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GRAPHS WITH FEW EIGENVALUES AND AN EXTREME NUMBER OF SPANNING TREES

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Abstract. The graphs with which we work have labeled vertices. A problem of theoretical and practical interest is to identify the graphs with n vertices and m edges that have a maximal (or minimal) number of spanning trees. It is demonstrated here that the seven known triangle-free strongly regular graphs, such as the Higman–Sims graph, are graphs with a maximum number of spanning trees among all graphs of the same order and degree; their complements are shown to have a minimum number of spanning trees. A generalization to almost regular graphs with two or three distinct eigenvalues of the Laplacian is then presented.

These results, along with several helpful heuristics, motivate us to formulate conjectures that describe the structure of the graphs having a maximum number of spanning trees in terms of a sieving process involving the traces of the Laplacian.

1. Introduction

In this paper we work with graphs that have a finite number of labeled vertices, at most one (undirected) edge between any two vertices, and no loops. By the *order* of a graph we understand the number of its vertices, and by *size* the number of its edges. Standard terminology is used and we assume that the reader is familiar with such notions as degree of a vertex, path, graph connectivity, tree and spanning tree; see [2]. The *adjacency matrix* of a graph of order n is a $n \times n$ matrix with the entry (i, j) equal to 1 if $\{i, j\}$ is an edge, and equal to 0 otherwise. For clarity we remind that a *walk* of length k (or k-walk) is a sequence of vertices and edges $v_1e_1v_2e_2 \cdots v_ke_kv_{k+1}$, where e_j is the edge joining vertices v_j and v_{j+1}. Vertices and edges may be repeated in this sequence. The walk is *closed* if $v_1 = v_{k+1}$. An *m-cycle* is a sequence of vertices and edges $v_1e_1v_2e_2 \cdots v_me_mv_{m+1}$, where all vertices v_i are distinct except for v_1 and v_{m+1} which are the same; $m \geqslant 2$. A *triangle* is a 3-cycle. A graph is said to be *tree-maximal* (respectively, *tree-minimal*) if it has a maximum (respectively, minimum) number of spanning trees among all graphs of the same order and size. We aim, as far as we can, to understand the structure of such graphs.

Denote by D the diagonal matrix with the degrees of the vertices of graph G as entries (written always in the same fixed order), by A the adjacency matrix and by $L = D - A$ the Laplacian. Recall that A^r has the number of walks of length r that start and end at vertex v_i as the i^{th} diagonal entry. Kirchhoff's theorem states that the number of spanning trees of a graph (up to sign) is equal to the determinant of any principal minor of L obtained by deleting a row and a column of L. It is an easy consequence of Kirchhoff's theorem that:

The number of spanning trees of G is equal to $\frac{1}{n+1}x_1x_2 \cdots x_n$ where $n + 1$ is the order of G and $x_1 \geqslant x_2 \geqslant x_3 \geqslant \ldots \geqslant x_n \geqslant x_{n+1}(= 0)$ are the eigenvalues of the Laplacian L of G.

For simplicity of notation we write $e_n = x_1x_2\cdots x_n$, and also write $t(G)$ for the number of spanning trees of graph G.

In spite of the fact that $t(G)$ is expressed as the determinant of (any) principal minor of the Laplacian of G, this does not easily reveal the actual graph features that optimize the number of spanning trees; embarrassingly perhaps, it is still not known whether tree-maximal graphs are found among the set of graphs whose degrees differ by at most one. [This seems intuitive since any vertex appears to initially hold equal importance in building spanning trees.]

A graph of order n and size m is called *almost regular* if its degrees differ by at most 1; when all the degrees are equal, the graph is called *regular*. It is not hard to realize that, unlike regular graphs, almost regular graphs exist for any fixed order and fixed size. In this paper, we only consider spanning tree optimization over the set of almost regular graphs. We write $g(n, d)$ for the set of almost regular graphs with n vertices in which any vertex has degree d of $d + 1$. Assume that $G^* \in g(n, d)$. In Section 2 we demonstrate that if G^* has two non-zero eigenvalues of the Laplacian and a minimum number of triangles, then G^* is tree-maximal over $g(n, d)$. In particular, as Section 3 highlights, all the triangle-free strongly regular graphs (such as the Higman–Sims or Hoffman–Singleton graphs) are tree-maximal. The same is true about the complete multipartite graph G^* whose part orders differ by at most 1; in this case G^* has three distinct eigenvalues of the Laplacian. Relying on analogous techniques of proof to those employed in Section 2, Section 4 presents results on tree-minimality. Tree-maximality results presented in this paper, along with additional evidence and heuristics, lead us to formulate specific Conjectures that describe the general structure of the tree-maximal graphs of any order and size. The Conjectures are described in Section 5.

2. Tree-maximal almost regular graphs

In this section we present and prove Theorem 4, a main result of the paper. This result allows the identification of certain classes of tree-maximal graphs over g_2. Technical details are captured in the three lemmas preceding the theorem.

