Spectra of a new class of graphs with extremal properties

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Abstract

The class of graphs $G_D^*(n_1, n_2, ..., n_{D+1})$, consisting of $D+1$ cliques $K_{n_1}, K_{n_2}, ..., K_{n_{D+1}}$, placed on a line and fully-interconnected between neighboring cliques, contains the graph with the largest possible algebraic connectivity (second smallest eigenvalue of the Laplacian matrix) and the graph with the largest possible spectral radius (largest eigenvalue of the adjacency matrix) among all graphs with N nodes and diameter D. The spectrum of both the Laplacian and adjacency matrix of G_D^* is computed: $N-D-1$ eigenvalues are exactly known, while the remaining $D+1$ eigenvalues – among which the algebraic connectivity and spectral radius, respectively – are the zeros of an orthogonal polynomial. For the Laplacian, the coefficients of these orthogonal polynomials are exactly determined and bounds on the algebraic connectivity and spectral radius are given.

1 Introduction

Let G be a graph and let $\mathcal{N}$ denote the set of nodes and $\mathcal{L}$ the set of links, with $N = |\mathcal{N}|$ nodes and $L = |\mathcal{L}|$ links, respectively. The Laplacian matrix of G with N nodes is a $N \times N$ matrix $Q = \Delta - A$, where $\Delta = \text{diag}(d_i)$ and d_i is the degree of node $i \in \mathcal{N}$ and A is the adjacency matrix of G. The Laplacian eigenvalues are all real and nonnegative [2]. The set of all N Laplacian eigenvalues $\mu_N = 0 \leq \mu_{N-1} \leq ... \leq \mu_1$ is called the Laplacian spectrum of G. We denote the set of eigenvalues of the adjacency matrix by $\lambda_N \leq \lambda_{N-1} \leq \cdots \leq \lambda_1$, where λ_1 is called the spectral radius.

In a companion article [14], we determine, among all graphs with fixed diameter D and same number of nodes N, the largest possible second smallest eigenvalue μ_{N-1}, also called after Fiedler's seminal paper [4], the algebraic connectivity. The algebraic connectivity is the eigenvalue of the Laplacian, that is studied in most detail, because it features many interesting properties. In our investigations, a particular class of graphs with extremal properties is constructed as follows. The class of graphs $G_D^*(n_1, n_2, ..., n_{D+1})$ is composed of $D+1$ cliques $K_{n_1}, K_{n_2}, K_{n_3}, ..., K_{n_D}$ and $K_{n_{D+1}}$, where the variable $n_i \geq 1$ with $1 \leq i \leq D+1$ is the size or number of nodes of the i-th clique. Each clique K_{n_i} is fully connected with its neighboring cliques $K_{n_{i-1}}$ and $K_{n_{i+1}}$ for $2 \leq i \leq D$. Two graphs G_1 and G_2 are fully connected if each node in G_1 is connected to all the nodes in G_2. An example of a member of the class $G_D^*(n_1, n_2, ..., n_{D+1})$ is shown in Fig. 1. The total number of nodes

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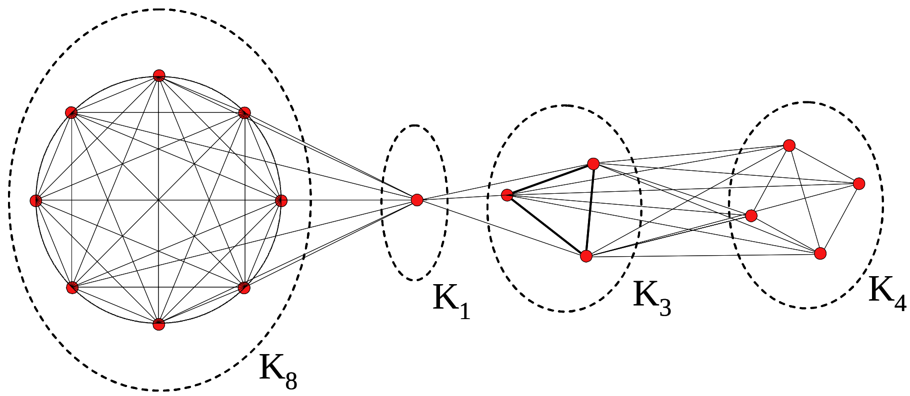

Figure 1: A chain of cliques $G_4^*(8,1,3,4)$

in $G_D^*(n_1, n_2, ..., n_{D+1})$ is

$$N = \sum_{j=1}^{D+1} n_j \tag{1}$$

The total number of links in G_D^* is

$$L = \sum_{j=1}^{D+1} \binom{n_j}{2} + \sum_{j=1}^{D} n_j n_{j+1} \tag{2}$$

where the first sum equals the number of intra-cluster links and the second the number of inter-cluster links.

The main motivation to study the class of graphs $G_D^*(n_1, n_2, ..., n_{D+1})$ with $n_j \geq 1$ are its extremal properties, that are proved elsewhere [14]:

Theorem 1 *Any graph $G(N, D)$ with N nodes and diameter D is a subgraph of at least one graph in the class $G_D^*(n_1 = 1, n_2, ..., n_D, n_{D+1} = 1)$.*

Theorem 2 *The maximum of any Laplacian eigenvalue $\mu_i(G_D^*)$, $i \in [1, N]$ achieved in the class $G_D^*(n_1 = 1, n_2, ..., n_D, n_{D+1} = 1)$ is also the maximum among all the graphs with N nodes and diameter D.*

Theorem 3 *The maximum number of links in a graph with given size N and diameter D is $L_{\max}(N, D) = \binom{N-D+2}{2} + D - 3$, which can only be obtained by either $G_D^*(1, ..., 1, n_j = N - D, 1, ..., 1)$ with $j \in [2, D]$, where only one clique has size larger than one, or by $G_D^*(1, ..., 1, n_j > 1, n_{j+1} > 1, 1, ..., 1)$ with $j \in [2, D-1]$ where only two cliques have size larger than one and they are next to each other.*

Another valuable theorem, due to Van Dam [12] and related to Theorem 3, is

Theorem 4 *The graph $G_D^*(n_1, n_2, ..., n_{D+1})$ with $n_{\left[\frac{D+1}{2}\right]} = N - D$ and all other $n_j = 1$ is the graph with largest spectral radius (i.e. largest eigenvalue of the adjacency matrix) among all graphs with a same diameter D and number of nodes N.*

Since the spectral radius is bounded by $d_{av} = \frac{2L}{N} \leq \lambda_1 \leq d_{\max}$, a combination of Theorems 3 and 4 leads to

$$N - 2D + 3 + \frac{(D-1)\,D - 4}{N} \leq \max_{G(N,D)} \lambda_1 \leq N - D + 1$$

If $D = N - 1$, we see that

$$2 - \frac{2}{N} \leq \max_{G(N,D)} \lambda_1 \leq 2$$

In this article, we show that the spectrum of the Laplacian and adjacency matrix of the graphs $G_D^*(n_1, n_2, ..., n_{D+1})$ can be computed: $N - D - 1$ eigenvalues are exactly known, while the remaining $D + 1$ eigenvalues are the zeros of an orthogonal polynomial. The focus of this article is to deduce the spectrum and to link it to a class of yet unknown orthogonal polynomials. Although there is an extensive classification being performed by Koekoek and Swarttouw [8], our set of orthogonal polynomials is not easy to classify, due to the very general parametrization. For the special case of $n_i = 1$, $G_D^*(1, 1, ..., 1)$ reduces to a simple chain or line topology, whose spectrum is completely known and thus also the related Chebyshev orthogonal polynomials. But, in general, little is known. Since our orthogonal set of polynomials are related to a graph with extremal properties, we attempt to provide as much properties as possible of this "new" general set.

Section 2 starts with the algebraic computation of the eigenvalues of the Laplacian $Q_{G_D^*}$ of the graph G_D^*, from which a recursive structure or a continued fraction pops up, that is a basic property of orthogonal polynomials, as shown in Section 3. We show that the non-trival eigenvalues of the Laplacian $Q_{G_D^*}$, including the algebraic connectivity, are the zeros of an orthogonal polynomial $p_D(\mu)$, and equivalently, of a Jacobi $(D+1) \times (D+1)$ matrix. Likewise, all eigenvalues of the adjacency matrix $A_{G_D^*}$, different from $\lambda = -1$, are the zeros of an orthogonal polynomial $w_D(\lambda + 1)$. The Jacobi matrix is computationally interesting, because the eigenvalue problem is reduced from a $N \times N$ to a $(D+1) \times (D+1)$ tri-diagonal matrix. In addition, in most practical cases, the diameter D of a graph is considerably smaller than its size N. Section 4 presents the exact coefficients of the orthogonal polynomial $p_D(\mu)$, while Section 5 gives bounds for the algebraic connectivity z_D and the largest zero z_1 of $p_D(\mu)$. The final Section 6 applies all previous deduced results for the Laplacian to the adjacency matrix.

2 Eigenvalues of the Laplacian of $G_D^*(n_1, n_2, ..., n_{D+1})$

Theorem 5 *The characteristic polynomial of the Laplacian $Q_{G_D^*}$ of $G_D^*(n_1, n_2, ..., n_{D+1})$ equals*

$$\det\left(Q_{G_D^*} - \mu I\right) = p_D(\mu) \prod_{j=1}^{D+1} (d_j + 1 - \mu)^{n_j - 1} \tag{3}$$

where $d_j = n_{j-1} + n_j + n_{j+1} - 1$ denotes the degree of a node in clique j. The polynomial $p_D(\mu) = \prod_{j=1}^{D+1} \theta_j$ is of degree $D+1$ in μ and the function $\theta_j = \theta_j(D; \mu)$ obeys the recursion

$$\theta_j = (d_j + 1 - \mu) - \left(\frac{n_{j-1}}{\theta_{j-1}} + 1\right) n_j \tag{4}$$

with initial condition $\theta_0 = 1$ and with the convention that $n_0 = n_{D+2} = 0$.

Two proofs are given of Theorem 5: an elementary one is given in Appendix B, while the proof below uses the concept of a quotient matrix (see e.g. [6]), that we first define. Consider the k-partition of a graph G that separate the node set $\mathcal{N}$ of G into $k \in [1, N]$ disjoint, non-empty subsets $\{\mathcal{N}_1, \mathcal{N}_2, ..., \mathcal{N}_k\}$. Correspondingly, the quotient matrix A^π of the adjacency matrix of G is a $k \times k$ matrix where $A^\pi_{i,j}$ is the average number of neighbors in $\mathcal{N}_j$ of nodes in $\mathcal{N}_i$. Similarly, the quotient matrix Q^π of the Laplacian matrix Q of G is a $k \times k$ matrix where

$$Q^\pi_{i,j} = \begin{cases} -A^\pi_{i,j}, \text{ if } i \neq j \\ \sum_{i \neq k} A^\pi_{i,k}, \text{ if } i = j \end{cases}$$

A partition is called regular or equitable if for all $1 \leq i, j \leq k$ the number of neighbors in $\mathcal{N}_j$ is the same for all the nodes in $\mathcal{N}_i$. The eigenvalues derived from the quotient matrix A^π (Q^π) of the adjacency A (Laplacian Q) matrix are also eigenvalues of $A(Q)$ given the partition is equitable.

