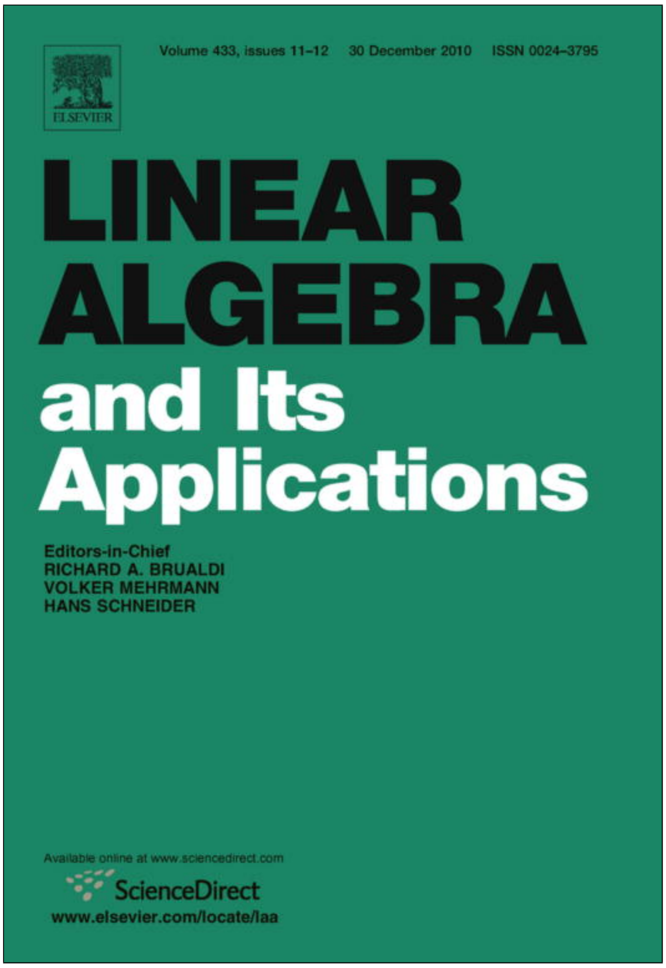
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Graphs with given diameter maximizing the algebraic connectivity

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ABSTRACT

We propose a class of graphs $G^*_D(n_1, n_2, \ldots, n_{D+1})$, containing of a chain of $D+1$ cliques $K_{n_1}, K_{n_2}, \ldots, K_{n_{D+1}}$, where neighboring cliques are fully-interconnected. The class of graphs has diameter D and size $N = \sum_{1 \leqslant i \leqslant D+1} n_i$. We prove that this class of graphs can achieve the maximal number of links, the minimum average hopcount, and more interestingly, the maximal of any Laplacian eigenvalue among all graphs with N nodes and diameter D. The algebraic connectivity is the eigenvalue of the Laplacian that has been studied most, because it features many interesting properties. We determine the graph with the largest algebraic connectivity among graphs with N nodes and diameter $D \leqslant 4$. For other diameters, numerically searching for the maximum of any eigenvalue is feasible, because (a) the searching space within the class $G^*_D(n_1, n_2, \ldots, n_{D+1})$ is much smaller than within all graphs with N nodes and diameter D; (b) we reduce the calculation of the Laplacian spectrum from a $N \times N$ to a $(D+1) \times (D+1)$ matrix.
The maximum of any Laplacian eigenvalue obtained either theoretically or by numerical searching is applied to (1) investigate the topological features of graphs that maximize different Laplacian eigenvalues; (2) study the correlation between the maximum algebraic connectivity $a_{\max}(N, D)$ and N as well as D and (3) evaluate two upper bounds of the algebraic connectivity that are proposed in the literature.

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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 [1]. The set of all N Laplacian eigenvalues $\mu_N = 0 \leqslant \mu_{N-1} \leqslant \cdots \leqslant \mu_1$ is called the Laplacian spectrum of G.

The second smallest eigenvalue μ_{N-1}, also called after Fiedler's seminal paper [2], the algebraic connectivity, can be denoted as $\mu_{N-1} = a(G)$ for simplicity. The algebraic connectivity $a(G)$ is widely studied in the literature due to (a) its importance for the connectivity, a basic measure for the robustness of a graph. The larger the algebraic connectivity is, the larger the relative number of links required to be cut-away to generate a bipartition [3]; (b) its correlation with properties of dynamic processes, such as synchronization of dynamic processes at the nodes of a network and random walks on graphs which model, e.g. the dispersion phenomena or exploring graph properties [3]. A network has a more robust synchronized state if the algebraic connectivity of the network is large [4,5]. Random walks move and disseminate efficiently in topologies with large algebraic connectivity.

The diameter D of a graph is the maximum distance in terms of the number of hops or links over all pairs of nodes in G. The diameter is one of the graph metrics that is not only of theoretical interest but that also has many practical applications. In communication networks, the diameter plays a key role in network design when the network performance, such as the delay or signal degradation, is proportional to the number of links that a packet traverses. Numerous applications include circuit design, data representation, and parallel and distributive computing [6]. The complete graph has the maximal algebraic connectivity $a(K_N) = N$. However, real-world networks are always far sparser and their diameters are mostly larger. In order to construct a certain relative large diameter, links have to be removed, but this reduces the algebraic connectivity. It is essential to understand how the maximum algebraic connectivity $a_{\max}(N, D)$ decreases while increasing the diameter D, at constant N.

In this work, we propose a class of graphs $G_D^*(n_1, n_2, \ldots, n_D, n_{D+1})$ where D is the diameter and the variables n_i, with $1 \leqslant i \leqslant D + 1$, are the sizes of the cliques contained in G_D^*. This structure was employed by van Dam [7] to determine the graphs with the maximal spectral radius (largest eigenvalue of the adjacency matrix) among those on N nodes and diameter D. Here, we claim that the maximum algebraic connectivity of the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ is also the maximum $a_{\max}(N, D)$ over all graphs $G(N, D)$ with N nodes and diameter D. More generally, we prove that $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ can achieve the maximum of any Laplacian eigenvalue μ_i, $1 \leqslant i \leqslant N - 1$, the maximum link density, the minimum average hopcount among all graphs $G(N, D)$.