We make the following definitions:

$$g_0 = \{\text{all connected graphs on } n + 1 \text{ vertices having at most } m \text{ edges}\},$$

and, for $r \geqslant 1$,

$$g_r = \{G \in g_{r-1} : (-1)^{r-1} \operatorname{Tr}(L^r) \text{ is maximal}\}.$$

Here $\operatorname{Tr}(M)$ denotes the trace of matrix M.

Evidently,

$$g_0 \supseteq g_1 \supseteq g_2 \supseteq \cdots \supseteq g_r \supseteq \cdots,$$

and g_r is *non-empty* for all $r \geqslant 0$. In words, g_0 consists of graphs with $n + 1$ vertices and at most m edges. Set g_1 consists of graphs with $n + 1$ vertices and exactly m edges. Set g_2 consists of graphs with $n + 1$ vertices that are almost regular with each vertex of degree either d or $d+1$, where d is the integral part of $\frac{2m}{n+1}$. When we want to highlight the degree d, which is often fixed, we write $g(n+1, d)$ for g_2. Our optimization approach is to impose restrictions on the traces of powers of Laplacians. This brings into focus walks and cycles. Although such constraints are quite intuitive, it may be

possible to use other bases of symmetric functions for this purpose. A promising choice may consist of a basis that highlights cycle-free graph substructures; see [8].

For fixed order $n+1$ and fixed size m our aim is to identify graphs with a maximum number of spanning trees. This is equivalent to maximizing e_n, the product of the non-zero Laplacian eigenvalues. Observe first that, by the monotonicity of the logarithm, e_n is maximal if and only if $\log e_n = \sum_{i=1}^{n} \log x_i$ is maximal. We generally prefer to work with the function $f = f(x_1, \ldots, x_n) = \sum_{i=1}^{n} \log x_i = \log e_n$. Being in g_1 assures us that the graphs have $n+1$ vertices and that $\mathrm{Tr}(L) = \sum x_i = 2m$. We maximize f subject to the constraint $\sum x_i = 2m$. By Lagrange multipliers the answer is that f is maximal if and only if all the x_i are equal to $\frac{2m}{n}$. Key issue to always raise is this: *Are there any graphs with this Laplacian eigenstructure*?

It is instructive to examine this simple case. For arbitrary m it is easy to see that this approach does not yield much information. Specifically, a graph G with this eigenstructure (that is with all x_i equal to $\frac{2m}{n}$, $1 \leqslant i \leqslant n$) exists if and only if $G = K_{n+1}$, the complete graph with $n+1$ vertices. Remarkably, this forces the number of edges m to be $m = \binom{n+1}{2}$, and the degree d to be n. [To see this, first note that L satisfies its minimum polynomial $L^2 - xL = 0$, with $x = \frac{2m}{n}$. Look at the i^{th} diagonal element of $L^2 - \frac{2m}{n}L = 0$ to conclude that the graph is in fact regular of degree $d = \frac{2m}{n} - 1$. By regularity we must also have $2m = (n+1)d$. Now $nd + d = 2m = nd + n$ yields $d = n$, forcing the graph to be complete.] The overarching conclusion is that the discreteness of the set of graphs severely limits the spectral approach, at least initially. The continuous constraint $\sum x_i = 2m$ forces the "ideal" eigenstructure with all x_i equal as sole solution, and *only the graph* K_{n+1} conforms to that.

With that out of the way, we now focus on g_2. Let $s := \min_{L \in g_1} \mathrm{Tr}(L^2)$ be the minimal value that $\mathrm{Tr}(L^2)$ takes among all graphs with $n+1$ vertices and m edges. It follows that g_2 is the set of almost regular graphs with $n+1$ vertices and m edges, with $d = 2m/(n+1)$. We thus seek to maximize $f = \sum \log x_i$ subject to constrains $\mathrm{Tr}\, L = \sum x_i = 2m$ and $\mathrm{Tr}(L^2) = \sum x_i^2 = s$. Lagrange tells us that

$$\mathrm{grad}\, f = \left(\frac{1}{x_1}, \ldots, \frac{1}{x_n}\right) = \lambda_1(1, \ldots, 1) + \lambda_2(x_1, \ldots, x_n). \tag{1}$$

This forces $\frac{1}{x_i} = \lambda_1 + \lambda_2 x_i$, for all i. The x_i are therefore roots of the quadratic $\lambda_2 x^2 + \lambda_1 x - 1 = 0$. Note that λ_2 cannot be zero, else the x_i would emerge as all equal again, and we would be in the previous case. Thus the eigenvalues x_i ($i \neq 0$) of the Laplacian L of G take *exactly two distinct values.*

For convenience we write $r = 2m$. As mentioned, s is the value of the sum of squares of degrees attained by any almost regular graph with $n+1$ vertices and m edges. Let x_1 and x_2 be the two distinct non-zero eigenvalues of L with respective multiplicities n_1 and n_2. We set $x_1 > x_2 > 0$. The constraints $n_1 x_1 + (n - n_1)x_2 = r$ and $n_1 x_1^2 + (n - n_1)x_2^2 = s$ yield, with $z = \sqrt{ns - r^2}$,

$$x_1 = \frac{r}{n} + \frac{z}{n}\sqrt{\frac{n - n_1}{n_1}} \text{ and } x_2 = \frac{r}{n} - \frac{z}{n}\sqrt{\frac{n_1}{n - n_1}}. \tag{2}$$