Proof: The partition that separates the graph $G^*_D(n_1, n_2, ..., n_{D+1})$ into the $D+1$ cliques $K_{n_1}, K_{n_2}, ..., K_{n_{D+1}}$ is equitable. The quotient matrix Q^π of the Laplacian matrix Q of G is

$$Q^\pi = \begin{bmatrix} n_2 & -n_2 & & & & \\ -n_1 & n_1+n_3 & -n_3 & & & \\ & -n_2 & n_2+n_4 & -n_4 & & \\ & & & \ddots & & \\ & & & -n_{D-1} & n_{D-1}+n_{D+1} & -n_{D+1} \\ & & & & -n_D & n_D \end{bmatrix}$$

We apply the method of subsequent expansion using (39) to

$$\det(Q^\pi - \mu I) = \begin{bmatrix} n_2-\mu & -n_2 & & & & \\ -n_1 & n_1+n_3-\mu & -n_3 & & & \\ & -n_2 & n_2+n_4-\mu & -n_4 & & \\ & & & \ddots & & \\ & & & -n_{D-1} & n_{D-1}+n_{D+1}-\mu & -n_{D+1} \\ & & & & -n_D & n_D-\mu \end{bmatrix}$$

$$= (n_2-\mu)\det \begin{bmatrix} n_1+n_3-\mu-\frac{n_1 n_2}{n_2-\mu} & -n_3 & & & \\ -n_2 & n_2+n_4-\mu & -n_4 & & \\ & & \ddots & & \\ & & -n_{D-1} & n_{D-1}+n_{D+1}-\mu & -n_{D+1} \\ & & & -n_D & n_D-\mu \end{bmatrix}$$

We repeat the method and obtain

$$\det(Q^\pi - \mu I) = (n_2-\mu)\left(n_1+n_3-\mu-\frac{n_1 n_2}{n_2-\mu}\right) \times$$

$$\det \begin{bmatrix} n_2+n_4-\mu-\frac{n_2 n_3}{\left(n_1+n_3-\mu-\frac{n_1 n_2}{n_2-\mu}\right)} & -n_4 & & \\ & \ddots & & \\ & -n_{D-1} & n_{D-1}+n_{D+1}-\mu & -n_{D+1} \\ & & -n_D & n_D-\mu \end{bmatrix}$$

Eventually, we find

$$\det\left(Q^{\pi}-\mu I\right)=\prod_{j=1}^{D+1}\theta_j$$

where θ_j follows the recursion

$$\theta_j=\left(n_{j-1}+n_{j+1}-\lambda\right)-\frac{n_{j-1}n_j}{\theta_{j-1}}$$

with initial condition $\theta_0=1$ and with the convention that $n_0=n_{D+2}=0$. When written in terms of the degree $d_j=n_{j-1}+n_j+n_{j+1}-1$, we obtain (4).

Any two nodes s and t in a same clique K_{n_i} of G_D^* are connected to each other and they are connected to the same set of neighbors. The two rows in $\det\left(Q_{G_D^*}-\mu I\right)$ corresponding to node s and t are the same when $\mu=d_i+1$, where d_i is the degree of all nodes in clique K_{n_i}. In this case, $\det\left(Q_{G_D^*}-\mu I\right)=0$ since the rank of $Q_{G_D^*}-\mu I$ is reduced by 1. Hence, $\mu=d_i+1$ is an eigenvalue of the Laplacian matrix $Q_{G_D^*}$. The corresponding eigenvector x has only two non-zero components, $x_s=-x_t\neq 0$. Since the $D+1$ partitions of $G_D^*(n_1,n_2,...,n_{D+1})$ are equitable, the $D+1$ eigenvalues of Q^{π}, which are the roots of $\det\left(Q^{\pi}-\mu I\right)=0$, are also the eigenvalues of the Laplacian matrix $Q_{G_D^*}$. Each eigenvector of $Q_{G_D^*}$, belonging to the $D+1$ eigenvalues, has the same elements $x_s=x_t$ if the nodes s and t belong to the same clique. Hence, the Laplacian matrix $Q_{G_D^*}$ has $D+1$ nontrivial eigenvalues, which are the roots of $\det\left(Q^{\pi}-\mu I\right)=0$ and trivial eigenvalues d_j+1 with multiplicity n_j-1 for $1\leq j\leq D+1$. $\square$

Theorem 5 shows that the Laplacian $Q_{G_D^*}$ has eigenvalues at $\mu_j=n_{j-1}+n_j+n_{j+1}=d_j+1$ with multiplicity n_j-1 for $1\leq j\leq D+1$, with the convention that $n_0=n_{D+2}=0$. The less trivial zeros are solutions of the polynomial $p_D\left(\mu\right)$, where θ_j is recursively defined via (4). Thus, the polynomial of interest is

$$p_D\left(\mu\right)=\prod_{j=1}^{D+1}\theta_j\left(D;\mu\right)=\sum_{k=0}^{D+1}c_k\left(D\right)\mu^k=\prod_{k=1}^{D+1}\left(z_k-\mu\right) \tag{5}$$

where the dependence of θ_j on the diameter D and on μ is explicitly written and where the product with the non-negative zeros $z_{D+1}\leq z_D\leq\cdots\leq z_1$ follows from the definition of the eigenvalue equation (see [13, p. 435-436]). Moreover, each $z_j\in[0,N]$ because each Laplacian eigenvalue of any graph is contained in the interval $[0,N]$.

Corollary 1 *At least three Laplacian eigenvalues of G_D^*, the two smallest Laplacian eigenvalues $\mu_N=0$ and μ_{N-1} and the largest one μ_1, are equal to the zero $z_{D+1}=0$, z_D and z_1 of the polynomial $p_D\left(\mu\right)$, respectively.*

Proof: Since all the explicit Laplacian eigenvalues $\mu_j=d_j+1$ of G_D^* in (3) are larger than zero and since $\mu=0$ is an eigenvalue of any Laplacian, the polynomial $p_D\left(\mu\right)$ must have a zero at $\mu=0$. Grone and Merris [7] succeeded to improve Fiedler's lower bound and proved that, for any graph, $\mu_{N-1}\leq d_{\min}$, where $d_{\min}$ is the minimum degree in the graph. All trivial eigenvalues are larger than the minimum degree since $\mu_j=d_j+1>d_j\geq d_{\min}$, which implies that the algebraic connectivity $\mu_{N-1}=z_D$, the smallest positive zero of $p_D\left(\mu\right)$.

The largest Laplacian eigenvalue obeys $\mu_1\geq d_{\max}+1$. Brouwer and Haemers [3] further show that the equality holds if and only if there is a node connecting to all the other nodes in the graph. Hence, when the diameter $D > 2$, the largest eigenvalue is always a nontrivial eigenvalue, i.e. $\mu_1 = z_1$. When $D = 2$, the zeros of

$$p_D(\mu) = \mu\left(\mu^2 - (N + n_2)\mu + Nn_2\right) = \mu(\mu - N)(\mu - n_2)$$

are $z_3 = 0, z_2 = n_2$ and $z_1 = N$. Since the largest eigenvalue $\mu_1 \in [0, N]$, $\mu_1 = z_1$. $\square$

Since $p_D(0) = 0$, we rewrite (5) as

$$p_D(\mu) = \mu \sum_{k=0}^{D} c_{k+1}(D)\mu^k = -\mu \prod_{k=1}^{D}(z_k - \mu)$$

Our main goal is to find the smallest positive zero z_D of the polynomial

$$q_D(\mu) = \frac{p_D(\mu)}{-\mu} = -\sum_{k=0}^{D} c_{k+1}(D)\mu^k = \prod_{k=1}^{D}(z_k - \mu) \tag{6}$$

which is the algebraic connectivity $z_D = \mu_{N-1}$ of the Laplacian $Q_{G_D^*}$. Notice that all coefficients of $q_D(-\mu) = \frac{p_D(-\mu)}{\mu}$ are strict positive.

3 Orthogonal polynomials

In the sequel, we will show that $p_D(\mu)$ belongs to a set of orthogonal polynomials. We refer to Szego's classical book [11] for the beautiful theory of orthogonal polynomials.

3.1 The recursive nature of (4)

Lemma 6 *For all $j \geq 0$, the functions $\theta_j(D;x)$ are rational functions*

$$\theta_j(D;x) = \frac{t_j(D;x)}{t_{j-1}(D;x)} \tag{7}$$

where $t_j(x)$ is a polynomial of degree j in $x = -\mu$ and $t_0(D;x) = 1$.

Proof: It holds for $j = 1$ as verified from (4) because $\theta_0(D;x) = 1$. Let us assume that (4) holds for $j-1$ (induction argument). Substitution of (7) into the right hand side of (4),

$$\theta_j(D;x) = \begin{cases} \frac{(x+n_{j-1}+n_{j+1})t_{j-1}(D;x) - n_{j-1}n_j t_{j-2}(D;x)}{t_{j-1}(D;x)} & 1 \leq j \leq D \\ \frac{(x+n_D)t_D(D;x) - n_D n_{D+1} t_{D-1}(D;x)}{t_D(D;x)} & j = D+1 \end{cases}$$

indeed shows that the left hand side is of the form (7) for j. This demonstrates the induction argument and proves the lemma. $\square$

Introducing (7) into the definition (5) yields

$$p_D(-x) = \frac{\prod_{j=1}^{D+1} t_j(D;x)}{\prod_{j=1}^{D+1} t_{j-1}(D;x)} = t_{D+1}(D;x)$$

We rewrite (7) as $t_j(D;x) = \theta_j(D;x)\, t_{j-1}(D;x)$ and with (4), we obtain the set of polynomials

$$\begin{cases} t_{D+1}(D;x) = (x + n_D)\, t_D(D;x) - n_D n_{D+1} t_{D-1}(D;x) \\ t_j(D;x) = (x + n_{j-1} + n_{j+1})\, t_{j-1}(D;x) - n_{j-1} n_j t_{j-2}(D;x) \quad \text{for } 1 \leq j \leq D \\ t_1(D;x) = (x + n_2)\, t_0(D;x) \end{cases} \tag{8}$$

where $t_0(D;x) = 1$. By iterating the equation upwards, we find that

$$t_j(D;0) = \begin{cases} \displaystyle\prod_{m=2}^{j+1} n_m & 1 \le j \le D \\ 0 & j = D+1 \end{cases} \tag{9}$$

Thus, $t_{D+1}(D;0) = 0$ (and thus $\theta_{D+1}(D;0) = 0$) implies that $p_D(\mu)$ must have a zero at $\mu = 0$, which is, indeed, a general property of any Laplacian as mentioned in Corollary 1. From (7), it then follows that

$$\theta_j(D;0) = n_{j+1} > 0$$

For a fixed D, the sequence $\{t_j(D;x)\}_{0\le j\le D+1}$ is an orthogonal set of polynomials because it obeys Favard's three-term recurrence relation (see e.g. [5]). The zeros of any set of orthogonal polynomials are all simple, real and lying in the orthogonality interval $[a,b]$, which is here for the Laplacian equal to $[0,N]$. Moreover, the zeros of $t_j(D;x)$ and $t_{j-1}(D;x)$ are interlaced. In other words, in between two zeros of $t_{j-1}(D;x)$, there is precisely one zero of $t_j(D;x)$ and between two zeros of $t_j(D;x)$ there is at least one zero of $t_k(D;x)$ with $k > j$. This property shows that the set $\{t_j(D;x)\}_{0\le j\le D+1}$ is finite and cannot be extended beyond $D+1$, because the smallest zero of the highest degree polynomial $t_{D+1}(D;x)$ coincides with the lower boundary of the orthogonality interval. The special equation for $t_{D+1}(D;x)$ in (8), with n_D instead of $n_{D-1} + n_{D+1}$, guarantees this zero at $x = 0$; it is the basic difference in structure compared to the orthogonal set (33) of the corresponding adjacency matrix (see Section 6).

