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Nodal domain counts and the chromatic number of graphs

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Abstract

A function f, defined on the vertices of a graph G, induces nodal domains on the graph. Nodal domains of discrete and metric graphs are of growing interest among physicists and mathematicians. In this paper, several results regarding the nodal domain counts of discrete graphs are derived. One such result is a global upper bound for the number of nodal domains of G, in terms of its chromatic number. Another result is a criterion of resolution of (Laplacian) isospectral graphs via their nodal counts. Several additional results are also shown.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The research of nodal domains has been developing since the 19th century. The first pioneering work was conducted by Chladni on the nodal structures on vibrating plates. Following Chladni's work, Sturm discovered his well-known theorem which stated the following: a vibrating string is divided into exactly n nodal intervals by the zeros of the nth eigenfunction of the Laplace operator. In an attempt to generalize Sturm's theorem to more than one dimension, Courant formulated a nodal domain theorem suitable for vibrating membranes [1], which bounded the number of nodal domains of the nth eigenfunction by n.

Similar results were proven for metric and discrete graphs. In combinatorial trees, it was shown that the nth eigenvector of the Laplacian has exactly n nodal domains [2]. This is a generalization of Sturm's theorem from the interval to a tree. A similar theorem was proven for metric graphs [3–6]. For non-tree combinatorial graphs, as well as for metric graphs, an analogue of Courant's nodal domain theorem was proven [7, 8].

Nodal domains come to play in various branches of physics and mathematics. For example, it was shown that the nodal domain statistics can be used as a criterion for quantum chaos [9]. Moreover, there is a growing body of evidence which shows that the nodal sequence

stores geometrical information about the domain. Gnutzmann *et al* [10] derived a trace formula for the nodal domain counts in separable systems. It expresses the nodal domain count in terms of the periodic geodesics on the domain, and some other constants which depend on the shape parameters of the system. The geometrical information stored in the nodal sequence is not identical to that stored in the spectrum. Indeed, it was conjectured [11, 12] that isospectral, yet not isometric domains can be distinguished by their nodal domain sequences. This conjecture was proven to be valid in a few particular cases—flat tori in 4d [13] and for simple metric graphs [12].

In the present paper, several results on nodal domains of discrete graphs are presented. We start by describing a simple observation about the maximal number of nodal domains of bipartite graphs, which can be formulated as a criterion for resolving isospectrality of pairs of graphs, of which only one is bipartite.

Next, we address a more general question: what limits the maximal possible number of nodal domains on a graph? We derive an exact and optimal upper bound for the maximal possible number of nodal domains of a given graph G. This bound is global, i.e. it is a property of the graph, and it is a consequence of the complexity of the graph connectivity. In particular, this result is applicable to discrete Laplacians, and to discrete nodal domain counts on *metric graphs* (see [12]), since as a topological object, a metric graph is similar to a discrete graph.

The paper is arranged as follows: the next section will consist of the necessary definitions and background. The third section will present the main results: at first we discuss nodal domains of Laplacians, and their use in bipartite and isospectral graphs. Then we provide an upper bound for nodal domain counts, with possible applications. The final section is devoted to discussions and miscellaneous results.

2. Definitions and notations

A *graph* $G = (V, E)$ is a set of vertices $V = \{v_1, v_2, \ldots, v_n\}$ and a set of undirected edges (bonds) E such that $\{v_1, v_2\} \in E$ if vertices v_1 and v_2 are connected by an edge. In this case we say that vertices v_1 and v_2 are *adjacent*. The *degree* (*valency*) of a vertex is the number of edges which are connected to it. Throughout this paper, we only deal with connected graphs with no multiple edges or loops (an edge which connects a vertex to itself). For convenience, whenever we need the cardinality of the vertex set $|V|$, we shall simply write V.

The *complete graph* on V vertices, denoted by K_V, is the graph where all pairs of vertices are adjacent.

A graph G is said to be *properly colored* if each vertex is colored so that adjacent vertices have different colors. G is *k-colorable* if it can be properly colored by k colors. The *chromatic number* $\chi(G)$ is k if G is k-colorable and not $(k-1)$-colorable. A very simple observation, which we will use later, is that $\chi(G) \leqslant V$ where V is the number of vertices in G.