For fixed (n, r, s), and hence fixed z, it is not clear how many graphs with such eigenstructure exist, if any. But the above expression for x_1 and x_2 indicates that they can

be indexed by n_1; for notational ease write x for n_1. We may now write our optimizing function as $f = x\log x_1 + (n-x)\log x_2$, and view it solely as a function of x. Specifically,

$$f = x\log\left(r + \frac{(n-x)z}{\sqrt{x(n-x)}}\right) + (n-x)\log\left(r - \frac{xz}{\sqrt{x(n-x)}}\right) - n\log(n),$$

$$\text{for } 1 \leqslant x \leqslant n-1.$$

We first address a couple of technical steps.

Lemma 1. *The function f is strictly decreasing in x, $1 \leqslant x \leqslant n-1$.*

Proof. It suffices to show that f', the derivative of f with respect to x, is negative for $1 < x < n-1$. With n, r, s (and hence z) fixed, we view the roots x_1 and x_2, written explicitly in (2), as functions of x. Write $f = x\log x_1 + (n-x)\log x_2$ and differentiate with respect to x to obtain

$$f' = \log x_1 - \log x_2 + \frac{xx_1'}{x_1} + \frac{(n-x)x_2'}{x_2}.$$

We observe that $xx_1' = (n-x)x_2' = \frac{-z}{2\sqrt{x(n-x)}} = \frac{-1}{2}(x_1 - x_2)$. This yields

$$f' = \log\left(\frac{x_1}{x_2}\right) - \frac{1}{2}(x_1 - x_2)\left(\frac{1}{x_1} + \frac{1}{x_2}\right).$$

Consider now the substitution $t = t(x) = \frac{x_1 - x_2}{x_2}$, and define function $g(t) = \log(1+t) - \frac{1}{2}t(\frac{2+t}{1+t})$, for $t \geqslant 0$. Observe first that $f'(x) = g(t(x)) = g(t)$. The derivative $g'(t) = \frac{-t^2}{2(1+t^2)}$ is negative for all $t > 0$. It follows that g is a strictly decreasing function of t. Since also $g(0) = 0$, we conclude that $g(t) < 0$ for all $t > 0$. This shows that $f'(x) = g(t(x)) = g(t) < 0$, for all x, as asserted. □

Lemma 1 tells us that of two almost regular graphs, with the same order and size, and each having two distinct non-zero eigenvalues of the Laplacian, the one that has a lesser multiplicity of its larger eigenvalue has more spanning trees. To shed further clarity on how to identify the tree-maximal graphs over g_2, we examine $\mathrm{Tr}(L^3) = \sum x_i^3$. It is easy to see that $\sum x_i^3 = \mathrm{Tr}(L^3) = \sum d_i^3 + 3\sum d_i^2 - 6\Delta$, with d_i being the degrees and Δ the number of triangles in the graph. Furthermore, since the graphs are in g_2, each d_i has value either d or $d+1$. It follows that $\sum d_i^2 = s$, for all graphs in g_2. It is also equally clear that $\sum d_i^3$ takes the same fixed value for all graphs in g_2. We therefore conclude that *for any two graphs G_1 and G_2 in g_2 with Laplacians L_1 and L_2, we have $\mathrm{Tr}(L_1^3) \geqslant \mathrm{Tr}(L_2^3)$ if and only if $\Delta_1 \leqslant \Delta_2$, with the Δs indicating the respective numbers of triangles.*

For a graph in g_2 with Laplacian L and eigenvalues $x_1 > x_2$ with multiplicities $n_1 = x$ and $n_2 = n - x$, define now the function

$$c = \mathrm{Tr}(L^3) = xx_1^3 + (n-x)x_2^3.$$

Substituting the values of x_1 and x_2 we obtain

$$c = \mathrm{Tr}(L^3) = x\left(r + \frac{(n-x)z}{\sqrt{x(n-x)}}\right)^3 + (n-x)\left(r - \frac{xz}{\sqrt{x(n-x)}}\right)^3.$$

Lemma 2. *The function c is strictly decreasing in x, $1 \leqslant x \leqslant n-1$.*

Proof. Let $y = \sqrt{x(n-x)}$. The derivative of y with respect to x is $y' = \frac{n-2x}{2y}$. We may now write

$$c(x) = y^{-3}[x(ry + (n-x)z)^3 + (n-x)(ry - xz)^3].$$

Upon expanding the third powers and sorting monomials we obtain

$$c(x) = nr^3 + 3nrz^2 + 2nz^3y'.$$

It is now easy to check that the derivative c' is negative. Indeed, routine calculations yield

$$c'(x) = 2nz^3y'' = \frac{-n^3z^3}{2(\sqrt{x(n-x)})^3} < 0.$$

This verifies the fact that function c is decreasing in x. □

Using Lemmas 1 and 2 and employing a composition of bijections, along with the observation we made that $\mathrm{Tr}(L^3)$ is decreasing in the number of triangles, we may now conclude as follows.