3.2 Jacobi Matrix of the set $\{t_j(D,x)\}_{1\le j\le D+1}$

As known in the theory of orthogonal polynomials [5], it is instructive to rewrite the j-equation in (8) as

$$x t_{j-1}(D;x) = n_{j-1}n_j t_{j-2}(D;x) - (n_{j-1} + n_{j+1}) t_{j-1}(D;x) + t_j(D;x)$$

and, in matrix form by defining the vector $\tau(D;x) = \begin{bmatrix} t_0(D;x) & t_1(D;x) & \cdots & t_{D-1}(D;x) & t_D(D;x) \end{bmatrix}^T$,

$$x \begin{bmatrix} t_0 \\ t_1 \\ \vdots \\ t_{D-1} \\ t_D \end{bmatrix} = \begin{bmatrix} -n_2 & 1 & & & \\ n_1 n_2 & -(n_1+n_3) & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & n_{D-1}n_D & -(n_{D-1}+n_{D+1}) & 1 \\ & & & n_D n_{D+1} & -n_D \end{bmatrix} \begin{bmatrix} t_0 \\ t_1 \\ \vdots \\ t_{D-1} \\ t_D \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ t_{D+1} \end{bmatrix}$$

where $t_j = t_j(D;x)$. Thus, the three-term recursion set of polynomials (8) is written in matrix form as

$$x\tau(D;x) = M\tau(D;x) + t_{D+1}(D;x)\, e_{D+1} \tag{10}$$

where the basic vector $e_{D+1} = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \end{bmatrix}^T$ and the $(D+1) \times (D+1)$ Jacobi matrix is

$$M = \begin{bmatrix} -n_2 & 1 & & & \\ n_1 n_2 & -(n_1+n_3) & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & n_{D-1}n_D & -(n_{D-1}+n_{D+1}) & 1 \\ & & & n_D n_{D+1} & -n_D \end{bmatrix} \tag{11}$$

When $x = z_k$ is a zero of $t_{D+1}(D;x) = p_D(-x)$, then (10) reduces to the eigenvalue equation

$$M\tau(D;z_k) = z_k \tau(D;z_k)$$

such that z_k is an eigenvalue of M belonging to the eigenvector $\tau(D;z_k)$. This eigenvector is never equal to the zero vector because the first component $t_0(x;D) = 1$. The special case where $z_{D+1} = 0$ leads again to (9) and all components of $\tau(D;0)$ are positive.

The quotient matrix Q^π has the same eigenvalues as the Jacobian M, such that both are also related by a similarity transform. In addition, there must be a similarity transform to make the matrix M symmetric (since all eigenvalues are real). The simplest similarity transform is $H = \text{diag}(h_1, h_2, \ldots, h_{D+1})$ such that

$$\widetilde{M} = HMH^{-1} = \begin{bmatrix} -n_2 & \frac{h_1}{h_2} & & & \\ \frac{h_2}{h_1}n_1 n_2 & -(n_1+n_3) & \frac{h_2}{h_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{h_D}{h_{D-1}}n_{D-1}n_D & -(n_{D-1}+n_{D+1}) & \frac{h_D}{h_{D+1}} \\ & & & \frac{h_{D+1}}{h_D}n_D n_{D+1} & -n_D \end{bmatrix}$$

Thus, in order to have $\widetilde{M} = \widetilde{M}^T$, we need to require that $\left(\widetilde{M}\right)_{i,i-1} = \left(\widetilde{M}\right)_{i-1,i}$ for all $2 \le i \le D+1$, implying that

$$\frac{h_i}{h_{i-1}} n_{i-1} n_i = \frac{h_{i-1}}{h_i}$$

whence,

$$\frac{h_{i-1}}{h_i} = \sqrt{n_{i-1} n_i}$$

and $h_i = \frac{1}{\sqrt{n_{i-1}n_i}} h_{i-1}$ for $2 \le i \le D+1$ and $h_1 = 1$. Thus,

$$H = \text{diag}\left(1, \frac{1}{\sqrt{n_1 n_2}}, \ldots, \frac{1}{\sqrt{n_1 n_j}\prod_{k=2}^{j-1} n_k}, \ldots, \frac{1}{\sqrt{n_1 n_{D+1}}\prod_{k=2}^{D} n_k}\right)$$

and the eigenvector belonging to zero equals $\widetilde{\tau}(D;0) = H\tau(D;0) = \begin{bmatrix} 1 & \sqrt{\frac{n_2}{n_1}} & \cdots & \sqrt{\frac{n_{D-1}}{n_1}} & \sqrt{\frac{n_D}{n_1}} \end{bmatrix}^T$.

After the similarity transform H, the result is

$$\widetilde{M} = HMH^{-1} = \begin{bmatrix} -n_2 & \sqrt{n_1 n_2} & & & \\ \sqrt{n_1 n_2} & -(n_1+n_3) & \sqrt{n_2 n_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{n_{D-1} n_D} & -(n_{D-1}+n_{D+1}) & \sqrt{n_D n_{D+1}} \\ & & & \sqrt{n_D n_{D+1}} & -n_D \end{bmatrix}$$

In summary, all non-trivial eigenvalues of $Q_{G_D^*}$ are also eigenvalues of the (much simpler and smaller) matrix $-M$ or $-\widetilde{M}$.

3.3 Deductions from the Jacobian $\widetilde{M}$

A number of consequence can be deduced. First, Gerschgorin's theorem [9] tells us that there lies a zero z_k of $p_D(x)$ centered around $n_{j-1} + n_{j+1}$ with radius $1 + n_j n_{j-1}$ or, from $-\widetilde{M}$, centered around $n_{j-1} + n_{j+1}$ with radius $\sqrt{n_j}\left(\sqrt{n_{j-1}} + \sqrt{n_{j+1}}\right)$, which leads to sharper bounds. However, not always. In particular as follows from $-M$, there lies a zero of $p_D(x)$ in the interval $[n_2 - 1, n_2 + 1]$.

A second consequence from the Jacobian symmetric matrix $-\widetilde{M}$ is the following asymptotic result

Theorem 7 *For a constant diameter D and large N, all non-trivial eigenvalues of both the adjacency and Laplacian matrix of any graph in the class $G_D^*(n_1, n_2, ..., n_D, n_{D+1})$ scale linearly with N, the number of nodes.*

Proof: Each non-trivial eigenvalue μ of the Laplacian satisfies the eigenvalue equation $-\widetilde{M}y = \mu y$, where y is the corresponding normalized eigenvector such that the Euclidian norm $y^T y = \|y\|_2^2 = 1$. We now define the rational number $\alpha_j = \frac{n_j}{N}$, for each $1 \leq j \leq D+1$. It follows from (1) and $n_j \geq 1$ that $0 < \alpha_j < 1$ and $\sum_{j=1}^{D+1} \alpha_j = 1$. The Jacobian matrix then becomes $\widetilde{M} = N.\widetilde{R}$, where

$$\widetilde{R} = \begin{bmatrix} -\alpha_2 & \sqrt{\alpha_1 \alpha_2} & & & \\ \sqrt{\alpha_1 \alpha_2} & -(\alpha_1+\alpha_3) & \sqrt{\alpha_2 \alpha_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\alpha_{D-1} \alpha_D} & -(\alpha_{D-1}+\alpha_{D+1}) & \sqrt{\alpha_D \alpha_{D+1}} \\ & & & \sqrt{\alpha_D \alpha_{D+1}} & -\alpha_D \end{bmatrix}$$

For small N, the dependence[1] of α_j on N will influence μ. For large N, on the other hand, since the norm of $\widetilde{R}$ is bounded for a constant D independent of N, and the eigenvector y is normalized, we observe from the eigenvalue equation that $\mu = -Ny^T\widetilde{R}y = N(c + o(1))$, where c is only dependent on D. This means that, for large N, the eigenvalue μ scales linearly with N. Since the argument holds as well for the adjacency matrix (see Section 6), the theorem is proved. $\square$

Combining Theorem 7 and 2 and Corollary 1 implies that, for large N, the highest possible achievable algebraic connectivity in networks $G(N, D)$ is a linear function of N, provided the diameter D is independent from N.

[1] In particular, for $n_1 = n_{D+1} = 1$, the dependence on N is obvious because $\alpha_1 = \alpha_{D+1} = \frac{1}{N}$.

Finally, we mention that the corresponding squareroot matrix B of the Gram matrix $-M = B^T B$ can be computed explicitly as

$$B = \begin{bmatrix} \sqrt{n_2} & -\sqrt{n_1} & & & \\ 0 & \sqrt{n_3} & -\sqrt{n_2} & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & \sqrt{n_{D+1}} & -\sqrt{n_D} \\ & & & 0 & 0 \end{bmatrix}$$

in contrast to the general theory of orthogonal polynomials, where each element of the squareroot matrix of a positive semi-definite Jacobi matrix is a continued fraction. Although all eigenvalues and eigenvectors of B are explicitly known, there does not seem to exist a general method to link these $\sqrt{n_j}$ eigenvalues of B to those of M (or $\widetilde{M}$).

4 Coefficients $c_k(D)$ of the polynomial $p_D(x)$

In this section, we will show that all the coefficients of the characteristic polynomial of M, i.e. the polynomial $p_D(x)$, can be exactly computed.

For $1 \le j \le D+1$, we write the polynomials as

$$t_j(D; x) = \sum_{k=0}^{j} b_k(j; D)\, x^k \tag{12}$$

and (5) relates $b_k(D+1; D) = (-1)^k c_k(D)$. Moreover, (9) shows that, for $1 \le j \le D$,

$$b_0(j; D) = \prod_{m=2}^{j+1} n_m \tag{13}$$

while $b_0(D+1; D) = 0$. Introduction of (12) into the recursive set (8) of polynomials yields, for $j = D+1$,

$$\begin{aligned} \sum_{k=0}^{D+1} b_k(D+1; D)\, x^k &= (x + n_D) \sum_{k=0}^{D} b_k(D; D)\, x^k - n_D n_{D+1} \sum_{k=0}^{D-1} b_k(D-1; D)\, x^k \\ &= \sum_{k=1}^{D+1} b_{k-1}(D; D)\, x^k + \sum_{k=0}^{D} n_D b_k(D; D)\, x^k - \sum_{k=0}^{D-1} n_D n_{D+1} b_k(D-1; D)\, x^k \\ &= n_D b_0(D; D) - n_D n_{D+1} b_0(D-1; D) + b_D(D; D)\, x^{D+1} \\ &\quad + \sum_{k=1}^{D} \{ b_{k-1}(D; D) + n_D b_k(D; D) - n_D n_{D+1} b_k(D-1; D) \}\, x^k \end{aligned}$$

After equating corresponding powers in x (higher than zero),

$$\begin{aligned} b_{D+1}(D+1; D) &= b_D(D; D) \\ b_k(D+1; D) &= b_{k-1}(D; D) + n_D b_k(D; D) - n_D n_{D+1} b_k(D-1; D) \end{aligned}$$

Similarly, we find for $1 \leq j \leq D$, that

$$\begin{aligned}
b_j(j;D) &= b_{j-1}(j-1;D) \\
b_k(j;D) &= b_{k-1}(j-1;D) + (n_{j-1}+n_{j+1})\, b_k(j-1;D) - n_{j-1}n_j b_k(j-2;D)
\end{aligned}$$

while for $j=1$, $t_1(D;x) = x + n_2$ and $t_1(D;x) = b_1(1;D)\,x + b_0(1;D)$. Thus, $b_1(1,D) = 1$, which shows that $b_j(j;D) = 1$ for all $1 \leq j \leq D+1$.