For $D \leqslant 4$, we determine rigorously the graph in the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ that achieves the maximum algebraic connectivity $a_{\max}(N, D)$. For larger diameters, the maximum of any Laplacian eigenvalue is searched numerically, which is feasible, because we search within the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ instead of all graphs $G(N, D)$. And, we reduce the computation of the Laplacian eigenvalue from a $N \times N$ to a $(D + 1) \times (D + 1)$ matrix. Numerical exhaustive searching is applied in this paper to (1) examine the topological features of graphs that maximize different Laplacian eigenvalues; (2) investigate the maximum algebraic connectivity $a_{\max}(N, D)$ for various N and D and (3) finally, we evaluate the upper bounds on the algebraic connectivity that are proposed in the literature.

2. The class of graphs $G_D^*(n_1, n_2, \ldots, n_{D+1})$

2.1. Definition

Definition 1. The class of graphs $G_D^*(n_1, n_2, \ldots, n_{D+1})$ is composed of $D + 1$ cliques[1] $K_{n_1}, K_{n_2}, \ldots, K_{n_D}$ and $K_{n_{D+1}}$, where the variable $n_i \geqslant 1$ with $1 \leqslant i \leqslant D + 1$ is the size or number of nodes of the ith clique.

[1] A clique is a subset of nodes that every two nodes in the subset are connected by a link.

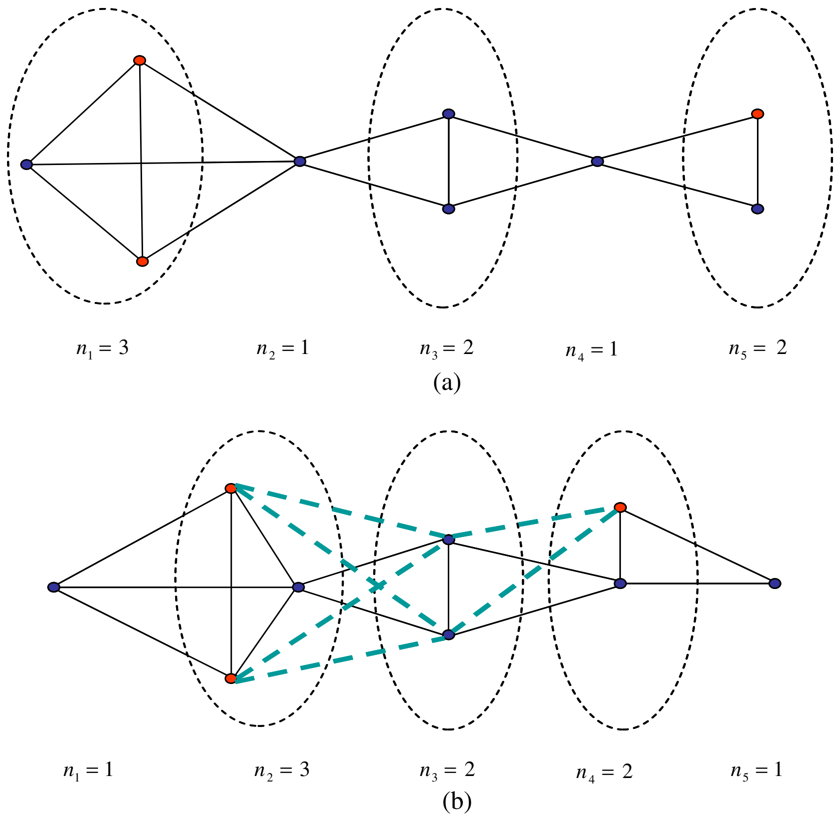

Fig. 1. The graph (a) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ and (b) $G^*_{D=4}(n_1 = 1, n_2 = 3, n_3 = 2, n_4 = 2, n_5 = 1)$.

Each clique K_{n_i} is fully connected with its neighboring cliques $K_{n_{i-1}}$ and $K_{n_{i+1}}$ for $2 \leqslant i \leqslant D$. 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.

Two examples, $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ and $G^*_{D=4}(n_1 = 1, n_2 = 3, n_3 = 2, n_4 = 2, n_5 = 1)$, are shown in Fig. 1. Obviously, the class of graphs $G^*_D(n_1, n_2, \ldots, n_{D+1})$ has diameter D, which equals the distance between nodes in clique K_{n_1} and nodes in $K_{n_{D+1}}$. The size of each clique must be larger than or equal to 1, i.e. $n_i \geqslant 1$ for $1 \leqslant i \leqslant D + 1$. The degree of a node is the number of links that connects to the node. The degree of any node in K_{n_i} is $n_i - 1 + n_{i+1} + n_{i-1}$ for $2 \leqslant i \leqslant D$. The degree is $n_1 - 1 + n_2$ for any node in K_{n_1} and is $n_{D+1} - 1 + n_D$ for nodes in clique $K_{n_{D+1}}$.

2.2. Properties

Each node in the class of graphs $G^*_D(n_1, n_2, \ldots, n_{D+1})$ is fully connected within the clique and with neighboring cliques. We now define a node shifting action performed on a graph of the class $G^*_D(n_1, n_2, \ldots, n_{D+1})$. The resultant graph also belongs to this class and differs from the initial graph in that one node is shifted to a neighboring clique.