Lemma 3. *On graphs in g_2 with two distinct eigenvalues of the Laplacian, the function f is strictly decreasing as a function of the number of triangles in the graph.*

We now state and prove a result that identifies tree-maximal graphs over g_2. Recall that $g_2 = g(n+1, d)$ consists of all graphs with $n+1$ vertices and m edges whose degrees differ by at most 1.

Theorem 4. *If a graph G^* in g_2 has two distinct non-zero eigenvalues of the Laplacian and a minimal number of triangles among all graphs in g_2, then the graph G^* is tree-maximal among all graphs in g_2. Such a graph is unique up to Laplacian cospectrality.*

Proof. Let G^* be a graph that satisfies the enunciated assumptions in the theorem. If $G \in g_2$ then $\mathrm{Tr}(L) = 2m$ and $\mathrm{Tr}(L^2) = s$, where s is the sum of squares of the degrees of G; recall that s is the same for all graphs in g_2. Insisting that G be tree-maximal over g_2 forces L to have exactly two distinct non-zero eigenvalues (by using the Lagrange multipliers argument). For arbitrary n and m typically there are no graphs like that; but, by our assumption, we have G^* in hand, which *is* like that. Our setting therefore allows such graphs to exist and, in accordance with Lagrange, we need only examine these to pick the optimal one among them. The tool employed to that purpose is Lemma 3 which tells us that, from among them, we should select a graph with a minimal number of triangles. Graph G^* is like that, and is thence tree-maximal. Uniqueness of G^* also follows from Lemma 3 since picking the smallest number of triangles identifies n_1 uniquely. Knowing n_1 determines $n - n_1$ and hence the eigenvalues x_1 and x_2 of the Laplacian uniquely. We conclude that G^* is unique up to Laplacian cospectrality. □

3. Examples of tree-maximal graphs

Theorem 4 has some instantiations worth mentioning, and we explore them in this section. It is known that a regular graph having two non-zero eigenvalues of the Laplacian is necessarily strongly regular [2]. Furthermore, a strongly regular graph is determined, up to isomorphism, by its two eigenvalues and their multiplicities.

Corollary 5. (a) *If a strongly regular graph G^* with a minimal number of triangles over g_2 exists in g_2, then G^* is tree-maximal over g_2, and it is unique up to isomorphism.*

(b) *If there exists non-regular $G^* \in g_2$ of order $n+1$ whose degrees are d or $d+1$, and G^* has two distinct non-zero eigenvalues of the Laplacian then n necessarily divides $d(d+1)$. Furthermore, if such G^* also has a minimum number of triangles, then G^* is a tree-maximal graph. Non-exhaustive examples of such graphs are the complete graphs with some parallel edges removed.*

Proof. (a) By Theorem 4 we conclude that if g_2 contains a strongly regular graph G^* that has a minimal number of triangles over g_2, then G^* is the tree-maximal graph over g_2 and is unique up to isomorphism.

(b) Let us turn now to the setting in which g_2 does not contain regular graphs. A graph in $g_2 = g(n+1, d)$ has $n+1$ vertices, m edges, with d and $d+1$ being the two distinct degrees. Let further x_1 and x_2 be the two non-zero eigenvalues of the Laplacian L of G. Denote by J the matrix with all entries 1. Then L satisfies the functional equation $(L - x_1 I)(L - x_2 I) = \frac{x_1 x_2}{n+1} J$, obtained from its minimum polynomial; see also [4, p. 33]. Write $x_1 + x_2 = p$ and $x_1 x_2 = q$. Identifying a diagonal element on both sides of this functional equation we conclude that both d and $d+1$ are roots of the quadratic $z^2 - (p-1)z + \frac{nq}{n+1} = 0$. View this as a system in p and q. It yields $\frac{q}{n+1} = \frac{d(d+1)}{n}$. Select any vertices i and j in G that are not joined by an edge. Examination of the (i, j) entry of the above functional equation yields that the number of vertices in G joined to both i and j is $\frac{q}{n+1}$, and integer, necessarily. Integrality of $\frac{q}{n+1} = \frac{d(d+1)}{n}$ forces n to divide $d(d+1)$. We shall not attempt to classify here all almost regular graphs that satisfy this arithmetic condition. It suffices to just observe that a graph G that is a complete graph with some non-intersecting (shall we say, parallel) edges removed satisfies this condition.

It is not hard to verify that a complete graph with some parallel edges removed is in fact tree-maximal among all graphs of the same order and size. □

A notable special case of Corollary 5, Part (a), are the triangle-free strongly regular graphs.

Corollary 6. *Each of the seven triangle-free strongly regular graphs is tree-maximal over the set of all regular graphs with the same number of vertices and the same degree as itself. These graphs are: the 5-cycle, the Petersen, Clebsch, Hoffman–Singleton, Gewirtz, Mesner and Higman–Sims graphs.*

Proof. Being strongly regular these graphs have exactly two non-zero Laplacian eigenvalues. Since they are triangle-free, evidently they also have a minimum number of triangles. □

The graphs in Corollary 6 have quite large symmetry groups. Notably, the index-two subgroup of the symmetry group of the Higman–Sims graph is known as the Higman–Sims group; it is one of the 26 sporadic simple groups discovered by Higman and Sims in 1968; cf. [5].