In summary, the coefficients $c_k(D) = (-1)^k b_k(D+1;D)$ of $p_D(\mu)$ obey the recursion

$$b_k(D+1;D) = b_{k-1}(D;D) + n_D b_k(D;D) - n_D n_{D+1} b_k(D-1;D) \tag{14}$$

and

$$b_k(j;D) = b_{k-1}(j-1;D) + (n_{j-1}+n_{j+1})\, b_k(j-1;D) - n_{j-1}n_j b_k(j-2;D) \tag{15}$$

for all $1 \leq j \leq D$ and $0 < k < D+1$, while $c_{D+1}(D) = (-1)^{D+1}$ and $c_0(D) = 0$. Since all zeros of $p_D(\mu)$ are real and non-negative, $b_k(D+1;D) > 0$ for all $k > 0$.

4.1 A two-term recursion for $b_k(j;D)$

Lemma 8 *The k-th coefficient $b_k(j;D)$ of the polynomial $t_j(D;x) = \sum_{k=0}^{j} b_k(j;D)\,x^k$ obeys, for $j \leq D$ and $k \geq 1$, beside the three-term recursion (15), also the two-term recursion,*

$$b_k(j;D) = \sum_{q=k}^{j} \sum_{m=k}^{q} \frac{b_{k-1}(m-1;D)}{n_q n_{q+1}} \prod_{s=m}^{j+1} n_s \tag{16}$$

Proof: We can rewrite (15) as

$$b_k(j;D) - n_{j+1} b_k(j-1;D) = b_{k-1}(j-1;D) + n_{j-1}\left\{ b_k(j-1;D) - n_j b_k(j-2;D) \right\}$$

Let

$$r_k(j;D) = b_k(j;D) - n_{j+1} b_k(j-1;D) \tag{17}$$

then the recursion equation (15) is

$$r_k(j;D) = b_{k-1}(j-1;D) + n_{j-1} r_k(j-1;D)$$

Iterating $l = j-k+1$ times until $b_{k-1}(j-l;D) = b_{k-1}(k-1;D) = 1$ yields

$$\begin{aligned}
r_k(j;D) &= b_{k-1}(j-1;D) + n_{j-1} b_{k-1}(j-2;D) + n_{j-2}n_{j-1} r_k(j-2;D) \\
&= b_{k-1}(j-1;D) + n_{j-1} b_{k-1}(j-2;D) + n_{j-2}n_{j-1} b_{k-1}(j-3;D) \\
&\quad + n_{j-3}n_{j-2}n_{j-1} r_k(j-3;D) \\
&= \cdots
\end{aligned}$$

such that

$$r_k(j;D) = \sum_{l=1}^{j-k+1} \left(\prod_{s=j+1-l}^{j-1} n_s \right) b_{k-1}(j-l;D)$$

or, with $m = j - l$,

$$r_k(j;D) = \sum_{m=k-1}^{j-1} \left(\prod_{s=m+1}^{j-1} n_s \right) b_{k-1}(m;D) \tag{18}$$

from which (or from the definition (17))

$$r_k(k;D) = b_k(k;D) - n_{j+1} b_k(k-1;D) = 1$$

Analogously, for a given $r_k(j;D)$, the definition (17) of $r_k(j;D)$ is also a recursion in $b_k(j;D)$ that can be iterated,

$$\begin{aligned}
b_k(j;D) &= r_k(j;D) + n_{j+1} b_k(j-1;D) \\
&= r_k(j;D) + n_{j+1} r_k(j-1;D) + n_{j+1} n_j b_k(j-2;D) \\
&= r_k(j;D) + n_{j+1} r_k(j-1;D) + n_{j+1} n_j r_k(j-2;D) + n_{j+1} n_j n_{j-1} b_k(j-3;D) \\
&= \cdots \\
&= \sum_{l=0}^{j-k} \left(\prod_{s=j+2-l}^{j+1} n_s \right) r_k(j-l;D)
\end{aligned}$$

Combined with (18) leads, for $j \le D$, to

$$b_k(j;D) = \sum_{l=0}^{j-k} \sum_{m=0}^{j-k-l} \left(\prod_{s=j+2-l}^{j+1} n_s \right) \left(\prod_{s=j-l-m}^{j-l-1} n_s \right) b_{k-1}(j-l-m-1;D) \tag{19}$$

With $\prod_{s=j+2-l}^{j+1} n_s \prod_{s=j-l-m}^{j-l-1} n_s = \frac{1}{n_{j-l} n_{j+1-l}} \prod_{s=j-l-m}^{j+1} n_s$, we have

$$b_k(j;D) = \sum_{l=0}^{j-k} \sum_{m=0}^{j-k-l} \frac{b_{k-1}(j-l-m-1;D)}{n_{j-l} n_{j+1-l}} \prod_{s=j-l-m}^{j+1} n_s$$

After letting $q = j - k$, we obtain a closed expression that relates, for $j \le D$, the coefficients $b_k(j;D)$ to $b_{k-1}(j;D)$,

$$b_k(j;D) = \sum_{q=k}^{j} \sum_{m=0}^{q-k} \frac{b_{k-1}(q-m-1;D)}{n_q n_{q+1}} \prod_{s=q-m}^{j+1} n_s$$

which is (16). $\square$

A number of consequences can be drawn from Lemma 8. First, relation (19) shows that, since $b_0(j;D)$ is an integer, all $b_k(j;D)$ are integers and, hence, all coefficients $c_k(D)$. Moreover, an increase in any size $n_j \ge 1$ of clique j cannot decrease $b_k(j;D)$.

Next, relation (14) is simplified with the definition (17) as

$$b_k(D+1;D) = b_{k-1}(D;D) + n_D r_k(D;D) \tag{20}$$

Introducing (18) in (20) and the convention that $\prod_{j=a}^{b} f(j) = 1$ if $a > b$ yields

$$b_k(D+1;D) = \sum_{m=k-1}^{D} \left(\prod_{s=m+1}^{D} n_s \right) b_{k-1}(m;D) \tag{21}$$

The general relation (16) immediately leads, for $k=1$ and using (13), to

$$\begin{aligned}
b_1(j;D) &= \sum_{q=1}^{j}\sum_{m=0}^{q-1}\frac{1}{n_q n_{q+1}}\prod_{s=q-m}^{j+1} n_s \prod_{k=2}^{q-m} n_k \\
&= \prod_{s=2}^{j+1} n_s \sum_{q=1}^{j}\frac{1}{n_q n_{q+1}}\sum_{m=0}^{q-1} n_{q-m}
\end{aligned}$$

Thus, for $j \le D$, we have

$$b_1(j;D) = \prod_{s=2}^{j+1} n_s \sum_{q=1}^{j}\frac{\sum_{k=1}^{q} n_k}{n_q n_{q+1}} \tag{22}$$

Using (13) in (21) yields, with (1),

$$c_1(D) = -b_1(D+1;D) = -N\prod_{m=2}^{D} n_m \tag{23}$$

From (6), it follows that

$$c_1(D) = -\prod_{k=1}^{D} z_k$$

The number of minimum spanning trees, also called the complexity $\xi(G_D^*)$, of G_D^* equals, using (23) and (3),

$$\begin{aligned}
\xi(G_D^*) &= \frac{1}{N}\prod_{j=1}^{N-1}\mu_j = \frac{1}{N}\textstyle\prod_{j=1}^{D+1}(d_j+1)^{n_j-1}\displaystyle\prod_{k=1}^{D} z_k \\
&= \textstyle\prod_{j=1}^{D+1}(d_j+1)^{n_j-1}\displaystyle\prod_{m=2}^{D} n_m
\end{aligned}$$

4.2 The general solution

Lemma 9 *The k-th coefficient $b_k(j;D)$ of the polynomial $t_j(D;x) = \sum_{k=0}^{j} b_k(j;D)\,x^k$ is, for $j \le D$ and $k \ge 1$, equal to*

$$b_k(j;D) = \prod_{s=2}^{j+1} n_s \sum_{q_{k+1}=k+1}^{j+1}\frac{1}{n_{q_{k+1}-1}n_{q_{k+1}}}\sum_{q_k=k}^{q_{k+1}-1}\frac{\left(\sum_{t=q_k}^{q_{k+1}-1} n_t\right)}{n_{q_k-1}n_{q_k}}\sum_{q_{k-1}=k-1}^{q_k-1}\frac{\left(\sum_{t=q_{k-1}}^{q_k-1} n_t\right)}{n_{q_{k-1}-1}n_{q_{k-1}}}\cdots\sum_{q_2=2}^{q_3-1}\frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1}n_{q_2}}\sum_{q_1=1}^{q_2-1} n_{q_1} \tag{24}$$

while $b_0(j;D)$ is given by (13).

Proof (by induction): The case for $k=1$, given in (22), is of the form of (24). We assume that (24) is correct and compute $b_{k+1}(j;D)$ by substituting (24) into (16),

$$b_{k+1}(j;D) = \left(\prod_{s=2}^{j+1} n_s\right)\sum_{q=k+1}^{j}\sum_{m=k+1}^{q}\frac{n_m}{n_q n_{q+1}}\sum_{q_{k+1}=k+1}^{m}\frac{1}{n_{q_{k+1}-1}n_{q_k}}\sum_{q_k=k}^{q_{k+1}-1}\frac{\left(\sum_{t=q_k}^{q_{k+1}-1} n_t\right)}{n_{q_k-1}n_{q_k}}\cdots\sum_{q_2=2}^{q_3-1}\frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1}n_{q_2}}\sum_{q_1=1}^{q_2-1} n_{q_1}$$

Reversing the m- and q_{k+1}-sum

$$b_{k+1}(j;D) = \left(\prod_{s=2}^{j+1} n_s\right)\sum_{q=k+1}^{j}\frac{1}{n_q n_{q+1}}\sum_{q_{k+1}=k+1}^{q}\frac{\sum_{m=q_{k+1}}^{q} m}{n_{q_{k+1}-1}n_{q_k}}\sum_{q_k=k}^{q_{k+1}-1}\frac{\left(\sum_{t=q_k}^{q_{k+1}-1} n_t\right)}{n_{q_k-1}n_{q_k}}\cdots\sum_{q_2=2}^{q_3-1}\frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1}n_{q_2}}\sum_{q_1=1}^{q_2-1} n_{q_1}$$

After letting $q = q_{k+2} - 1$, we verify that $b_{k+1}(j; D)$ satisfies (24) for $k+1$. The proves the lemma. $\square$

Theorem 10 *The k-th coefficient $c_k(D)$ of the polynomial $p_D(\mu)$, defined in (5), is an integer and, for $k \geq 2$, equal to*

$$(-1)^k c_k(D) = \left(\prod_{s=2}^{D} n_s\right) \sum_{q_k=k}^{D+1} \frac{\left(\sum_{t=q_k}^{D+1} n_t\right)}{n_{q_k-1} n_{q_k}} \sum_{q_{k-1}=k-1}^{q_k-1} \frac{\left(\sum_{t=q_{k-1}}^{q_k-1} n_t\right)}{n_{q_{k-1}-1} n_{q_{k-1}}} \sum_{q_{k-2}=k-2}^{q_{k-1}-1} \frac{\left(\sum_{t=q_{k-2}}^{q_{k-1}-1} n_t\right)}{n_{q_{k-2}-1} n_{q_{k-2}}} \cdots \sum_{q_2=2}^{q_3-1} \frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1} n_{q_2}} \sum_{q_1=1}^{q_2-1} n_{q_1} \tag{25}$$

while $c_0(D) = 0$ and $c_1(D)$ is given by (23).