G is called *bipartite* if its chromatic number is 1 or 2. However, since a chromatic number 1 corresponds to a graph with no edges, and we are dealing only with connected graphs, we can exclude this trivial case and say that for a bipartite graph, $\chi = 2$. The vertex set of a bipartite graph G can be partitioned into two disjoint sets, say V_1 and V_2, in such a way that every edge of G connects a vertex from V_1 with a vertex from V_2. We then have the following notation: $G = (V_1 \cup V_2, E)$ [14].

The *adjacency matrix* (*connectivity*) of G is the symmetric $V \times V$ matrix $C = C(G)$ whose entries are given by

$$C_{ij} = \begin{cases} 1, & \text{if} \quad v_i \text{ and } v_j \text{ are adjacent} \\ 0, & \text{otherwise.} \end{cases}$$

The *combinatorial Laplacian*, or simply the Laplacian of G, is the matrix $L(G) = D - C$ where D is the diagonal matrix whose ith diagonal entry is the degree of the vertex v_i, and C is the adjacency matrix of G.

The eigenvalues of $L(G)$, along with their multiplicities, are known as the *spectrum* of G. To each eigenvalue corresponds (at least one) eigenvector whose entries are labeled by the vertices indexes.

A *nodal domain* is a maximally connected subgraph of G such that all vertices have the same sign with respect to f, where $f \in \mathbb{R}^V$. The number of nodal domains with respect to a vector f is called a *nodal domain count*. It will be denoted by $\nu(f)$. The maximal number of nodal domains which can be achieved by a graph G will be denoted by ν_G. The *nodal sequence* of a graph is the number of nodal domains of eigenvectors of the Laplacian, arranged by increasing eigenvalues.

The definition of nodal domains should be sharpened if we allow a zero entry in f. Two definitions are then natural: A strong positive (negative) nodal domain is a maximally connected subgraph H of G such that $f(v) > 0$ ($f(v) < 0$) for all $v \in H$. A weak positive (negative) nodal domain is a maximally connected subgraph H of G such that $f(v) \geqslant 0$ ($f(v) \leqslant 0$) for all $v \in H$. In both cases, a positive (negative) nodal domain must consist of at least one positive (negative) vertex.

According to these definitions, it is clear that the weak nodal domain count is always smaller or equal to the strong one.

Two non-isomorphic graphs, G and H, are said to be *isospectral* if they posses the same spectrum (same eigenvalues with the same multiplicities).

3. Main results

We start by considering the nodal domains induced by the eigenvectors of the Laplacian of a graph G. We provide a criterion for bipartite graphs, and identify a class of isospectral graphs, which can be resolved using this criterion.

Theorem 3.1. *Let f_V be the eigenvector corresponding to the largest eigenvalue of the Laplacian of a connected graph G. Then $\nu(f_V) = \nu_G = V$, if and only if G is bipartite.*

Proof. If $\nu(f_V) = V$ then each nodal domain must consist of exactly one vertex. We should note that since the nodal domain count is maximal, then there can be no zero vertices (with respect to f). Hence, we can color G in the following way: a positive vertex will be colored in red and a negative one will be colored in blue. Adjacent vertices have different colors, because otherwise there will be at least one nodal domain which consists of more than one vertex, in contradiction to $\nu(f_V) = V$. Hence G is bipartite.

If G is bipartite then we can use a theorem by Robert Roth [15], later proven in a different way by Bıyıkoglu, Leydold and Stadler [16], which can be formulated for our needs as the following.

Let $G = (V_1 \cup V_2, E)$ be a connected bipartite graph with $V = |V_1 \cup V_2|$ vertices, and let L be the Laplacian of G. Then there is an eigenvector f_V which corresponds to the largest eigenvalue of L, such that f_V is positive on V_1 and negative on V_2 or vice versa and hence $\nu(f_V) = V$. □

Note that a tree T is a special case of a bipartite graph. Theorem 3.1 is consistent with the discrete nodal domain theorem for trees [2]: if we order the eigenvalues of the Laplacian of a tree in a non-decreasing order, then $\nu(f_n) = n$, where f_n is the eigenvector corresponding