In Part (b) of Corollary 5 we mention that a complete graph with any number of parallel edges removed is tree-maximal. Such a graph is a very special case of a complete multipartite graph; specifically one in which the part orders are either 1 or 2. Allow

now for the possibility that the complete multipartite graph $G^* = K_{q,\dots,q}$, having p parts of cardinality q each, exists in g_2. The Laplacian of G^* has two non-zero eigenvalues: $x_1 = pq$ of multiplicity $p(q-1)$ and $x_2 = pq - q$ of multiplicity $p-1$. This graph is also known to have a minimal number of triangles among all graphs in g_2. By Theorem 4 it follows that graph $K_{q,\dots,q}$ is tree-maximal over the set of graphs with the same order and the same degree as itself. We take this a step further in our next theorem. Specifically, we prove the tree-maximality over g_2 of the almost regular complete multipartite graphs. These graphs have at most three distinct non-zero Laplacian eigenvalues and a minimum number of triangles over the set g_2.

Theorem 7. *A complete multipartite graph G^* whose parts have almost equal orders is tree-maximal over the set of almost regular graphs having the same order and the same degree sequence as G^*.*

Proof. Denote by G^c the complement of graph G. Look at the complement of G^*, which we denote by K; thus $K^c = G^*$. We express $K = m_1K_{d+1} + m_2K_{d+2}$ as a disjoint union of m_1 complete graphs K_{d+1} and m_2 complete graphs K_{d+2}. If K has $n+1$ vertices and m parts, then $m = m_1 + m_2$ and $n+1 = m_1(d+1) + m_2(d+2)$. Graph K is almost regular with degrees d and $d+1$. It follows that, for $d > 0$, the three non-zero eigenvalues of the Laplacian of G^* are: $n+1$ of multiplicity $m-1$; $n-d$ of multiplicity dm_1; and $n-d-1$ of multiplicity $(d+1)m_2$.

Let H be any graph with degrees d_i and Laplacian $L = (c_{ij})$. More generally, for a non-negative integer k, write $L^k = (c_{ij}^{(k)})$. When $k = 0$ we set $L^0 = I$, the identity matrix. Diagonalization of L by an orthonormal matrix and a subsequent application of the Cauchy–Schwarz inequality immediately yield $c_{ii}^{(k+1)} \cdot c_{ii}^{(k-1)} \geqslant (c_{ii}^{(k)})^2$. [Specifically, write $L = V\Lambda V^t$, with $V = (v_{ij})$ orthonormal, and $\Lambda = diag(\lambda_1, \dots, \lambda_{n+1})$. Then we have $L^k = (c_{ij}^{(k)})$, with $c_{ij}^{(k)} = \sum_{j=1}^{n+1} \lambda_j^k v_{ij}^2$. Let $w_j = v_{ij}^2$, with $\sum w_j = 1$ and $w_j \geqslant 0$. Set $a_j = \sqrt{\lambda_j^{k+1} w_j}$ and $b_j = \sqrt{\lambda_j^{k-1} w_j}$. Apply Cauchy–Schwarz to vectors $(a_1, \dots, a_{n+1})$ and $b = (b_1, \dots, b_{n+1})$ to obtain the stated inequality.] We may express this inequality by, equivalently, stating that the function $q_i(k) := c_{ii}^{(k)}/c_{ii}^{(k-1)}$ is increasing in k for any fixed i, $1 \leqslant i \leqslant n+1$. This yields

$$c_{ii}^{(k)} = q_i(k) \cdot q_i(k-1) \cdots q_i(1) \geqslant q_i(2)^{k-1} \cdot q_i(1) = (d_i+1)^{k-1} d_i,$$

since $q_i(2) = c_{ii}^{(2)}/c_{ii}^{(1)} = (d_i^2 + d_i)/d_i$, and $q_i(1) = d_i$. Take traces, by summing over i, to obtain $\mathrm{Tr}(L^k) \geqslant \sum_{i=1}^{n+1} d_i(d_i+1)^{k-1}$. This proves to be a useful lower bound.

Recall also that

$$\mathrm{Tr}(L^3) = \sum d_i^3 + 3\sum d_1^2 - 6\Delta = M + \sum d_i(d_i+1)^2,$$

where $M = \sum d_i(d_i-1) - 6\Delta$. It is well-known, and going back to Turán, that $M \geqslant 0$ for any graph H with the same number of vertices and edges as K, and $M = 0$ if and only if H is isomorphic to K.