Proof: The fact that all coefficients $c_k(D)$ are integers has been shown in Section 4.1. Introducing (24) in (21) yields

$$\begin{aligned} b_k(D+1; D) &= \left(\prod_{s=2}^{D} n_s\right) \sum_{m=k-1}^{D} \sum_{q_k=k}^{m+1} \frac{n_{m+1}}{n_{q_k-1} n_{q_k}} \sum_{q_{k-1}=k-1}^{q_k-1} \frac{\left(\sum_{t=q_{k-1}}^{q_k-1} n_t\right)}{n_{q_{k-1}-1} n_{q_{k-1}}} \cdots \sum_{q_2=2}^{q_3-1} \frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1} n_{q_2}} \sum_{q_1=1}^{q_2-1} n_{q_1} \\ &= \left(\prod_{s=2}^{D} n_s\right) \sum_{m=k}^{D+1} \sum_{q_k=k}^{m} \frac{n_m}{n_{q_k-1} n_{q_k}} \sum_{q_{k-1}=k-1}^{q_k-1} \frac{\left(\sum_{t=q_{k-1}}^{q_k-1} n_t\right)}{n_{q_{k-1}-1} n_{q_{k-1}}} \cdots \sum_{q_2=2}^{q_3-1} \frac{\left(\sum_{t=q_2}^{q_3-1} n_t\right)}{n_{q_2-1} n_{q_2}} \sum_{q_1=1}^{q_2-1} n_{q_1} \end{aligned}$$

Reversing the m- and q_k- sum leads to (25). $\square$

Theorem 10 specifies all coefficients of the characteristic polynomial of $Q_{G_D^*}$, as follows from (3). Moreover, since all coefficients of $p_D(\mu) = \mu \sum_{k=0}^{D} c_{k+1}(D) \mu^k$ are integers and $c_{D+1}(D) = (-1)^{D+1}$, $p_D(\mu)$ cannot have rational zeros, but only integer zeros and irrational zeros.

4.2.1 Case $k = D$

Although (25) also specifies $c_D(D)$, we present an alternative, simpler form. Using (1), the coefficient $c_D = (-1)^D \sum_{j=1}^{D+1} z_j = (-1)^D \text{trace}(-M)$ directly follows from the Jacobi matrix M in (11) as

$$c_D = (-1)^D (2N - n_1 - n_{D+1}) \tag{26}$$

We conclude, knowing that $z_{D+1} = 0$, that

$$\sum_{j=1}^{D} z_j = 2N - n_1 - n_{D+1}$$

Thus, the average of the zeros is

$$\overline{z} = \frac{1}{D} \sum_{j=1}^{D} z_j = \frac{2N - n_1 - n_{D+1}}{D} \tag{27}$$

which is extremal for $n_1 = n_{D+1} = 1$, given N and D.

4.2.2 Case $k = D - 1$

Recursion (14) gives, for $k = D$,

$$\begin{aligned} b_D(D+1;D) &= b_{D-1}(D;D) + n_D b_D(D;D) - n_D n_{D+1} b_D(D-1;D) \\ &= b_{D-1}(D;D) + n_D \end{aligned}$$

while (15) gives, for $j = k+1$ and $k < D$,

$$\begin{aligned} b_k(k+1;D) &= b_{k-1}(k;D) + (n_k + n_{k+2})\, b_k(k;D) - n_k n_{k+1} b_k(k-1;D) \\ &= b_{k-1}(k;D) + n_k + n_{k+2} \end{aligned}$$

Let $y[k] = b_k(k+1;D)$, then $y[0] = b_0(1;1) = n_2$ and

$$y[k] = y[k-1] + n_k + n_{k+2}$$

This difference equation[2] has the general solution

$$y[k] = b_k(k+1;D) = \sum_{j=1}^{k} n_j + \sum_{j=2}^{k+2} n_j \tag{28}$$

Turning to the case $k = D-1$, recursion (14) gives

$$\begin{aligned} b_{D-1}(D+1;D) &= b_{D-2}(D;D) + n_D b_{D-1}(D;D) - n_D n_{D+1} b_{D-1}(D-1;D) \\ &= b_{D-2}(D;D) + n_D b_{D-1}(D;D) - n_D n_{D+1} \end{aligned}$$

and with (28),

$$b_{D-1}(D+1;D) = b_{D-2}(D;D) + n_D \left(\sum_{j=1}^{D-1} n_j + \sum_{j=2}^{D} n_j \right) \tag{29}$$

The term $b_{D-2}(D;D)$ obeys the (15) for $j = k+2$ and $k \le D-2$,

$$b_k(k+2;D) = b_{k-1}(k+1;D) + (n_{k+1} + n_{k+3})\, b_k(k+1;D) - n_{k+1} n_{k+2}$$

With (28) and denoting $w[k] = b_k(k+2;D)$, we obtain

$$\begin{aligned} w[k] &= w[k-1] + (n_{k+1} + n_{k+3}) \left(\sum_{j=1}^{k} n_j + \sum_{j=2}^{k+2} n_j \right) - n_{k+1} n_{k+2} \\ &= w[k-1] + n_{k+1} \sum_{j=1}^{k} n_j + n_{k+1} \sum_{j=2}^{k+1} n_j + n_{k+3} \sum_{j=1}^{k} n_j + n_{k+3} \sum_{j=2}^{k+2} n_j \end{aligned}$$

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[2] The difference equation

$$y[k] = y[k-1] + f[k]$$

has the general solution $y[k] = y[a-1] + \sum_{j=a}^{k} f[j]$ for some integer a. Indeed, summing both sides over $a \le k \le K$ verifies the claim.

whose solution is, with $w[0] = b_0(2;D) = n_2 n_3$ by (9),

$$\begin{aligned}
w[k] &= n_2 n_3 + \sum_{j=1}^{k} n_{j+1} \sum_{q=1}^{j} n_q + \sum_{j=1}^{k} n_{j+1} \sum_{q=2}^{j+1} n_q + \sum_{j=1}^{k} n_{j+3} \sum_{q=1}^{j} n_q + \sum_{j=1}^{k} n_{j+3} \sum_{q=2}^{j+2} n_q \\
&= n_2 n_3 + \sum_{j=2}^{k+1} n_j \sum_{q=1}^{j-1} n_q + \sum_{j=2}^{k+1} n_j \sum_{q=2}^{j} n_q + \sum_{j=4}^{k+3} n_j \sum_{q=1}^{j-3} n_q + \sum_{j=4}^{k+3} n_j \sum_{q=2}^{j-1} n_q \\
&= n_2 n_3 + n_1 \left(\sum_{j=2}^{k+1} n_j + \sum_{j=4}^{k+3} n_j \right) + 2 \sum_{j=2}^{k+1} n_j \sum_{q=2}^{j-1} n_q + 2 \sum_{j=4}^{k+3} n_j \sum_{q=2}^{j-3} n_q \\
&\quad + \sum_{j=2}^{k+1} n_j^2 + \sum_{j=4}^{k+3} n_j n_{j-1} + \sum_{j=4}^{k+3} n_j n_{j-2}
\end{aligned}$$

Using this expression for $k = D-2$ into (29) yields, for $D > 1$,

$$\begin{aligned}
b_{D-1}(D+1;D) = n_2 n_3 &+ n_1 \left(\sum_{j=2}^{D-1} n_j + \sum_{j=4}^{D+1} n_j \right) + 2 \sum_{j=2}^{D-1} n_j \sum_{q=2}^{j-1} n_q + 2 \sum_{j=4}^{D+1} n_j \sum_{q=2}^{j-3} n_q \\
&+ n_D \left(\sum_{j=2}^{D-1} n_j + \sum_{j=1}^{D} n_j \right) + \sum_{j=2}^{D-1} n_j^2 + \sum_{j=4}^{D+1} n_j n_{j-1} + \sum_{j=4}^{D+1} n_j n_{j-2} \qquad (30)
\end{aligned}$$

Since $c_{D-1} = (-1)^{D-1} b_{D-1}(D+1;D)$ and $\sum_{j=1}^{D} z_j^2 = c_D^2 - 2c_{D-1}$, the variance of the zeros equals

$$\mathrm{Var}[z] = \frac{1}{D} \sum_{j=1}^{D} (z_j - \overline{z})^2 = \frac{1}{D}\left(1 - \frac{1}{D}\right) c_D^2 - \frac{2c_{D-1}}{D}$$

4.3 Explicit expressions

We end this section by listing some explicit expression. From (25) in Theorem 10, and with $N = \sum_{m=1}^{D+1} n_m$, we have

$$\begin{aligned}
c_0(D) &= 0 \\
-c_1(D) &= \left(\prod_{s=2}^{D} n_s \right) N \\
c_2(D) &= \left(\prod_{s=2}^{D} n_s \right) \sum_{q=2}^{D+1} \frac{\left(N - \sum_{k=1}^{q-1} n_k \right)}{n_{q-1} n_q} \sum_{k=1}^{q-1} n_k \\
-c_3(D) &= \left(\prod_{s=2}^{D} n_s \right) \sum_{q=3}^{D+1} \frac{\left(N - \sum_{k=1}^{q-1} n_k \right)}{n_{q-1} n_q} \sum_{i=2}^{q-1} \frac{\left(\sum_{t=i}^{q-1} n_t \right)}{n_{i-1} n_i} \sum_{k=1}^{i-1} n_k \\
c_4(D) &= \left(\prod_{s=2}^{D} n_s \right) \sum_{q=4}^{D+1} \frac{\left(N - \sum_{k=1}^{q-1} n_k \right)}{n_{q-1} n_q} \sum_{i=3}^{q-1} \frac{\sum_{t=i}^{q-1} n_t}{n_{i-1} n_i} \sum_{l=2}^{i-1} \frac{\sum_{t=l}^{i-1} n_t}{n_{l-1} n_l} \sum_{k=1}^{l-1} n_k \\
&\vdots \\
c_D &= (-1)^D (2N - n_1 - n_{D+1}) \\
c_{D+1} &= (-1)^{D+1}
\end{aligned}$$

Listing the first few polynomials $q_D(\mu)$, using (1),

$$
\begin{aligned}
q_1(\mu) &= -(\mu - N) \\
q_2(\mu) &= \mu^2 - (N + n_2)\mu + Nn_2 = (\mu - N)(\mu - n_2) \\
q_3(\mu) &= -\mu^3 + (2N - n_1 - n_4)\mu^2 - \left(n_2^2 + n_3^2 + n_1 n_2 + n_1 n_3 + n_1 n_4 + 3n_2 n_3 + n_2 n_4 + n_3 n_4\right)\mu + Nn_2 n_3 \\
q_4(\mu) &= \mu^4 - (2N - n_1 - n_5)\mu^3 \\
&\quad + \left(n_2^2 + n_3^2 + n_4^2 + n_4 n_5 + n_3(3n_4 + n_5) + n_2(3n_3 + 3n_4 + 2n_5) + n_1(n_2 + n_3 + 2n_4 + n_5)\right)\mu^2 \\
&\quad - \left(n_3 n_4(n_3 + n_4 + n_5) + n_2\left\{n_3^2 + n_4^2 + 4n_3 n_4 + (n_3 + n_4)n_5 + n_2(n_3 + n_4 + n_5)\right\}\right. \\
&\quad \left. + n_1(n_2 + n_4)(n_3 + n_4 + n_5)\right)\mu + Nn_2 n_3 n_4
\end{aligned}
$$

shows that the coefficients rapidly become involved without a simple structure. There is one exception: $G_D^*(n_1, n_2, ..., n_{D-1}, n_D, n_{D+1})$ with all unit size cliques, $n_j = 1$, is a D-hop line topology, whose spectrum is exactly known such that

$$
q_D\left(\mu; \{n_j = 1\}_{1 \le j \le D+1}\right) = \prod_{k=1}^{D}\left(2\left(1 - \cos\left(\frac{k\pi}{D+1}\right)\right) - \mu\right)
$$

5 Bounds for the smallest positive zero of $p_D(\mu)$ or $q_D(\mu)$

In this section, we present bounds of three different types deduced from: (a) the interlacing properties of zeros of orthogonal polynomials, (b) the Newton identities and (c) Rayleigh's principles of eigenvalues.