Definition 2. Node shifting within the class $G^*_D(n_1, \ldots, n_{i-1}, n_i, n_{i+1}, \ldots, n_{D+1})$: Any node in clique K_{n_i} for $2 \leqslant i \leqslant D$ can be shifted to its neighboring clique $K_{n_{i+1}}$ (or $K_{n_{i-1}}$) by removing links between this node and all the nodes in clique $K_{n_{i-1}}$ (or $K_{n_{i+1}}$) and by adding links between this node and all

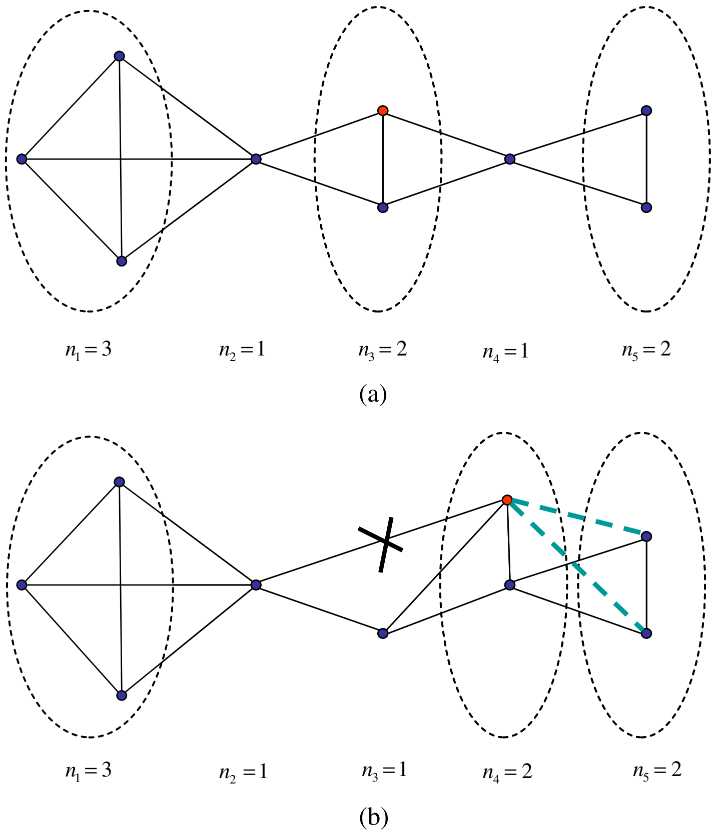

Fig. 2. The graph (a) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ and (b) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 1, n_4 = 2, n_5 = 2)$. The line with cross mark is to be removed and the dotted blue links are added.

the nodes in clique $K_{n_{i+2}}$ $(K_{n_{i-2}})$, if $n_i > 1$. The resultant graph after one of such node shifting actions is $G^*_D(n_1, \ldots, n_{i-1}, n_i - 1, n_{i+1} + 1, \ldots, n_{D+1})$ or $G^*_D(n_1, n_2, \ldots, n_{i-1} + 1, n_i - 1, n_{i+1}, \ldots, n_{D+1})$. A node in clique K_{n_1} (or $K_{n_{D+1}}$) can only be shifted to clique K_{n_2} (or K_{n_D}) by adding links between it and all nodes in clique K_{n_3} (or $K_{n_{D-1}}$), which results in $G^*_D(n_1 - 1, n_2 + 1, \ldots, n_{D-1}, n_D, n_{D+1})$ (or $G^*_D(n_1, n_2, \ldots, n_{D-1}, n_D + 1, n_{D+1} - 1)$).

Fig. 2 illustrates an example of node shifting. From (a) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ to (b) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 1, n_4 = 2, n_5 = 2)$, a node (red[2]) in K_{n_3} is shifted to K_{n_4} by removing the link (marked with cross) between that node and nodes in clique K_{n_2} and by adding links (the blue dotted line) between the node and all nodes in K_{n_5}. In fact, any two graphs in the class $G^*_D(n_1, n_2, \ldots, n_D, n_{D+1})$ with the same number N of nodes can be transformed from one to the other by a set of node shifting actions. For example, Fig. 1(b) can be obtained from Fig. 1(a) by shifting two nodes from K_{n_1} to K_{n_2} and one node from K_{n_5} to K_{n_4}. When a node in clique K_{n_i}, where $2 \leqslant i \leqslant D$ and $n_i > 1$, is shifted to clique $K_{n_{i+1}}$, n_{i-1} links are removed and n_{i+2} links are added. Hence, if we shift $m < n_i$ nodes from clique K_{n_i} to clique $K_{n_{i+1}}$, $n_{i-1} \cdot m$ links are removed and $n_{i+2} \cdot m$ links are added. This node shifting operation will be frequently used to prove several interesting properties of the class $G^*_D(n_1, n_2, \ldots, n_D, n_{D+1})$.

[2] For interpretation of color in Figs. 1-7, the reader is referred to the web version of this article.

Based on the sizes of the first and last clique, the class of graphs $G_D^*(n_1, n_2, \ldots, n_D, n_{D+1})$ can be divided into two sets: (1) $n_1 = n_{D+1} = 1$, e.g. Fig. 1(b), and (2) at least one of n_1, n_{D+1} is larger than 1, e.g. Fig. 1(a). The set 1 is generally denser than the set 2, in the sense that

Lemma 3. *A graph $G_D^*(n_1, n_2, \ldots, n_D, n_{D+1})$, where at least one of n_1 and n_{D+1} is larger than one, is a subgraph of $G_D^*(1, n_1 - 1 + n_2, \ldots, n_{D-1}, n_D + n_{D+1} - 1, 1)$.*

Proof. According to the definition of node shifting, links are only added and not removed, when a node is shifted from K_{n_1} to K_{n_2} or from $K_{n_{D+1}}$ to K_{n_D}. $G_D^*(1, n_1 - 1 + n_2, \ldots, n_{D-1}, n_D + n_{D+1} - 1, 1)$ can be obtained from $G_D^*(n_1, n_2, \ldots, n_{D-1}, n_D, n_{D+1})$ by shifting $n_1 - 1$ nodes from K_{n_1} to K_{n_2} and by shifting $n_{D+1} - 1$ nodes from $K_{n_{D+1}}$ to K_{n_D} by purely adding links. Hence, $G_D^*(n_1, n_2, \ldots, n_{D-1}, n_D, n_{D+1})$ is a subgraph of $G_D^*(1, n_1 - 1 + n_2, \ldots, n_{D-1}, n_D + n_{D+1} - 1, 1)$, when either n_1 or n_{D+1} is larger than one. □

Fig. 1 gives an example of Lemma 3, i.e. $G_{D=4}^*(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ is a subgraph of $G_{D=4}^*(n_1 = 1, n_2 = 3, n_3 = 2, n_4 = 2, n_5 = 1)$. Both graphs contain the same set of nodes, while the latter consists of more links, the blue dotted ones.

The motivation to study the set of graphs $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ lies in the following properties.