Assume now that H is a graph of the same order and having the same degree sequence as graph K. Thus, the degrees of H are $d_i \in \{d, d+1\}$. If the eigenvalues of H are $x_1 \geqslant \cdots \geqslant x_n \geqslant x_{n+1}$, and $x_{n+1} = 0$ is the eigenvalue associated to the eigenvector $\mathbf{1}$, then the eigenvalues of H^c are $n+1-x_i$, $1 \leqslant i \leqslant n$, and 0 (associated again to $\mathbf{1}$). We attempt to maximize the number of spanning trees over the set of almost

regular graphs to which $G^* = K^c$ and H^c belong. Maximizing the number of spanning trees is equivalent to maximizing $\prod_{i=1}^{n}(n+1-x_i)$ or, by dividing to a fixed power of $n+1$, maximizing $\prod_{i=1}^{n}(1-\frac{x_i}{n+1})$. By the monotonicity of the logarithm, this is further equivalent to maximizing $\sum_{i=1}^{n}\log(1-\frac{x_i}{n+1})$. Expanding the logarithm in a power series, and subsequently sorting by traces of powers of the Laplacian, we obtain

$$\sum_{i=1}^{n}\log\left(1-\frac{x_i}{n+1}\right) = -\sum_{k\geqslant 1}\frac{\mathrm{Tr}(H^k)}{k(n+1)^k} \leqslant -\frac{M}{3(n+1)^3} + C.$$

Here we set

$$C = \sum_{k\geqslant 1}\frac{(\sum_{i=1}^{n+1} d_i(d_i+1)^{k-1})}{k(n+1)^k} = \sum_{i=1}^{n+1}\frac{d_i}{d_i+1}\log\left(1-\frac{d_i+1}{n+1}\right),$$

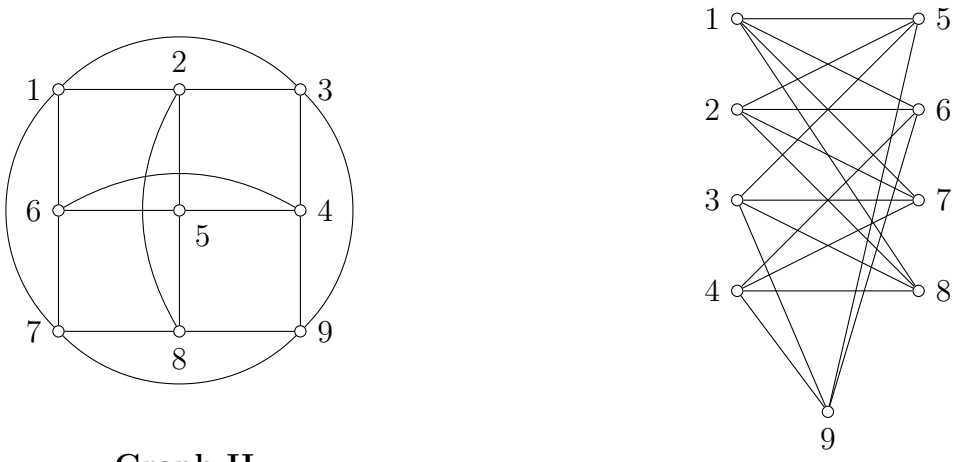
and use the trace inequalities $\mathrm{Tr}(L^k) \geqslant \sum_{i=1}^{n+1} d_i(d_i+1)^{k-1}$. There are a few final observations to make. Note that the value of C is *the same* for all graphs with $n+1$ vertices and the same (non-increasing) degree sequence as K; this is true because C is a function of degrees only. We also know that $M \geqslant 0$ and is equal to 0 if and only if the graph H is isomorphic to K. Lastly, for graph K we actually obtain the equality $\sum_{i=1}^{n}\log(1-\frac{x_i}{n+1}) = C$, justifying the statement about the tree-maximality of $K^c = G^*$. Indeed, exponentiation of both sides yields

$$\begin{aligned}
\exp\left(\sum\log\left(1-\frac{x_i}{n+1}\right)\right) &= \prod_{i=1}^{n+1}\left(1-\frac{x_i}{n+1}\right)\\
&= \left(1-\frac{d+1}{n+1}\right)^{m_1 d}\left(1-\frac{d+2}{n+1}\right)^{m_2(d+1)}\\
&= \left[\left(1-\frac{d+1}{n+1}\right)^{\frac{d}{d+1}}\right]^{m_1(d+1)}\left[\left(1-\frac{d+2}{n+1}\right)^{\frac{d+1}{d+2}}\right]^{m_2(d+2)}\\
&= \prod_{i=1}^{n+1}\left(1-\frac{d_i+1}{n+1}\right)^{\frac{d_i}{d_i+1}} = \exp C.
\end{aligned}$$

It is easy to confirm the convergence of all the series expansions involved. □

A simple example, given next, helps us understand why insistence upon having a minimum number of triangles is essential in achieving tree-maximality. We look at graphs on 9 vertices with 18 edges. The first contender is the Lattice graph H on 9 vertices of degree 4, a strongly regular graph with eigenvalues of the Laplacian 3 and 6, each of multiplicity 4. Graph H has 11664 spanning trees. It is very pleasing to the eye, in the sense that its symmetry group is of order at least 72. We do not believe any other graph in its class to be more symmetric. To top it off, H is also self-complementary! Hands down, on looks alone, it should be the winner on tree-maximality as well. However, the graph H is not tree-maximal. Consider the second contender, a graph G with 9 vertices, regular of degree 4, with edges 15, 16, 17, 18, 25, 26, 27, 28, 35, 37, 38, 39, 46, 47, 48, 49, 59, 69. G *is* the tree-maximal graph. With only 4 symmetries, it is less pleasing to the eye than H, but its number of spanning trees is 12480, exceeding that of H. Surprisingly, perhaps, graph G has six distinct non-zero eigenvalues. The key point is that G has only two triangles, while H has six. The two

graphs are displayed in the figure below. We observe that the graph feature of having a



