prod_{j=1}^{n} x_j$$
$$= \sum_{I,|I|=n-1} a_I\, x_{i_I} \prod_{k=1}^{n} x_k \prod_{j=1}^{n} x_j = \sum_{I,|I|=n-1} x_{i_I}\, a_I\,.$$

(2) On any path from $\mathbf{1}$ to $-\mathbf{1}$ the number of negative coordinates of x 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 $\widehat{\vartheta}$ changes sign. Since $\prod_{j=1}^{n} x_j$ has alternating signs on every path, the sign of $\vartheta(x) = \widehat{\vartheta}(x)\prod_{j=1}^{n} x_j$ changes except along the edge e. □

First assume that ψ does not vanish on any vertex. Then using Lemma 2 it is easy to show that for every path of length n from the absolute maximum of ψ to its antipodal point, ψ 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 $\psi(x) = 0$ for some vertex $x \in V$ then we can use the same idea as in the proof of Lemma 2. However we find on this path (at most) one vertex x where ψ vanishes.

Now on each edge of this path ψ either changes sign or joins x with a vertex of positive of negative sign. Again the result follows. □

Our experiments show that this bound is not sharp, see Table 2.

7. 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 1 that the maximum number of strong nodal domains (listed in the lower part of Table 2) must be non-decreasing with n for fixed p. As trivial consequence of Theorem 2 we have therefore

Corollary 3. *The eigenvalue* $2p$ *has an associated eigenvector* ξ *with at least* $\mathrm{SND}(\xi) \geq \mathrm{WND}(\xi) \geq 2^p$ *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.

8. Open Questions

We suspect that the bounds in Tab. 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 $\mathrm{WND}(\psi) = 2$ for almost all eigenvectors is sharp for e.g. for all expander graphs.

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