Theorem 4. *Any graph $G(N, D)$ with N nodes and diameter D is a subgraph of at least one graph in the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ with $N = \sum_{i=1}^{D+1} n_i$.*

Proof. There is at least one node pair in $G(N, D)$ that is D hops away from each other, because the diameter of $G(N, D)$ is D. We select a node s from one such node pair and denote it as cluster $C_1 = s$. We define the set of clusters C_i $(2 \leqslant i \leqslant D + 1)$ as the set of $|C_i|$ nodes that is i hops away from s or cluster C_1. There can be more than one node that is D hops away from s, when $|C_{D+1}| \geqslant 1$. First, $G(N, D)$ is a subgraph of the graph $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1})$ when $n_i = |C_i|$ for $1 \leqslant i \leqslant D + 1$, because of two reasons: (a) within each cluster C_i of $G(N, D)$, for $1 \leqslant i \leqslant D + 1$, these $|C_i|$ nodes are at best fully connected as in the corresponding clique K_{n_i} with size $n_i = |C_i|$ in $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1})$ and (b) in $G(N, D)$, nodes in cluster $C_i (2 \leqslant i \leqslant D)$ cannot be connected to nodes in other clusters except for C_{i-1} and C_{i+1}, or else, the distance between $C_1 = s$ and nodes in C_{D+1} is smaller than D. Similarly, each clique K_{n_i} is only but fully connected to its neighboring cliques $K_{n_{i-1}}$ and $K_{n_{i+1}}$ in $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1})$.

Based on Lemma 3, $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1})$ is a subgraph of $G_D^*(1, n_2, \ldots, n_{D-1}, n_D + n_{D+1} - 1, 1)$. Hence, any graph $G(N, D)$ with N nodes and diameter D is a subgraph of at least one graph in the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$. □

Since $\sum_{i=1}^{D+1} n_i = N$ and $n_1 = n_{D+1} = 1$ always hold, the graph $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ contains $D - 2$ variables: the sizes of the cliques and $n_i > 0$ for $1 \leqslant i \leqslant D + 1$.

Fiedler [2] showed that, if G_1 is a subgraph of G with the same size, then $a(G_1) \leqslant a(G)$. Hence, by virtue of Theorem 4, we have:

Corollary 5. *The maximum algebraic connectivity of the graphs in the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ is also the maximum among all the graphs with the same size N and diameter D, i.e. $a_{\max}(G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)) = a_{\max}(N, D)$.*

However, given size N and diameter D, the graph that has the maximum algebraic connectivity $a_{\max}(N, D)$ may not be unique. For example, the graph in $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ maximizing the algebraic connectivity $a_{\max}(N, D)$ may possess the same algebraic connectivity after a set of links is deleted. In other words, different graphs may have the same algebraic connectivity $a_{\max}(N, D)$.

Theorem 6. *The maximum of any eigenvalue $\mu_i(G_1)$, $i \in [1, N]$ achieved in the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ is also the maximum among all the graphs with N nodes and diameter D.*

Proof. Our proof is based on the well-known interlacing property (see, e.g., [8]): Let G be a general graph of N nodes. Let $G+e$ be the graph obtained by adding a link e between two nodes that are not directly connected in G. Then, the eigenvalues of G interlace with those of $G+e$, that is,

$$\begin{aligned}\mu_N(G) &\leqslant \mu_N(G+e) \leqslant \mu_{N-1}(G) \leqslant \mu_{N-1}(G+e)\\ &\leqslant \mu_{N-2}(G)\cdots \leqslant \mu_1 \leqslant \mu_1(G+e).\end{aligned}$$

Therefore, if G_1 is a subgraph of G with the same size N, $\mu_i(G_1) \leqslant \mu_i(G)$, for $i \in [1,N]$. Together with Theorem 4, the proof can be completed. □

Theorem 7. *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* $G_D^*(1,\ldots,1,n_j = N-D,1,\ldots,1)$ *with* $j \in [2,D]$, *where only one clique has size larger than one, or by* $G_D^*(1,\ldots,1,n_j > 1, n_{j+1} > 1,1,\ldots,1)$ *with* $j \in [2,D-1]$ *where only two cliques have size larger than one and they are next to each other*.

Proof. First, according to Theorem 4, the maximum number of links $L_{\max}(N,D)$ can only be achieved within the class $G_D^*(n_1 = 1, n_2,\ldots,n_D,n_{D+1} = 1)$. Second, any other graph $G_D^*(n_1 = 1, n_2,\ldots,n_D,n_{D+1} = 1)$, where more than one clique has size larger than one, can be transformed into $G_D^*(1,\ldots,1,n_j = N-D,1,\ldots,1)$ by a set of node shifting operations. (a) When progressing from clique K_{n_2} to clique $K_{n_{D-1}}$, we label the first encountered clique that has size larger than one as K_{n_r} such that $n_i = 1$ for $i < r$. (b) We shift all but one (i.e. $n_r - 1$) nodes in clique K_{n_r} to clique $K_{n_{r+1}}$ by deleting $(n_r - 1)\cdot n_{r-1} = (n_r - 1)$ links and by adding $(n_r - 1)\cdot n_{r+2}$ links. The process (a and b) is repeated until there is only one clique having size larger than 1. Since $n_i \geqslant 1$ for $i \in [1, D+1]$ according to the definition of the class $G_D^*(n_1,n_2,\ldots,n_D,n_{D+1})$, $(n_r - 1)\cdot n_{r+2} \geqslant n_r - 1$. The inequality holds when $n_{r+2} > 1$, which happens at least one time during the recursive node shifting except for $G_D^*(1,\ldots,1,n_j > 1,n_{j+1} > 1,1,\ldots,1)$, $j \in [1,D-2]$ where only two cliques have size larger than one and they are next to each other. Hence, $G_D^*(1,\ldots,1,n_j = N-D,1,\ldots,1)$, $j \in [2,D]$ and $G_D^*(1,\ldots,1,n_j > 1,n_{j+1} > 1,1,\ldots,1)$, $j \in [2,D-1]$ possess the maximum number of links among graphs of size N and diameter D. The maximum number of links is $L_{\max}(N,D) = \binom{N-D}{2} + 2(N-D) + D - 2 = \binom{N-D+2}{2} + D - 3$. □