5.1 Interlacing properties of zeros of orthogonal polynomials

The general lower bound of Grone and Merris [7] for the algebraic connectivity in any graph is

$$
\mu_{N-1} \le d_{\min} = \min_{1 \le j \le D+1}(n_{i-1} + n_i + n_{i+1} - 1) \le n_2 + n_1 - 1
$$

The interlacing properties of the zeros of orthogonal polynomials imply that the smallest positive zero of $t_j(D; -\mu)$ for $D+1 \ge j > 1$, lies within $[0, n_2]$, irrespective of the value of n_1, because $t_1(x) = x + n_2$. Further, since

$$
t_2(D; x) = x^2 - (n_1 + n_2 + n_3)x + n_2 n_3
$$

with zeros

$$
x_\pm = \frac{1}{2}\left((n_1 + n_2 + n_3) \pm \sqrt{(n_1 + n_2 + n_3)^2 - 4n_2 n_3}\right)
$$

we thus find that, for all $t_j(D; x)$ with $D + 1 \ge j > 2$,

$$
z_D < \frac{1}{2}\left((n_1 + n_2 + n_3) - \sqrt{(n_1 + n_2 + n_3)^2 - 4n_2 n_3}\right) < n_2
$$

and that the largest zero $z_1 \le N$ is larger than

$$
z_1 > \frac{1}{2}\left((n_1 + n_2 + n_3) + \sqrt{(n_1 + n_2 + n_3)^2 - 4n_2 n_3}\right) > n_2
$$

Maximizing the bounds for z_D implies minimizing $(n_1+n_2+n_3)^2 - 4n_2n_3$ and, consequently, also minimizing the bounds for z_1. The sequence of increasingly sharper upper bounds for z_D can be continued for $j>2$. Indeed,

$$t_3(D;x) = -x^3 + (n_1+2n_2+n_3+n_4)\,x^2 - \left(n_1n_2+n_2^2+n_2n_3+n_1n_4+n_2n_4+n_3n_4\right)x + n_2n_3n_4$$

whose zeros can be determined by Cardano's formula.

5.2 Newton identities and Laguerre's method

The logarithmic derivative of $q_D(\mu)$ is

$$\frac{q_D^{'}(\mu)}{q_D(\mu)} = -\sum_{k=1}^{D} \frac{1}{z_k-\mu}$$

from which

$$\frac{q_D^{'}(0)}{q_D(0)} = -\sum_{k=1}^{D} \frac{1}{z_k} = \frac{c_2(D)}{c_1(D)}$$

Since $0 < z_D \le z_{D-1} \le \cdots \le z_1$, we see that

$$\frac{1}{z_D} \le -\frac{c_2(D)}{c_1(D)} = \sum_{k=1}^{D} \frac{1}{z_k} \le \frac{D}{z_D}$$

or

$$\frac{c_1(D)}{-c_2(D)} < z_D < \frac{Dc_1(D)}{-c_2(D)}$$

It seems that $z_D \approx \frac{(D+1)c_1(D)}{-2c_2(D)}$, which is the mean of the above lower and upper bounds.

We can proceed with

$$\sum_{k=1}^{D} \frac{1}{z_k^2} = \left(\frac{c_2(D)}{c_1(D)}\right)^2 - 2\left(\frac{c_3(D)}{c_1(D)}\right)$$

(and higher powers via Newton's relations (see e.g. [13, pp. 472-477])) to find closer bounds. Following Laguerre's method (see e.g. [1]), we now deduce a lower bound for the algebraic connectivity z_D. The above relation shows that

$$\frac{1}{z_D} + \sum_{k=1}^{D-1} \frac{1}{z_k} = -\frac{c_2(D)}{c_1(D)}$$

By the Cauchy-Schwarz inequality,

$$\left(\sum_{k=1}^{D-1} \frac{1}{z_k}\right)^2 \le (D-1) \sum_{k=1}^{D-1} \frac{1}{z_k^2}$$

we arrive at

$$\left(\frac{c_2(D)}{c_1(D)} + \frac{1}{z_D}\right)^2 \le (D-1)\left(\left(\frac{c_2(D)}{c_1(D)}\right)^2 - 2\left(\frac{c_3(D)}{c_1(D)}\right) - \frac{1}{z_D^2}\right)$$

or, with $y = \frac{1}{z_D}$,

$$y^2 + \frac{2}{D}\frac{c_2}{c_1}y - \left(\frac{D-2}{D}\right)\left(\frac{c_2}{c_1}\right)^2 + 2\left(\frac{D-1}{D}\right)\frac{c_3}{c_1} \le 0$$

Solving the quadratic equation yields

$$\begin{aligned}
y_{\pm} &= -\frac{c_2}{Dc_1} \pm \sqrt{\frac{1}{D^2}\left(\frac{c_2}{c_1}\right)^2 + \left(\frac{D-2}{D}\right)\left(\frac{c_2}{c_1}\right)^2 - 2\left(\frac{D-1}{D}\right)\frac{c_3}{c_1}} \\
&= -\frac{c_2}{Dc_1} \pm \sqrt{\left(1-\frac{1}{D}\right)^2\left(\frac{c_2}{c_1}\right)^2 - 2\left(\frac{D-1}{D}\right)\frac{c_3}{c_1}} \\
&= -\frac{c_2}{Dc_1} \pm \left(1-\frac{1}{D}\right)\sqrt{\left(\frac{c_2}{c_1}\right)^2 - \frac{2D}{D-1}\frac{c_3}{c_1}}
\end{aligned}$$

such that $y \in [y_-, y_+]$ and

$$z_D \geq \left(-\frac{c_2}{Dc_1} + \left(1-\frac{1}{D}\right)\sqrt{\left(\frac{c_2}{c_1}\right)^2 - \frac{2D}{D-1}\frac{c_3}{c_1}}\right)^{-1} \tag{31}$$

Again, sharper bounds can be deduced, however, by incorporating higher order coefficients c_k. Numerical computations, presented in [14], show that (31) is a fairly accurate.

5.3 Rayleigh's principle for the largest zero of $p_D(\mu)$ or $q_D(\mu)$

The Rayleigh principle [9] applied to the symmetric Jacobi matrix (11) for any vector y shows that the largest eigenvalue z_1 is bounded by

$$N \geq z_1 \geq \frac{y^T\left(-\widetilde{M}\right)y}{y^T y}$$

The common choice of the all one vector u is here inappropriate because, with $u^T u = D+1$,

$$\frac{u^T\left(-\widetilde{M}\right)u}{D+1} = \frac{(2N - n_1 - n_{D+1}) - 2\sum_{j=1}^{D}\sqrt{n_j n_{j+1}}}{D+1} < \overline{z}$$

where $\overline{z}$ is the average of the zeros (27). As shown in Section 3.2, the eigenvector $\widetilde{\tau}(D;0)$ of the symmetric matrix $\widetilde{M}$ belonging to $z_{D+1} = 0$ has all positive components (and only equal to u if all $n_j = 1$). This means that the eigenvector belonging to z_1 must have components with both signs (since eigenvectors of a symmetric matrix are orthogonal). This argument shows that the lower bound may be sharpened by considering a vector y in the Rayleigh inequality with some negative components. The choice, where the i-th vector component is $y_i = (-1)^i$ and $y^T y = D+1$, leads to a better lower bound

$$\overline{z} < \frac{y^T\left(-\widetilde{M}\right)y}{D+1} = \frac{(2N - n_1 - n_{D+1}) + 2\sum_{j=1}^{D}\sqrt{n_j n_{j+1}}}{D+1} \leq z_1$$

Notice that $u^T\left(-\widetilde{M}\right)u$ and $y^T\left(-\widetilde{M}\right)y$ are the sum of the elements and the sum of the absolute value of the elements of $-\widetilde{M}$, respectively.

6 Spectrum of the adjacency matrix

The spectrum of the adjacency matrix $A_{G_D^*}$ can be derived from its quotient matrix, since the partition that separates the graph $G_D^*(n_1, n_2, ..., n_{D+1})$ into cliques $K_{n_1}, K_{n_2}, ..., K_{n_{D+1}}$ is equitable. The corresponding quotient matrix of the adjacency matrix of G_D^*, as defined in Section 2, is

$$A^\pi = \begin{bmatrix} n_1-1 & n_2 & & & & \\ n_1 & n_2-1 & n_3 & & & \\ & n_2 & n_3-1 & n_4 & & \\ & & & \ddots & & \\ & & & n_{D-1} & n_D-1 & n_{D+1} \\ & & & & n_D & n_{D+1}-1 \end{bmatrix}$$

Using the same method and arguments as in the proof of Theorem 5, we find that the non-trivial eigenvalues of $A_{G_D^*}$ are the zeros of

$$\det\left(A^\pi - \lambda I\right) = \prod_{j=1}^{D+1} \phi_j$$

where ϕ_j follows the recursion

$$\phi_j = n_j - 1 - \lambda - \frac{n_{j-1}n_j}{\phi_{j-1}} \tag{32}$$

with initial condition $\phi_0 = 1$ and with the convention that $n_0 = n_{D+2} = 0$.

The characteristic polynomial of the adjacency matrix $A_{G_D^*}$ can be also deduced from Theorem 5. The eigenvalues of the adjacency matrix $A_{G_D^*}$, presented in Section B, are the solutions of $\det\left(A_{G_D^*} - \lambda I\right) = 0$, where

$$\det\left(A_{G_D^*} - \lambda I\right) =$$

$$\begin{bmatrix} J-xI & J_{n_1\times n_2} & & & & & & \\ J_{n_2\times n_1} & J-xI & J_{n_2\times n_3} & & & & & \\ & & & \ddots & & & & \\ & & & J_{n_i\times n_{i-1}} & J-xI & J_{n_i\times n_{i+1}} & & \\ & & & & & \ddots & & \\ & & & & & J_{n_D\times n_{D-1}} & J-xI & J_{n_D\times n_{D+1}} \\ & & & & & & J_{n_{D+1}\times n_{D+1}} & J-xI \end{bmatrix}$$

and where $x = \lambda + 1$. This determinant is equal to $(-1)^N \det\left(Q_{G_D^*} - \mu I\right)$ with $\delta_j = x$, for all $1 \le j \le D+1$. Theorem 5 shows that the characteristic polynomial of the adjacency matrix $A_{G_D^*}$ of $G_D^*(n_1, n_2, ..., n_{D+1})$ equals

$$\det\left(A_{G_D^*} - \lambda I\right) = (-1)^N w_D(x)\, x^{N-D-1}$$

where the polynomial $w_D(x) = \prod_{j=1}^{D+1} \phi_j$ is of degree $D+1$ in $x = \lambda+1$ and the function $\phi_j = \phi_j(D; x)$ obeys the recursion (32).