Graph H
Strongly regular
but not tree-maximal

Graph G
Tree-maximal

FIGURE 1. Comparison of the Lattice graph H and the tree-maximal graph G.

minimum number of triangles appears to be *essential* for tree-maximal graphs over g_2. In contrast, the fact that we insist on having two distinct non-zero eigenvalues of the Laplacian in Theorem 4 is actually non-essential and is merely used as a simplifying technical assumption to establish tree-maximality in certain settings. More detailed structural conjectures regarding tree-maximality are found in Section 5.

4. Almost regular tree-minimal graphs

Let us turn our attention now to connected tree-minimal graphs in the set g_2. This section establishes a connection between the Laplacian eigenstructure of a graph and of its complement. It also relates the number of triangles in a graph and its complement, which allows us to prove Theorem 9, an analogous result to Theorem 4, describing the structure of some tree-minimal graphs. Particularly helpful is the operation of graph complementation.

Recall that we write G^c for the complement of graph G. Assume that both G and G^c are connected graphs with $n+1$ vertices; G has m edges. Write L and L^c for the Laplacians of G and G^c. First, a few helpful observations.

Lemma 8.

(a) *x_i is a non-zero eigenvalue of L if and only if $n+1-x_i$ is a non-zero eigenvalue of L^c.*
(b) *G has two non-zero eigenvalues of the Laplacian if and only if G^c does.*
(c) *G is almost regular if and only if G^c is.*
(d) *The number of triangles in G and G^c satisfies*

$$\Delta(G) + \Delta(G^c) = \binom{n+1}{3} - nm + \frac{1}{2}\sum_i (d_i(G))^2,$$

where $\Delta(H)$ denotes the number of triangles in graph H, and $d_i(H)$ is the degree of vertex v_i in H.

(e) *G has a minimal number of triangles over the set of almost regular graphs to which G belongs if and only if G^c has a maximal number of triangles over the set of almost regular graphs to which G^c belongs.*

Proof. Statement (a) is easy to see, since $L + L^c$ equals the Laplacian of the complete graph, and x_i and $n + 1 - x_i$ share the same eigenvector. Assertion (b) follows immediately from (a). Statement (c) is obvious using complementation. Assertion (d) surfaces upon coloring the edges of G red, those of G^c blue, and counting the number of monochromatic triangles in the resulting bicolored complete graph; see also [9]. Statement (e) follows immediately from (d). □

Lemma 8 shows that the Laplacian spectra, degree sequences, and the number of triangles in a graph behave well under the operation of graph complementation. This allows us to formulate a "dual" result to Theorem 4 whose conclusions shed light on tree-minimality (rather than tree-maximality).

Theorem 9. *If a connected strongly regular graph G^* with a maximal number of triangles over g_2 exists in g_2, then G^* is tree-minimal over g_2, and it is unique up to isomorphism.*

Proof. Minimizing the number of spanning trees using Lagrange multipliers, as written in (1), allows us to conclude that such a graph should also ideally have just two nonzero eigenvalues of the Laplacian. Lemmas 1, 2, and 3 are also directly applicable. The statements listed in Lemma 8, and the monotonic behavior of the number of spanning trees in the number of triangles, allows us to complete the proof. □

In particular, the complement of each of the seven triangle-free strongly regular graphs mentioned in Corollary 6 is a tree-minimal graph over the set of all graphs with the same number of vertices and the same degree as itself. Along with the infinite families of the complements of the graphs described in Corollary 5, Theorem 9 answers, in part, a question raised by Peter Sarnak and Noga Alon; see [1].

The fact that tree-maximality is intimately linked to the absence of triangles (and small cycles, more generally) is interesting and useful. Theorem 4 and its corollaries point strongly to this fact. We take a few lines here to intuitively argue why small cycles are not favored by tree-maximal graphs. Start with any tree T. We are thinking of tossing in an extra edge ϵ in T (this means keeping the vertex set the same and just drawing an extra edge) and examine what happens to the resulting number of spanning trees. The resulting graph $T \cup \epsilon$ has a unique cycle, call it C. It is immediately clear that $T \cup \epsilon$ has exactly c spanning trees, where $c = |C|$. This tells us that the shorter the cycle C is the lesser spanning trees we have. [If we could only generalize this argument to arbitrary graphs!]