Theorem 8. *The minimum average hopcount in graphs with given size N and diameter D can be only obtained by* $G_D^*(1,\ldots,1,n_{\frac{D}{2}+1} = N-D,1,\ldots,1)$ *when D is even, or when D is odd, by* $G_D^*(1,\ldots,1,n_{\lfloor\frac{D}{2}\rfloor+1} \geqslant 1, n_{\lceil\frac{D}{2}\rceil+1} \geqslant 1,1,\ldots,1)$, *where only the two cliques in the middle can have size larger than one. The minimum average hopcount is*

$$\min_{\mathcal{G}\in G(N,D)} E[H(\mathcal{G})] = \begin{cases} \frac{N-D-1}{N(N-1)}\left(\frac{D^2}{2} + N\right) + \frac{\sum_{i=1}^{D} i(D-i+1)}{\binom{N}{2}}, & \text{when } D \text{ is even,}\\ \frac{N-D-1}{N(N-1)}\left(2\left\lfloor\frac{D}{2}\right\rfloor^2 + N + D\right) + \frac{\sum_{i=1}^{D} i(D-i+1)}{\binom{N}{2}}, & \text{when } D \text{ is odd.}\end{cases}$$

Proof. See Appendix B.1. □

In summary, the class $G_D^*(n_1 = 1,n_2,\ldots,n_D,n_{D+1} = 1)$ can achieve the maximum of any Laplacian eigenvalue μ_i, $1 \leqslant i \leqslant N-1$, the maximum link density, the minimum average hopcount among all graphs with given size N and diameter D. The graphs that possess the maximum link density and the minimum average hopcount are rigorously determined in Theorems 7 and 8. In the sequel, we focus on the Laplacian spectrum of the class $G_D^*(n_1 = 1,n_2,\ldots,n_D,n_{D+1} = 1)$.

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

The spectrum of both the Laplacian and adjacency matrix of G_D^* is computed in [9].

Theorem 9. *The characteristic polynomial of the Laplacian* $Q_{G_D^*} = \Delta_{G_D^*} - A_{G_D^*}$ *of* $G_D^*(n_1, n_2, \ldots, n_{D-1}, n_D, n_{D+1})$ *equals*

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

where d_j *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*

$$\theta_j = (d_j + 1 - \mu) - \left(\frac{n_{j-1}}{\theta_{j-1}} + 1\right) n_j \tag{2}$$

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

Proof. See [9]. □

Theorem 9 shows that the Laplacian $Q_{G_D^*}$ has eigenvalues at $n_{j-1} + n_j + n_{j+1} = d_j + 1$ with multiplicity $n_j - 1$ for $1 \leqslant j \leqslant D + 1$, with the convention that $n_0 = n_{D+2} = 0$. The less trivial zeros are solutions of the polynomial $p_D(\mu) = \prod_{j=1}^{D+1} \theta_j$, where θ_j is recursively defined via (2). Since all the explicit Laplacian eigenvalues $\mu_j = d_j + 1$ of G_D^* in (1) are larger than zero and since $\mu = 0$ is an eigenvalue of any Laplacian, the polynomial $p_D(\mu)$ must have a zero at $\mu = 0$. Thus, the polynomial of interest is

$$p_D(\mu) = \prod_{j=1}^{D+1} \theta_j(D; \mu) = \sum_{k=0}^{D+1} c_k(D)\, \mu^k = \prod_{k=1}^{D+1} (z_k - \mu), \tag{3}$$

where the dependence of θ_j on the diameter D and on μ is explicitly written and where the product with the zeros $0 = z_{D+1} \leqslant z_D \leqslant \cdots \leqslant z_1$ follows from the definition of the eigenvalue equation (see [10, pp. 435–436]).

The general lower bound [11] for the algebraic connectivity in any graph is $a \leqslant d_{\min}$ where $d_{\min}$ is the minimal degree of a graph. Hence, $a = z_D$, the algebraic connectivity is always a non-trivial eigenvalue of $Q_{G_D^*}$, i.e. the second smallest zero of the polynomial $p_D(\mu)$. The largest Laplacian eigenvalue follows

$$\mu_1 \geqslant d_{\max} + 1$$

the same as presented in [11–13]. Brouwer and Haemers [13] 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 $\mu_1 \in [0, N],\ \mu_1 = z_1$.

Furthermore, $p_D(\mu)$ is shown in [9] to belong to a set of orthogonal polynomials. All the non-trivial eigenvalues of $Q_{G_D^*}$ are also eigenvalues of the (much simpler and smaller) Jacobian matrix – $\widetilde{M}$, where

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

Table 1
Graphs with $D = 6$ that optimize the ith largest Laplacian eigenvalue μ_i or the spacing $\mu_i - \mu_{i+1}$.

$N = 50$						$N = 100$					
Value to optimize	n_2	n_3	n_4	n_5	n_6	Value to optimize	n_2	n_3	n_4	n_5	n_6
$\mu_{N-1} = \mu_{N-1} - \mu_N$	6	11	14	11	6	$\mu_{N-1} = \mu_{N-1} - \mu_N$	13	22	28	22	13
μ_{N-2}	16	15	1	1	15	μ_{N-2}	32	32	1	1	32
$\mu_{N-2} - \mu_{N-1}$	16	15	1	1	15	$\mu_{N-2} - \mu_{N-1}$	32	32	1	1	32
μ_{N-3}	1	22	1	1	23	μ_{N-3}	1	47	1	1	48
$\mu_{N-3} - \mu_{N-2}$	1	22	1	1	23	$\mu_{N-3} - \mu_{N-2}$	1	47	1	1	48
μ_{N-4}	1	22	1	23	1	μ_{N-4}	1	48	1	47	1
$\mu_{N-4} - \mu_{N-3}$	1	22	1	23	1	$\mu_{N-4} - \mu_{N-3}$	1	48	1	47	1
μ_{N-5}	1	1	44	1	1	μ_{N-5}	1	1	94	1	1
$\mu_{N-5} - \mu_{N-4}$	1	1	44	1	1	$\mu_{N-5} - \mu_{N-4}$	1	1	94	1	1
μ_{N-6}	1	1	1	30	15	μ_{N-6}	1	1	34	61	1
$\mu_{N-6} - \mu_{N-5}$	1	1	43	1	2	$\mu_{N-6} - \mu_{N-5}$	2	1	93	1	1
μ_{N-7}	1	1	1	35	10	μ_{N-7}	1	1	1	38	57
$\mu_{N-7} - \mu_{N-6}$	2	1	42	1	2	$\mu_{N-7} - \mu_{N-6}$	2	1	92	1	2