Clearly all eigenvalues, different from $\lambda = -1$ (or $x = 0$), are the zeros of $w_D(x)$. Similarly as for $p_D(x)$, $w_D(x)$ is also an orthogonal polynomial that obeys, with $\phi_j(x) = \frac{v_j(x)}{v_{j-1}(x)}$, the three-term recursion

$$v_j(x) = (x - n_j)\, v_{j-1}(x) - n_{j-1}n_j v_{j-2}(x) \quad \text{for } 1 \le j \le D+1 \tag{33}$$

where $v_{-1}(x) = 0$ and $v_0(x) = 1$. Thus, $w_D(x) = \prod_{j=1}^{D+1} \phi_j = v_{D+1}(x)$, whose zeros $y_{D+1} < y_D < \cdots < y_1$ are all real and simple, and lying in the orthogonality interval, which is here $[-N+2, N]$, as follows from the general properties of the adjacency spectrum after a unit-shift because $x = \lambda + 1$. The corresponding symmetrized Jacobi matrix is

$$\widetilde{A} = \begin{bmatrix} n_1 & \sqrt{n_1 n_2} & & & \\ \sqrt{n_1 n_2} & n_2 & \sqrt{n_2 n_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{n_{D-1} n_D} & n_D & \sqrt{n_D n_{D+1}} \\ & & & \sqrt{n_D n_{D+1}} & n_{D+1} \end{bmatrix}$$

The sum of all non-trivial eigenvalues is $\text{trace}\left(\widetilde{A}\right) = N$, while the product

$$\prod_{j=1}^{D+1} y_j = \det \widetilde{A} = 1_{\{D \neq 3\mathbb{N}+1\}} (-1)^{(D+1) \bmod 3} \prod_{k=1}^{D+1} n_k$$

Thus, $\det \widetilde{A} = 0$ if $D = 1, 4, 7, \ldots, 3\mathbb{N}+1$, implying that in those cases $w_D(x)$ has a zero at $x = 0$. In addition, inspite that the structure of (33) is simpler than that of (8), it turns out that finding an explicit expression for the coefficients of $w_D(x)$ is more complicated due to the lack of a two-term recursion derived in Section 4.1 for the Laplacian.

The largest eigenvalue y_1 is found by the Raileigh principle (section 5.3) applied to the non-symmetric Jacobian as Jacobian A instead of $\widetilde{A}$

$$d_{\max} + 1 = \max_{1 \leq j \leq D+1} (n_{j-1} + n_j + n_{j+1}) \geq y_1 \geq \frac{u^T A u}{D+1} = \frac{N + D + \sum_{j=1}^{D} n_j n_{j+1}}{D+1}$$

that, for small diameters D, can be better than the classical lower bound is $E[d] + 1 = \frac{2L}{N} + 1$, where the number of links is given in (2). The classical lower bound is very near to $\frac{w^T \widetilde{A} w}{w^T w}$ with $w = \begin{bmatrix} \sqrt{n_1} & \sqrt{n_2} & \cdots & \sqrt{n_{D+1}} \end{bmatrix}^T$,

$$y_1 \geq \frac{1}{N} \left(\sum_{j=1}^{D+1} n_j n_{j-1} + \sum_{j=1}^{D+1} n_j^2 + \sum_{j=1}^{D+1} n_j n_{j+1} \right)$$

The recursion (33) is simpler than the recursion (8) of the Laplacian, because of two reasons. First, the Laplacian recursion (8) had a special equation for $j = D+1$ which is crucial to establish a zero eigenvalue. As mentioned, this zero lies at the boundary of the orthogonality interval and, thus, prevents to extend that set for $j > D+1$. The set (33) has no such limitations which implies that, for all diameters D (but not constant N), the zeros of $w_D(x)$ are all interlacing (as opposed to $p_D(\mu)$ for the Laplacian)!

6.1 When $\widetilde{A}$ is bisymmetric

Numerical computations in [14] show that the largest algebraic connectivity is achieved, in most (but not in all) cases, when $G_D^*(n_1, n_2, ..., n_{D+1})$ is symmetric, $n_j = n_{D+2-j}$ for all $1 \leq j \leq D+1$.

Theorem 4 also confirms that a symmetric graph G_D^* attains the highest possible spectral radius. For the adjacency matrix, consequences of symmetry are tractable to analyse algebraically, as we will show below. Matters are more complicated for the Laplacian (mainly due to the asymmetry n_D, instead of $n_{D-1} + n_{D+1}$, in the bottom diagonal element of M (or $\widetilde{M}$) as mentioned earlier).

A matrix B is bisymmetric [10] if B is symmetric, $B = B^T$, and, in addition, persymmetric, $B = B^F$, where the flip-transpose B^F flips a matrix across its skew-diagonal (the lower-left to upper-right diagonal). Thus, a $2n \times 2n$ bisymmetric matrix B must have the block structure

$$B = \begin{bmatrix} B_1 & B_2^T \\ B_2 & B_1^F \end{bmatrix}$$

where the $n \times n$ matrix $B_1 = B_1^T$ is symmetric and $B_2 = B_2^F$ is persymmetric. Reid [10] shows that the eigenvalues of B are the eigenvalues of $B_1 + RB_2$ and $B_1 - RB_2$, where the matrix R has all ones on the skew-diagonal and zeros elsewhere. Also, $R = R^T$ and $B^F = RB^T R$. In addition, if y is an eigenvector of $B_1 + RB_2$, then $[y, Ry]^T$ is an eigenvector of B belonging to the same eigenvalue. Likewise, if w is an eigenvector of $B_1 - RB_2$, then $[-w, Rw]^T$ is an eigenvector of B belonging to the same eigenvalue.

Let $D = 2m - 1$, then the $2m \times 2m$ matrix $\widetilde{A}$ is bisymmetric if $n_j = n_{D+2-j}$ for all $1 \leq j \leq D + 1$ such that

$$\widetilde{A}_{2m\times 2m} = \begin{bmatrix} \widetilde{A}_{m\times m} & n_m e_m e_1^T \\ n_m e_1 e_m^T & \widetilde{A}^F_{m\times m} \end{bmatrix}$$

The eigenvalues of $\widetilde{A}_{2m\times 2m}$ are those of the matrix $T_\pm = \widetilde{A}_{m\times m} \pm n_m R e_1 e_m^T$. Since $Re_1 e_m^T = e_m e_m^T$ is the zero matrix with element $O_{mm} = 1$, we have explicitly that

$$T_\pm = \begin{bmatrix} n_1 & \sqrt{n_1 n_2} & & & \\ \sqrt{n_1 n_2} & n_2 & \sqrt{n_2 n_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{n_{m-2} n_{m-1}} & n_{m-1} & \sqrt{n_{m-1} n_m} \\ & & & \sqrt{n_{m-1} n_m} & n_m \pm n_m \end{bmatrix}$$

Thus,

$$\det (T_\pm - xI) = \begin{vmatrix} n_1 - x & \sqrt{n_1 n_2} & & & \\ \sqrt{n_1 n_2} & n_2 - x & \sqrt{n_2 n_3} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{n_{m-2} n_{m-1}} & n_{m-1} - x & \sqrt{n_{m-1} n_m} \\ & & & \sqrt{n_{m-1} n_m} & n_m - x \pm n_m \end{vmatrix}$$

We expand the determinant in cofactors of the last row

$$\det (T_\pm - xI) = -\sqrt{n_{m-1} n_m} \text{cofactor}_{m;m-1} T_\pm + (n_m - x \pm n_m) \text{cofactor}_{m;m} T_\pm$$

The first cofactor is

$$\begin{aligned} -\sqrt{n_{m-1} n_m} \text{cofactor}_{m;m-1} T_\pm &= -\sqrt{n_{m-1} n_m} \text{cofactor}_{m;m-1} \widetilde{A}_{m\times m} \\ &= -n_{m-1} n_m \det \left(\widetilde{A}_{(m-2)\times(m-2)} - xI \right) \end{aligned}$$

and the second is

$$
\begin{aligned}
(n_m - x \pm n_m)\,\mathrm{cofactor}_{m;m} T_{\pm} &= (n_m - x \pm n_m)\,\mathrm{cofactor}_{m;m} \widetilde{A}_{m\times m} \\
&= (n_m - x \pm n_m)\det\left(\widetilde{A}_{(m-1)\times(m-1)} - xI\right)
\end{aligned}
$$

Since

$$
\det\left(\widetilde{A}_{m\times m} - xI\right) = -\sqrt{n_{m-1}n_m}\mathrm{cofactor}_{m;m-1}\widetilde{A}_{m\times m} + (n_m - x)\,\mathrm{cofactor}_{m;m}\widetilde{A}_{m\times m}
$$

we obtain

$$
\det(T_{\pm} - xI) = \det\left(\widetilde{A}_{m\times m} - xI\right) \pm n_m \det\left(\widetilde{A}_{(m-1)\times(m-1)} - xI\right)
$$

Reid's theorem states that

$$
\det\left(\widetilde{A}_{2m\times 2m} - xI\right) = \det\left((T_-)_{m\times m} - xI\right)\det\left((T_+)_{m\times m} - xI\right)
$$

which leads to a relation for the "bisymmetric" orthogonal polynomials, denoted by $w^*_m(x)$, in terms of $v_m(x)$,

$$
\begin{aligned}
w^*_{2m}(x) &= (v_m(x) - n_m v_{m-1}(x))\,(v_m(x) + n_m v_{m-1}(x)) \\
&= v_m^2(x) - n_m^2 v_{m-1}^2(x)
\end{aligned}
\tag{34}
$$

In case of a bisymmetric Laplacian, the corresponding $\det(T_{\pm} - xI)$ cannot be rewritten solely in terms of $\det\left(\widetilde{M}_{m\times m} - xI\right)$, but Reid's theorem still tells us that the bisymmetric orthogonal polynomial $p^*_{2m}(x)$ can be factorized into two polynomials of degree m.

7 Conclusion

The Laplacian spectrum of the class $G^*_D(n_1, n_2, ..., n_{D+1})$ with extremal eigenvalue properties is computed and shown to be related to orthogonal polynomials. Afterall, it is not so surprising to see orthogonal polynomials appearing because of the block tri-diagonal structure of either the adjacency $A_{G^*_D}$ or Laplacian $Q_{G^*_D}$ matrix. Moreover, orthogonal polynomials are often optimizers of problems.

Although a first step is made, we believe that still more properties may be discovered such as spacing and other properties of the zeros of $p_D(\mu)$ and of $w_D(x)$. More fundamentally, the numerically observed fact that a bi-symmetric Jacobian [10], where $n_j = n_{D+2-j}$, almost always provides the largest possible algebraic connectivity is still open to prove rigorously. In some cases, though, small deviations from symmetry occur, that, at first glance, are unusual because they lead to an asymmetric graph G^*_D.

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A Results from linear algebra

If

$$X_{m\times m} = (J - (\lambda+1)\, I)_{m\times m} \tag{35}$$

then the inverse matrix of X is

$$X^{-1} = -\frac{1}{(\lambda+1)(\lambda+1-m)}\,(J + (\lambda+1-m)\, I)_{m\times m} \tag{36}$$

We now compute

$$\begin{aligned} Y &= J_{(N-m)\times m} X^{-1}_{m\times m} J_{m\times(N-m)} \\ &= -\frac{1}{(\lambda+1)(\lambda+1-m)} J_{(N-m)\times m} \left(J_{m\times m} + (\lambda+1-m)\, I_{m\times m}\right) J_{m\times(N-m)} \end{aligned}$$

Using $J_{k\times n} J_{n\times l} = n J_{k\times l}$ gives

$$\begin{aligned} Y &= -\frac{1}{(\lambda+1)(\lambda+1-m)} \left(m J_{(N-m)\times m} + (\lambda+1-m)\, J_{(N-m)\times m}\right) J_{m\times(N-m)} \\ &= -\frac{1}{(\lambda+1)(\lambda+1-m)} \left(m^2 J_{(N-m)\times(N-m)} + m\,(\lambda+1-m)\, J_{(N-m)\times(N-m)}\right) \end{aligned}$$

whence

$$Y = -\frac{m}{(\lambda+1-m)} J_{(N-m)\times(N-m)} \tag{37}$$

Finally, it is shown in [13, p. 481] that,

$$\det (J - xI)_{n\times n} = (-1)^n x^{n-1}\,(x-n) \tag{38}$$

and we will need [9]

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det A \det \left(D - CA^{-1}B\right) \tag{39}$$

where $D - CA^{-1}B$ is called the Schur complement of A.