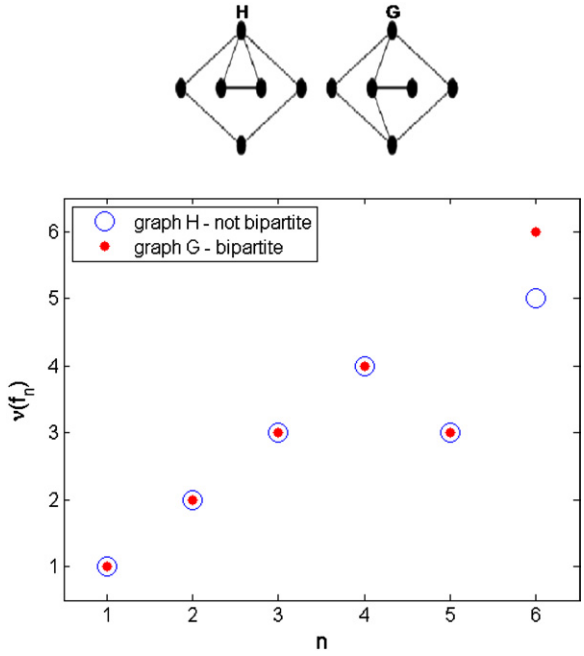

Figure 1. The upper figure presents a pair of isospectral graphs taken from [17]. Graph G, on the right is bipartite, whereas graph H, on the left, is not. The lower figure presents the nodal domain count, $\nu(f_n)$ versus the index n. As shown, the nodal domain count for the first five eigenvalues is equal for both graphs. However, the nodal count for the largest eigenvalue is different, as proven in theorem 3.2.

to λ_n. More precisely, theorem 3.1 applied on a tree, is identical to the discrete nodal domain theorem for trees, for the largest eigenvalue.

With this background, we can present a theorem, based on theorem 3.1, which provides a criterion for the resolution of a special class of isospectral graphs. The proof is obvious due to theorem 3.1

Theorem 3.2. *Let G and H be two isospectral graphs where one of them is bipartite and the other one is not (without loss of generality, G is bipartite and H is not). Then for the eigenvector corresponding to the largest eigenvalue λ_V, their nodal domain count will differ* $(\nu(G) = V, \nu(H) < V)$.

An example is given in figure 1. The number of nodal domains of a graph G on V vertices is at most V. But, can this number be achieved for any graph? The answer for this question is obviously negative. For example, we can clearly see that the maximal number of nodal domains on the complete graph K_3, is 2. More generally, $\nu_{k_V} = 2$ for all $2 \leqslant V \in \mathbb{N}$, as will be shown later. The following theorem provides an upper bound for the nodal domain count on discrete graphs.

Theorem 3.3. *Let G be a connected graph on V vertices, with chromatic number $\chi \geqslant 2$. Then ν_G satisfies the inequality:*

$$\nu_G \leqslant V - \chi + 2. \tag{1}$$

Before proving this theorem, we can get familiar with it using two extremal cases: the complete graph K_V and a bipartite graph H. The complete graph has a chromatic number $\chi(K_V) = V$

(this is the only graph for which this is true). Therefore, according to theorem 3.3 we expect that $\nu_{K_V} \leqslant 2$. This is obviously true because no matter how we distribute positive and negative signs (and zeros) on a vector defined on the vertices of K_V, they will form at most two nodal domains. This is a direct consequence of its high connectivity (highest chromatic number). On the other hand, a bipartite graph H possesses the lowest chromatic number a connected graph can have, $\chi = 2$. As a result: $\nu_H \leqslant V$. This is clearly true for any graph. However, as we have seen in theorem 3.1, the only graphs that can (and actually do) achieve this number are bipartite ones. It is therefore apparent that there is a trade off between ν_G and the chromatic number, which can be considered as a measure of the graph connectivity. Note that the two examples given above, show that the bound given in theorem 3.3 is optimal.