Therefore, exhaustively numerical searching for the maximum of any Laplacian eigenvalue is feasible because of two reasons: (a) the searching space within $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ is much smaller than the searching within all graphs with N nodes and diameter D. (b) the calculation of the Laplacian spectrum is reduced from a $N \times N$ matrix to a $(D + 1) \times (D + 1)$ tri-diagonal matrix.

4. The maximum of any Laplacian eigenvalue

Theorem 6 shows that the maximum of any eigenvalue among all graphs with size N and diameter D can be achieved within the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$. What is the topological implication when different eigenvalues are optimized? Table 1 presents the different topologies with $D = 6$ that optimize the ith largest Laplacian eigenvalue μ_i and the spacing $\mu_i - \mu_{i+1}$, for $i \in [N-1, N-7]$.

The graph in the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ that optimizes μ_i for $i \leqslant N-5$ possesses the maximal number of links, i.e. only one or two adjacent cliques have size larger than one, according to Theorem 7. In fact, μ_i for $i = N-6, N-7$ can be optimized by any graph in the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ that has the maximal number of links, not only the graph listed in the table. Theorem 9 shows that the Laplacian $Q_{G^*_D}$ has eigenvalues at $n_{j-1} + n_j + n_{j+1} = d_j + 1$ with multiplicity $n_j - 1$ for $1 \leqslant j \leqslant D+1$. Graphs that maximize the number of links have the maximal trivial eigenvalue $N - D + 2$ with the maximal multiplicity $N - D - 1$. Hence, a large set of eigenvalues, but not the largest one[3] μ_1, can be optimized by graphs possessing the maximal number of links. Graph that optimizes the eigenvalue μ_i, at the same time, maximizes the corresponding spacing $\mu_i - \mu_{i+1}$, for $i \geqslant N-5$. However, when $i < N-5$, the graph that optimizes the eigenvalue μ_i, has spacing $\mu_i - \mu_{i+1} = 0$, which is far from the maximal spacing.

The graph that maximizes the algebraic connectivity μ_{N-1} has larger sizes for cliques in the middle. It is dense in the core and sparse at borders. Such structure is robust for information transportation in the sense that traffic is more uniformly distributed, when traffic is injected between each node pair. Contrary, graphs that maximize other eigenvalues or spacing, have cliques with small size ($n_j = 1$) around the middle, which have to carry much more traffic and become the bottleneck for transportation. Graphs with many cliques of size one are vulnerable, because removal of such clique – which is in fact a node – disconnects the rest of the graph. Hence, the comparison of topologies in Table 1 provides us with an extra motivation to study the graphs maximizing the algebraic connectivity. Since $G^*_D(n_1, n_2, \ldots, n_D, n_{D+1})$ has $L = \sum_{i=2}^{D} \binom{n_i}{2} + \sum_{i=1}^{D} n_i n_{i+1}$ links, the number of links in the graph that maximizes the algebraic connectivity is far smaller than the maximum for $D > 3$ according to Theorem

[3] The largest eigenvalue μ_1 is always a nontrivial one according to Theorem 9. Hence, a lower bound for the maximal possible μ_1 follows $\mu_{1\,\max} \geqslant N - D + 2$.

7. Therefore, graphs that maximize the algebraic connectivity are robust for transportation, while, at the same time, efficient in the number of links.

5. The maximum algebraic connectivity $a_{\max}(N, D)$

5.1. Exact computation of $a_{\max}(N, D)$ for diameter $D = 2, 3, 4$

Before we start the $D = 2, 3$ cases, it should be mentioned that the graph $G(N, D = N - 1)$ with N nodes and diameter $N - 1$ is unique: a path graph. The algebraic connectivity of a path graph [14] is well-known: $a_{\max}(N, D = N - 1) = 2\left(1 - \cos\frac{\pi}{N}\right)$.

The complete Laplacian spectrum of $G^*_{D=2}(n_1, n_2, n_3)$ follows from Theorem 9 and the polynomial $p_D(\mu)$, as the zeros at $\mu_1 = n_1 + n_2$ with multiplicity $n_1 - 1$, $\mu_2 = n_1 + n_2 + n_3 = N$ with multiplicity $n_2 - 1$, $\mu_3 = n_2 + n_3$ with multiplicity $n_3 - 1$ and the simple zeros of

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

which are $z_3 = 0$, $z_2 = n_2$ and $z_1 = N$. Clearly, since $n_1 + n_2 + n_3 = N$, the largest possible algebraic connectivity $a_{\max}(N, D = 2) = n_2$ is $N - 2$.

This result is more directly found from Corollary 5. The maximum algebraic connectivity in graphs with N nodes and diameter D can be achieved in the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$, which is unique, i.e. $G^*_{D=2}(n_1 = 1, n_2 = N - 2, n_3 = 1)$ for $D = 2$. Hence, the graph $G^*_{D=2}(n_1 = 1, n_2 = N - 2, n_3 = 1)$, a clique of size N without one link $K_N - \{(i, j)\}$, has the maximum algebraic connectivity $N - 2$ among graphs with N nodes and diameter $D = 2$, i.e. $a_{\max}(N, D = 2) = N - 2$.

Theorem 10. *For graphs with N nodes and diameter $D = 3$, the graph $G^*_{D=3}\left(1, \left\lfloor\frac{N-2}{2}\right\rfloor, N - 2 - \left\lfloor\frac{N-2}{2}\right\rfloor, 1\right)$ has the maximum algebraic connectivity with $\left\lfloor\frac{N-2}{2}\right\rfloor - 1 \leqslant a_{\max}(N, D = 3) \leqslant \left\lfloor\frac{N-2}{2}\right\rfloor$.*

Proof. See Appendix B.2. □

We will give the solution for the case $D = 4$ through a number of theorems.