B Second proof of Theorem 5

The adjacency matrix of $G_D^*(n_1, n_2, ..., n_{D+1})$ is

$$A_{G_D^*} = \begin{bmatrix} \widetilde{J}_{n_1\times n_1} & J_{n_1\times n_2} & & & & & & \\ J_{n_2\times n_1} & \widetilde{J}_{n_2\times n_2} & J_{n_2\times n_3} & & & & & \\ & & & \ddots & & & & \\ & & & J_{n_i\times n_{i-1}} & \widetilde{J}_{n_i\times n_i} & J_{n_i\times n_{i+1}} & & \\ & & & & & \ddots & & \\ & & & & & J_{n_D\times n_{D-1}} & \widetilde{J}_{n_D\times n_D} & J_{n_D\times n_{D+1}} \\ & & & & & & J_{n_{D+1}\times n_{D+1}} & \widetilde{J}_{n_{D+1}\times n_{D+1}} \end{bmatrix}$$

where $\widetilde{J} = J - I$. The eigenvalues of corresponding Laplacian $Q_{G_D^*} = \Delta_{G_D^*} - A_{G_D^*}$ are the solutions of $\det\left(Q_{G_D^*} - \mu I\right) = 0$, where

$$\det\left(Q_{G_D^*} - \mu I\right) =$$
$$\begin{bmatrix} \delta_1 I - J & -J_{n_1\times n_2} & & & & & & \\ -J_{n_2\times n_1} & \delta_2 I - J & -J_{n_2\times n_3} & & & & & \\ & & & \ddots & & & & \\ & & & -J_{n_i\times n_{i-1}} & \delta_i I - J & -J_{n_i\times n_{i+1}} & & \\ & & & & & \ddots & & \\ & & & & & -J_{n_D\times n_{D-1}} & \delta_D I - J & -J_{n_D\times n_{D+1}} \\ & & & & & & -J_{n_{D+1}\times n_{D+1}} & \delta_{D+1} I - J \end{bmatrix}$$

where we have defined

$$\begin{aligned} \delta_1 &= n_1 + n_2 - \mu \\ \delta_i &= n_{i-1} + n_i + n_{i+1} - \mu \text{ for } i \in [2, D] \\ \delta_{D+1} &= n_D + n_{D+1} - \mu \end{aligned}$$

The dimensions of the block diagonal matrix are $n_i \times n_i$ (and omitted to make the matrix fit on the page). Clearly, the degree d_i of a node in clique i equals δ_i when $\mu = 1$. The submatrix of $Q_{G_D^*} - \mu I$ consisting of the last $D + 2 - j$ block rows and block columns is denoted by T_j; thus, T_j is the right bottom $\sum_{i=j}^{D+1} n_i \times \sum_{i=j}^{D+1} n_i$ sub-matrix of $Q_{G_D^*} - \mu I$, where $1 \le j \le D + 1$ and $T_1 = Q_{G_D^*} - \mu I$.

Applying (39) yields

$$\det T_1 = \det\left(\delta_1 I - J_{n_1\times n_1}\right)\det\left(T_2 - \begin{bmatrix} J_{n_2\times n_1} \\ 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times n_1}\end{bmatrix}\left(\delta_1 I - J_{n_1\times n_1}\right)^{-1}\begin{bmatrix} J_{n_2\times n_1} \\ 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times n_1}\end{bmatrix}^T\right)$$

$$= \det\left(\delta_1 I - J_{n_1\times n_1}\right)\det\left(T_2 - \begin{bmatrix} J_{n_2\times n_1}\left(\delta_1 I - J_{n_1\times n_1}\right)^{-1} J_{n_1\times n_2} & 0_{n_2\times\left(\sum_{i=3}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times n_2} & 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times\left(\sum_{i=3}^{i=D+1} n_i\right)}\end{bmatrix}\right)$$

Using (35) and (37) results in

$$J_{n_2\times n_1}\left(\delta_1 I - J_{n_1\times n_1}\right)^{-1} J_{n_1\times n_2} = \frac{n_1}{\delta_1 - n_1} J_{n_2\times n_2}$$

while application of (38) yields

$$\det\left(\delta_1 I - J_{n_1\times n_1}\right) = \delta_1^{n_1-1}\left(\delta_1 - n_1\right)$$

Thus, with the definition

$$\theta_1 = \delta_1 - n_1$$

we obtain

$$\det T_1 = \delta_1^{n_1-1}\theta_1 \det\widetilde{T}_2$$

where

$$\widetilde{T}_2 = T_2 - \begin{bmatrix} \frac{n_1}{\theta_1} J_{n_2\times n_2} & 0_{n_2\times\left(\sum_{i=3}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times n_2} & 0_{\left(\sum_{i=3}^{i=D+1} n_i\right)\times\left(\sum_{i=3}^{i=D+1} n_i\right)}\end{bmatrix}$$

We observe that the matrix at the right hand side has the same structure as that of T_2, except that the first block row and block column is now $\delta_2 I - \left(1 + \frac{n_1}{\theta_1}\right) J_{n_2\times n_2} = \delta_2 I - \frac{\delta_1}{\delta_1 - n_1} J_{n_2\times n_2}$. We apply the same operations on

$$\det\widetilde{T}_2 = \det\left(\delta_2 I - \frac{\delta_1}{\delta_1 - n_1} J_{n_2\times n_2}\right)\times$$

$$\det\left(T_3 - \begin{bmatrix} J_{n_3\times n_2} \\ 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times n_2}\end{bmatrix}\left(\delta_2 I - \frac{\delta_1}{\delta_1 - n_1} J_{n_2\times n_2}\right)^{-1}\begin{bmatrix} J_{n_3\times n_2} \\ 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times n_2}\end{bmatrix}^T\right)$$

$$= \delta_2^{n_2-1}\left(\delta_2 - \frac{\delta_1 n_2}{\delta_1 - n_1}\right)\det\left(T_3 - \begin{bmatrix} \frac{n_2}{\delta_2 - \frac{\delta_1 n_2}{\delta_1 - n_1}} J_{n_3\times n_3} & 0_{n_3\times\left(\sum_{i=4}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times n_3} & 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times\left(\sum_{i=4}^{i=D+1} n_i\right)}\end{bmatrix}\right)$$

$$= \delta_2^{n_2-1}\theta_2 \det\left(T_3 - \begin{bmatrix} \frac{n_2}{\theta_2} J_{n_3\times n_3} & 0_{n_3\times\left(\sum_{i=4}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times n_3} & 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times\left(\sum_{i=4}^{i=D+1} n_i\right)}\end{bmatrix}\right)$$

where $\theta_2 = \delta_2 - \frac{\delta_1 n_2}{\delta_1 - n_1} = \delta_2 - \left(\frac{n_1}{\theta_1} + 1\right) n_2$. Since the matrix

$$\widetilde{T}_3 = T_3 - \begin{bmatrix} \frac{n_2}{\theta_2} J_{n_3\times n_3} & 0_{n_3\times\left(\sum_{i=4}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times n_3} & 0_{\left(\sum_{i=4}^{i=D+1} n_i\right)\times\left(\sum_{i=4}^{i=D+1} n_i\right)}\end{bmatrix}$$

again possesses a similar structure, we claim that

$$\widetilde{T}_j = T_j - \begin{bmatrix} \frac{n_{j-1}}{\theta_{j-1}} J_{n_j \times n_j} & 0_{n_j \times \left(\sum_{i=j+1}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=j+1}^{i=D+1} n_i\right) \times n_j} & 0_{\left(\sum_{i=j+1}^{i=D+1} n_i\right) \times \left(\sum_{i=j+1}^{i=D+1} n_i\right)} \end{bmatrix} \tag{40}$$

obeys the recursion

$$\det \widetilde{T}_j = \delta_j^{n_j - 1} \theta_j \det \widetilde{T}_{j+1} \tag{41}$$

where θ_j is defined by the recursion (4) with the convention that $n_0 = 0$ and $\theta_0 = 1$, because $\theta_1 = \delta_1 - n_1$.

We have shown that (40), (41) and (4) hold for $j = 1$ and $j = 2$. Assuming that (40) holds for $j + 1$ (induction argument), we compute $\det \widetilde{T}_{j+1}$ similarly,

$$\begin{aligned}
\det \widetilde{T}_{j+1} = \det &\left(\delta_{j+1} I - \left(\frac{n_j}{\theta_j} + 1 \right) J_{n_{j+1} \times n_{j+1}} \right) \times \\
&\det \left(T_{j+2} - \begin{bmatrix} J_{n_{j+2} \times n_{j+1}} \\ 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times n_{j+1}} \end{bmatrix} \left(\delta_{j+1} I - \left(\frac{n_j}{\theta_j} + 1 \right) J_{n_{j+1} \times n_{j+1}} \right)^{-1} \times \begin{bmatrix} J_{n_{j+2} \times n_{j+1}} \\ 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times n_{j+1}} \end{bmatrix}^T \right) \\
&= \delta_{j+1}^{n_j} \left(\delta_{j+1} - \left(\frac{n_j}{\theta_j} + 1 \right) n_{j+1} \right) \\
&\quad \times \det \left(T_{j+2} - \begin{bmatrix} \frac{n_{j+1}}{\delta_{j+1} - \left(\frac{n_j}{\theta_j} + 1 \right) n_{j+1}} J_{n_{j+2} \times n_{j+2}} & 0_{n_{j+2} \times \left(\sum_{i=j+3}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times n_{j+2}} & 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times \left(\sum_{i=j+3}^{i=D+1} n_i\right)} \end{bmatrix} \right) \\
&= \delta_{j+1}^{n_j} \theta_{j+1} \det \left(T_{j+2} - \begin{bmatrix} \frac{n_{j+1}}{\theta_{j+1}} J_{n_{j+2} \times n_{j+2}} & 0_{n_{j+2} \times \left(\sum_{i=j+3}^{i=D+1} n_i\right)} \\ 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times n_{j+2}} & 0_{\left(\sum_{i=j+3}^{i=D+1} n_i\right) \times \left(\sum_{i=j+3}^{i=D+1} n_i\right)} \end{bmatrix} \right)
\end{aligned}$$

where $\theta_{j+1} = \delta_{j+1} - \left(\frac{n_j}{\theta_j} + 1 \right) n_{j+1}$. Hence, (40) holds for $j + 2$ and the recursion (41) are (4) are followed. By induction, (40), (41) and (4) hold for any $1 \leq j \leq D + 1$. But,

$$\begin{aligned}
\widetilde{T}_{D+1} &= T_{D+1} - \frac{n_D}{\theta_D} J_{n_{D+1} \times n_{D+1}} \\
&= \delta_{D+1} I - \left(1 + \frac{n_D}{\theta_D} \right) J_{n_{D+1} \times n_{D+1}}
\end{aligned}$$

such that, with (38),

$$\det \widetilde{T}_{D+1} = \delta_{D+1}^{n_{D+1} - 1} \left(\delta_{D+1} - \left(1 + \frac{n_D}{\theta_D} \right) n_{D+1} \right) = \delta_{D+1}^{n_{D+1} - 1} \theta_{D+1}$$

Iterating (41) back finally yields

$$\det \left(Q_{G_D^*} - \mu I \right) = \prod_{j=1}^{D+1} \delta_j^{n_j - 1} \prod_{j=1}^{D+1} \theta_j$$

which is (3).