Proof. Let us assume that we have found a vector f which maximizes the nodal domain count of G, i.e. $\nu(f) = \nu_G$. Generally speaking, f can have positive, negative or zero entries. Since we are looking for a maximal number of nodal domains, we can restrict ourselves to the *strong* nodal count as defined in the definitions section. We denote the set of zero entries in f by S: $S = \{v \in V | f(v) = 0\}$. There are ν_G^- negative nodal domains and ν_G^+ positive nodal domains in G, where

$$\nu_G^- + \nu_G^+ = \nu_G. \tag{2}$$

We denote the sizes of negative domains in G as a_i^-, $i = 1, 2, \ldots, \nu_G^-$ and the positive ones as a_i^+, $i = 1, 2, \ldots, \nu_G^+$. We order the $a_i^{\pm}{}'s$ in a non-ascending sequence:

$$a_1^- \geqslant a_2^- \geqslant \cdots \geqslant a_{\nu_G^-}^-$$
$$a_1^+ \geqslant a_2^+ \geqslant \cdots \geqslant a_{\nu_G^+}^+.$$

Since we are counting strong nodal domains (and hence all $v \in S$ are not included in any positive or negative nodal domains), it is obvious that

$$\sum_{k=1}^{\nu_G^-} a_k^- + \sum_{k=1}^{\nu_G^+} a_k^+ + |S| = V. \tag{3}$$

To prove theorem 3.3 we proceed by properly coloring G. Using the observation we made in the definitions section, we see that $\chi\left(a_1^-\right) \leqslant a_1^-$ and $\chi\left(a_1^+\right) \leqslant a_1^+$ (where $\chi\left(a_1^-\right)$ should be understood as the chromatic number of the subgraph which is the largest negative domain). It is obvious that there are no edges between different nodal domains of the same sign, in G. If, for example, there was an edge between two negative domains, a_i^- and a_j^- then neither of them would be maximal. This means that when we want to color another nodal domain, say a negative one a_2^-, no new colors are needed, since $a_2^- \leqslant a_1^-$. The zero vertices in G require at most $|S|$ new colors. Thus, the number of colors needed in order to properly color G is bounded from above in the following way:

$$\chi(G) \leqslant a_1^- + a_1^+ + |S| = V - \sum_{k=2}^{\nu_G^-} a_k^- - \sum_{k=2}^{\nu_G^+} a_k^+,$$

where we have used (3).

Each a_i^-, $i = 2, 3, \ldots, \nu_G^-$ and a_j^+, $j = 2, 3, \ldots, \nu_G^+$ is greater or equal to one, because each domain must consist of at least one vertex. Thus, using (2) we get

$$\chi(G) \leqslant V - \nu_G + 2$$

and so our result follows:

$$\nu_G \leqslant V - \chi + 2.$$

□

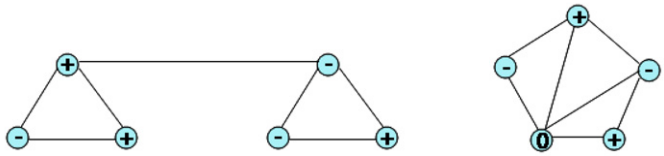

Figure 2. Two examples for the use of theorem 3.3.

Note that the proof remains valid if f has no zero entries. In that case $S = \emptyset$, $|S| = 0$, and the strong nodal count coincides with the regular one.

Let us examine two examples of applications of theorem 3.3. In figure 2, we see two graphs. On the left, a graph on six vertices and $\chi = 3$ is presented. By theorem 3.3, $\nu_G \leqslant 5$. The configuration given yields the largest possible number of nodal domains on the graph, as can easily be checked. This configuration has four nodal domains, and indeed $\nu_G = 4 \leqslant 5$. The graph on the right is an example of a graph, in which the maximal number of nodal domains is achieved only when the vector has a zero entry. This graph has five vertices and $\chi = 3$, so we expect $\nu_G \leqslant 4$. Indeed the proposed configuration yields $\nu_G = 4 \leqslant 4$.

Having proven theorem 3.3, we can discuss some of it applications. First, it can improve the upper bound of Courant's nodal domain theorem. Let us recall that this theorem states that for the nth eigenvector of the Laplacian, f_n, $\nu(f_n) \leqslant n$. However, for all n such that $n > V - \chi + 2$, we obtain an improved upper bound:

$$\nu(f_n) \leqslant V - \chi + 2.$$

Although finding the chromatic number of a graph is an NP-hard problem, a lower estimate of χ can be used. For example let us think of a graph G on 100 vertices which contain the complete graph on 10 vertices, K_{10}, as a subgraph. In this case, we know that $\chi(G) \geqslant 10$. By theorem 3.3 we know that $\nu_G \leqslant 100 - \chi + 2$, so it is certain that $\nu_G \leqslant 92$. So, even without knowing the actual chromatic number, it is still possible to say that for all $n > 92$, $\nu(f_n) \leqslant 92$, which is a lower bound than Courant's.