Since considerable understanding of the structure of regular graphs with a minimal number of triangles exists, cf. [7] and [6], this reflects favorably in identifying infinite families of tree-maximal graphs by way of Theorem 4 and its corollaries. Large classes of such graphs are described in [6, Theorem 1.6]. A more restricted but simple construction appears also in [7]. We explain the details. Let k and l be integers such that $k > l \geqslant 0$. Start with a complete bipartite graph $K_{2k+l,2k+l}$

with vertex set $\{x_1, \ldots, x_{2k+1}\}$ and $\{y_1, \ldots, y_{2k+l}\}$. Remove an $(l+1)$-factor from the graph induced by set $\{x_1, \ldots, x_k, y_1, \ldots, y_k\}$ and an l-factor from the graph induced by $\{x_{k+1}, \ldots, x_{2k+l}, y_{k+1}, \ldots, y_{2k+l}\}$. Join $x_1, \ldots, x_k, y_1, \ldots, y_k$ to a new vertex z. Denote by $g(k,l)$ the family of graphs so obtained. An element of $g(k,l)$ is a regular graph of degree $2k$ with $4k+2l+1$ vertices. It is shown in [7, Theorem 2.1] that for $k \geqslant 2^{20}$ and $k \geqslant 2l + 6\sqrt{10l} + 1$ a graph in $g(k,l)$ is the sole graph with $4k+2l+1$ vertices of degree $2k$ having a minimal number of triangles (exactly $k(k-l-1)$ triangles) among all graphs with the same number of vertices and of the same degree. When viewed in the context of Theorem 4 and Corollary 5 above, the results contained in [6, Theorem 1.6] and [7, Theorem 2.1] provide us with infinite families of tree-maximal graphs over g_2. As has been noted, the complements of these graphs are tree-minimal.

5. Conjectures on the structure of tree-maximal graphs

A graph is said to be *tree-maximal* if it has a maximal number of spanning trees among all graphs with (at most) the same number of vertices and (at most) the same number of edges as itself. We first state the conjectures and then present evidence in their support.

Conjecture 1. *Tree-maximal graphs, among all graphs with at most $n+1$ vertices and at most m edges, are found iteratively as follows:*

g_1*: They have $n+1$ vertices and m edges.*

g_2 *: They are as in g_1 and have almost equal degrees.*

g_3 *: They are as in g_2 and have a minimum number of triangles.*

For $r \geqslant 4$,

g_r *: They are in g_{r-1} and maximize $(-1)^{r-1}\operatorname{Tr}(L^r)$, where L is the Laplacian matrix.*

After finitely many (at most $n+1$) steps, condition g_r involves only cospectral tree-maximal graphs.

Settings in which regular graphs exist might be typically easier to handle, and we reformulate the above conjecture for this case.

Conjecture 2. *Tree-maximal graphs among all graphs with at most $n+1$ vertices and at most m edges, with $d = \frac{2m}{n+1}$ an integer, are found iteratively as follows:*

g_1 *: They have $n+1$ vertices and m edges.*

g_2 *: They are as in g_1 and have all degrees equal to d.*

g_3 *: They are as in g_2 and have a minimum number of triangles.*

For $r \geqslant 4$,

g_r *: They are in g_{r-1} and minimize the number of closed r-walks.*

After finitely many (at most $n+1$) steps, condition g_r involves only cospectral tree-maximal graphs.

Evidently Conjecture 1 implies Conjecture 2.

All graphs with 9 or fewer vertices and m edges, for all possible values of m, satisfy Conjecture 1. An asymptotic heuristic, available in [3, p. 157], also points strongly in the direction of these conjectures. We outline the pertinent case briefly here. Start with an arbitrary simple graph G and ask: what is the tree-maximal graph that emerges after superimposing x copies of the complete graph on G? Clearly the resulting graphs have multiple edges between two vertices; in fact there are x or $x+1$ edges between any two distinct vertices. If the (non-zero) eigenvalues of the Laplacian of G, a simple graph on $n+1$ vertices, are $x_1, \ldots, x_n$, then the resulting graph $G + xK_{n+1}$, obtained after superimposing x copies of K_{n+1} on G, has eigenvalues $x_1 + x, \ldots, x_n + x$. The logarithm of the number of spanning trees is

$$\sum_i \log(x_i + x) = \sum_i \log\left(x\left(1 + \frac{x_i}{x}\right)\right) = c(x) + \sum_i \log\left(1 + \frac{x_i}{x}\right)$$
$$= c(x) + \sum_i \sum_{j \geqslant 0} \frac{\log^{(j)}(1)}{j!}\left(\frac{x_i}{x}\right)^j = c(x) + \sum_{j \geqslant 0}\left(\sum_i x_i^j\right)\frac{\log^{(j)}(1)}{j!}(x^{-1})^j.$$

Here $c(x)$ is a fixed function of only x. Noting that the derivatives $\log^{(j)}(1)$ alternate in sign, this describes a strategy of selecting the base graph G. At the linear level, select G such that $\sum_i x_i = \operatorname{Tr} L$ is maximal; then, at the quadratic level, make $-\sum_i x_i^2 = \operatorname{Tr}(L^2)$ maximal, and so on. This is exactly the strategy described in Conjecture 1, sans asymptotics.

Supportive are also the results in Sections 2 and 3. These results establish tree-maximal graphs over the class of graphs g_2. If condition g_3 written in Conjecture 2 can be generally established, then large families of tree-maximal graphs can be revealed by relying on the asymptotic structure of graphs with a minimal number of triangles as described in the recent paper [6]. We do actually believe that the same results are in fact true over the larger class g_0. Observe that all graphs proved tree-maximal over g_2 in Section 2 are as Conjecture 1 affirms.

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