Theorem 11. *Among the graphs $G^*_{D=4}(1, m, N - 2m - 2, m, 1)$, the algebraic connectivity is maximal when $m = \left\lfloor\frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N - 8}\right\rfloor$ or $m = \left\lceil\frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N - 8}\right\rceil$ and $a_{\max}(N, D = 4) = \frac{N-1-m}{2} - \frac{1}{2}\sqrt{N^2 - 2N - 6Nm + 1 + 10m + 9m^2}$.*

Proof. See Appendix B.3. □

Theorem 12. *The graph $G^*_{D=4}(1, m + a, N - 2m - 2, m - a, 1)$, where $0 < a \leqslant m - 1$, has algebraic connectivity smaller than the graph $G^*_{D=4}(1, m, N - 2m - 2, m, 1)$.*

Proof. See Appendix B.4. □

Corollary 13. *For graphs with N nodes and diameter $D = 4$, if we consider the graphs $G^*_{D=4}(1, n_2, N - n_2 - n_4 - 2, n_4, 1)$, where n_2 and n_4 are real numbers, then the maximum algebraic connectivity is achieved for $n_2 = n_4 = \frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N - 8}$ and $a_{\max}(N, D = 4) = \frac{N}{3} - \frac{2}{9} - \frac{2}{9}\sqrt{6N - 8}$.*

Proof. The corollary follows directly from the proofs of Theorems 11 and 12. □

Theorem 14. *For graphs with N nodes and diameter $D = 4$, among the graphs $G^*_{D=4}(1, n_2, N - n_2 - n_4 - 2, n_4, 1)$, where n_2 and n_4 are integers, the maximum algebraic connectivity is achieved for either $(n_2, n_4) =$*

$(\lfloor m\rfloor, \lfloor m\rfloor)$, $(n_2, n_4) = (\lceil m\rceil, \lceil m\rceil)$ *or* $(n_2, n_4) = (\lfloor m\rfloor, \lceil m\rceil)$, *where* $m = \frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N-8}$. *Furthermore,* $a_{\max}(N, D = 4) \leqslant \frac{N}{3} - \frac{2}{9} - \frac{2}{9}\sqrt{6N-8}$.

Proof. See Appendix B.5. □

The $D = 4$ case deserves more discussions. In Appendix A we report the results of a numerical search for graphs that maximize the algebraic connectivity for various values of the diameter D. In the considered examples ($N = 26, 50, 100, 122$) the graph with maximum algebraic connectivity is each time unique and symmetric, namely $G^*_{D=4}(1, m, N - 2m - 2, m, 1)$, where m is obtained by rounding $\frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N-8}$ to an integer. However, we also found a number of examples where the maximum algebraic connectivity is realized for three different graphs, including the non-symmetric case mentioned in Theorem 14. For instance, the maximum algebraic connectivity for graphs on $N = 48$ nodes with diameter 4, is realized by $G^*_{D=4}(1, 14, 18, 14, 1)$, $G^*_{D=4}(1, 15, 16, 15, 1)$ and by $G^*_{D=4}(1, 15, 17, 14, 1)$. The algebraic connectivity for these graphs is an integer, namely 12. In fact, it is straightforward to prove that the maximum algebraic connectivity for graphs on $N = 4 + 10s + 6s^2$ nodes (where $s \in \mathbb{N}$) with diameter 4, is realized by $G^*_{D=4}(1, 2s^2 + 3s, 2s^2 + 4s + 2, 2s^2 + 3s, 1)$, $G^*_{D=4}(1, 2s^2 + 3s + 1, 2s^2 + 4s, 2s^2 + 3s + 1, 1)$ and by $G^*_{D=4}(1, 2s^2 + 3s + 1, 2s^2 + 4s + 1, 2s^2 + 3s, 1)$, with as algebraic connectivity is the integer $2s^2 + 2s$. Note that the case $N = 48$ corresponds with $s = 2$. Whether or not there exists a case where the non-symmetric graph $G^*_{D=4}(1, \lceil m\rceil, N - \lceil m\rceil - \lfloor m\rfloor - 2, \lfloor m\rfloor, 1)$ is the unique graph that realizes the maximum algebraic connectivity remains an interesting open problem.

5.2. $a_{\max}(N, D)$ in relation to N and D

The maximum algebraic connectivity $a_{\max}(N, D)$ used in this section is obtained via exhaustive searching in $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ for $D \geqslant 4$. We study first the $a_{\max}(N, D)$ in relation to N.

As shown in Fig. 3, the maximal algebraic connectivity seems linear in N for constant D, i.e. $a_{\max}(N, D) \cong \alpha + \beta \cdot N$. The slope β decreases fast from $\beta = 1$ to $\beta = 0.12$ when the diameter increases from $D = 2$ to $D = 6$. When $D = 2$, $a_{\max}(N, D = 2) = N - 2$, which is determined in Section 5.1. When $D = 3$, we have that $\beta = 0.5$, which follows from Theorem 10, i.e. $\left\lfloor \frac{N-2}{2} \right\rfloor - 1 \leqslant a_{\max}(N, D = 3) \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$. Moreover, we have proved in [9, Section 3.3] that, for large N, the highest possible achievable algebraic connectivity $a_{\max}(N, D)$ is a linear function of N, provided the diameter D is independent from N.

We start the investigation of the relation between $a_{\max}(N, D)$ and diameter D by examining, in general, $\mu_{i\max}(G(N, D))$, $i \in [1, N]$, the maximum of the ith largest Laplacian eigenvalue among all graphs $G(N, D)$ with N nodes and diameter D. Later we will prove that the $\mu_{i\max}(G(N, D))$, $i \in [1, N]$ is non-increasing as the diameter D increases based on the following clique merging operation.