We can further use this argument in order to bound the number of nodal domains of random graphs. In extremal graph theory, there are many theorems regarding the maximal number of edges of an undirected graph on V vertices, which does not contain a certain subgraph. For example, Turán (1941) found that the largest graph not containing K_n has $\left\lfloor \frac{(n-2)V^2}{2(n-1)} \right\rfloor$ edges (the Turán graph). So, if a graph G on V vertices has more edges than the Turán graph, then we can considerably bound its maximal nodal domain count. This could be useful when discussing the nodal domain distributions of random graphs, both discrete and metric.

Another potential use of theorem 3.3 could be in bounding the chromatic number of a graph, if we know the maximal number of nodal domains. There are quite efficient ways of counting nodal domains, which can be used to obtain numerically a bound on the nodal count. We can then use this to bound the chromatic number of a given graph.

4. Discussion and miscellaneous results

Throughout this section, we assume that f has no zero entries. The problem of maximal number of nodal domains can be rephrased as a coloring problem on a graph. From this point of view, the question we answered in this paper is the following: using two colors, what is the maximal number of maximally connected domains of the same color, can we have on a graph?

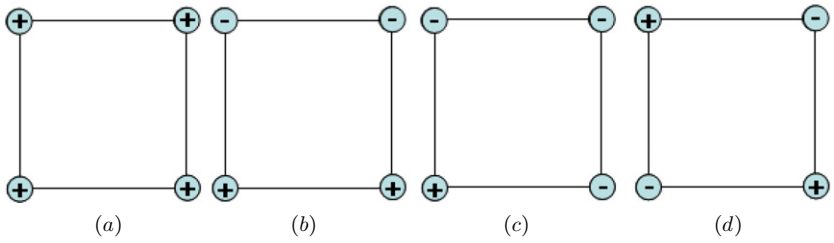

Figure 3. All possible nodal arrangements for C_4 up to trivial symmetries: (*a*) $\nu = 1$. (*b*) and (*c*) $\nu = 2$. (*d*) $\nu = 4$.

Nodal domains are of interest to physicists. However, we can generalize the question so it is applicable to an arbitrary number of colors: using k colors, what is the maximal number of maximally connected domains of the same color, can we have on a graph?

Using the same arguments, it is not hard to prove that in this case, the maximal number of nodal domains satisfies

$$\nu_G \leqslant V - \chi + k. \tag{4}$$

The question we dealt with in this paper, is only a special case of a more general question: given a graph G on V vertices, what are the numbers of nodal domains that can be supported by the graph? We only discussed the *maximal* number of nodal domains that can be supported by the graph. However, even if a graph can achieve the maximal nodal domain count, $\nu_G = V$ (i.e. it is bipartite), it is not guaranteed that it can support all the natural numbers smaller than V. For example, the cycle C_4 is bipartite, but cannot support $\nu = 3$ nodal domains (as shown in figure 3). There are non-tree graphs that can support the entire sequence $1, 2, \ldots, V$, but it is conjectured, although not yet proven, that the full sequence for the Laplacian, is only achieved by trees.

G Berkolaiko [19] showed that the nodal domain count of the nth eigenfunction f_n of the Laplacian of a graph G satisfies $\nu(f_n) \geqslant n - l$ where l is the number of edges that need to be removed from G in order to turn it into a tree (a so-called spanning tree of G). Combining Berkolaiko's result with (1) (for the highest eigenvalue) we get the following result:

$$V - l \leqslant \nu(f_V) \leqslant V - \chi + 2. \tag{5}$$

Considering the two extremes in this chain of inequalities, we end up with a graph theoretic property of any graph: $\chi \leqslant l + 2$. This can be independently shown using the following argument: let us start with a spanning tree of G, and denote it by T. As we know, T can be properly colored using two colors. Now we start adding edges to T in order to construct G. With each edge we add, the most we might need, is to add a new color. Since we need to add exactly l edges, the result follows.

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