Definition 15. Clique merging: In any graph with diameter D of the class $G^*_D(n_1, n_2, \ldots, n_i, n_{i+1}, \ldots, n_{D+1})$, any two adjacent cliques K_{n_i} and $K_{n_{i+1}}$ can be merged into one clique, resulting into a graph with diameter $D - 1$, i.e. $G^*_{D-1}(n_1, n_2, \ldots, n_i + n_{i+1}, \ldots, n_{D+1})$. The merging of clique K_{n_i} and $K_{n_{i+1}}$ is obtained by adding $n_i n_{i+2}$ links such that clique K_{n_i} is fully meshed with clique $K_{n_{i+2}}$ (if $i + 2 \leqslant D + 1$) and by adding $n_{i-1} n_{i+1}$ links such that the clique $K_{n_{i+1}}$ is fully meshed with clique $K_{n_{i-1}}$ (if $1 \leqslant i - 1$).

Fig. 4 presents an example of clique merging. Clique K_{n_3} and K_{n_4} in Fig. 4(a) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ are merged into one clique, which results in Fig. 4(b) $G^*_{D=3}(n_1 = 3, n_2 = 1, n_3 + n_4 = 3, n_5 = 2)$. The clique merging consists of purely adding links (the blue dotted line).

Theorem 16. *Given the network size N, the maximum of any eigenvalue* $\mu_{i\max}(G(N, D))$, $i \in [1, N]$ *is non-increasing as the diameter D increases, i.e.* $\mu_{i\max}(G(N, D + 1)) \leqslant \mu_{i\max}(G(N, D))$.

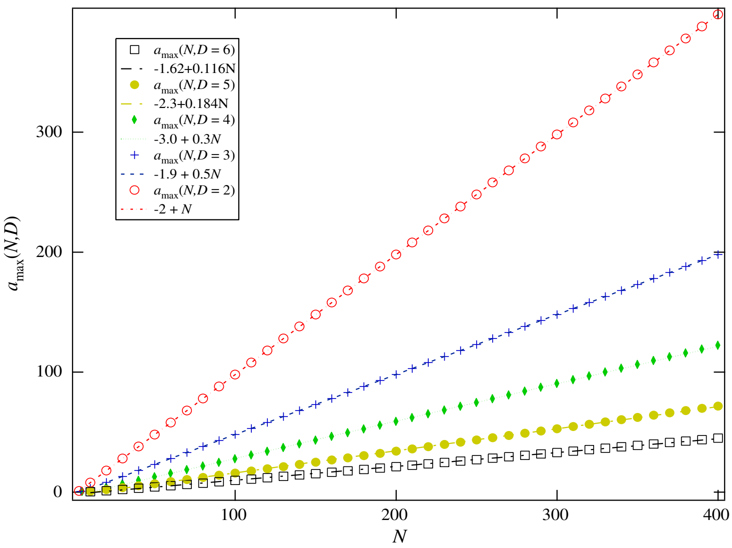

Fig. 3. The $a_{\max}(N,D)$ (marker) for $2 \leqslant D \leqslant 6$ and the corresponding linear fitting (dotted line).

Proof. Assume that the graph $G^*_{D+1}(n'_1 = 1, n'_2, \ldots, n'_i, \ldots, n'_{D+1}, n'_{D+2} = 1)$ possesses the maximum eigenvalue $\mu_{i\max}(G(N, D+1))$, $i \in [1, N]$ among all graphs with size N and diameter $D+1$. Any two adjacent cliques can be merged by only adding links, which results in $G^*_D(n'_1 = 1, n'_2, \ldots, n'_i + n'_{i+1}, \ldots, n'_{D+1}, n'_{D+2} = 1)$. Hence, the graph $G^*_{D+1}(n'_1 = 1, n'_2, \ldots, n'_i, \ldots, n'_{D+1}, n'_{D+2} = 1)$ is a subgraph of $G^*_D(n'_1 = 1, n'_2, \ldots, n'_i + n'_{i+1}, \ldots, n'_{D+1}, n'_{D+2} = 1)$. According to the interlacing property in the proof of Theorem 6, we have $\mu_{i\max}(G(N, D+1)) \leqslant \mu_i(G^*_D(n'_1 = 1, n'_2, \ldots, n'_i + n'_{i+1}, \ldots, n'_{D+1}, n'_{D+2} = 1))$. Furthermore, $G^*_D(n'_1 = 1, n'_2, \ldots, n'_i + n'_{i+1}, \ldots, n'_{D+1}, n'_{D+2} = 1)$ does not necessarily possess the maximum eigenvalue $\mu_{i\max}(G(N,D))$, i.e. $\mu_i(G^*_D(n'_1 = 1, n'_2, \ldots, n'_i + n'_{i+1}, \ldots, n'_{D+1}, n'_{D+2} = 1)) \leqslant \mu_{i\max}(G(N,D))$. Thus, $\mu_{i\max}(G(N, D+1)) \leqslant \mu_{i\max}(G(N,D))$. □

In view of the linear relation between $a_{\max}(N,D)$ and N, we present in Fig. 5 the scaled maximal algebraic connectivity $a_{\max}(G(N,D))/N$ in relation with the diameter D, when $10 \leqslant N \leqslant 122$. The maximal algebraic connectivity $a_{\max}(G(N,D))$ is presented for all possible diameters, i.e. $1 \leqslant D \leqslant N-1$ when $10 \leqslant N \leqslant 35$ and for $D < 10$ when N is large. The decrease of $a_{\max}(G(N,D))/N$ as a function of D is always slower than an exponential $c\exp(-\gamma N)$ and close to (but faster than) a power law $cN^{-\gamma}$. For large N, the scaled algebraic connectivity $a_{\max}(G(N,D))/N$ is expected to follow a universal function of diameter D.

The corresponding clique sizes of $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ that maximizes the algebraic connectivity are partially given in Appendix A and completely documented in [15]. A symmetric clique size $(n_1, n_2, \ldots, n_{D+1})$ or a symmetric structure seems to be necessary to maximize the algebraic connectivity $a_{\max}(N,D)$. The graphs that achieve the maximum algebraic connectivity in $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ have relative large sizes for cliques close to the middle.

5.3. Two proposed upper bounds for $a(N,D)$

Here, we discuss two upper bounds that are proposed in the literature [16,17]. Based on the upper bound

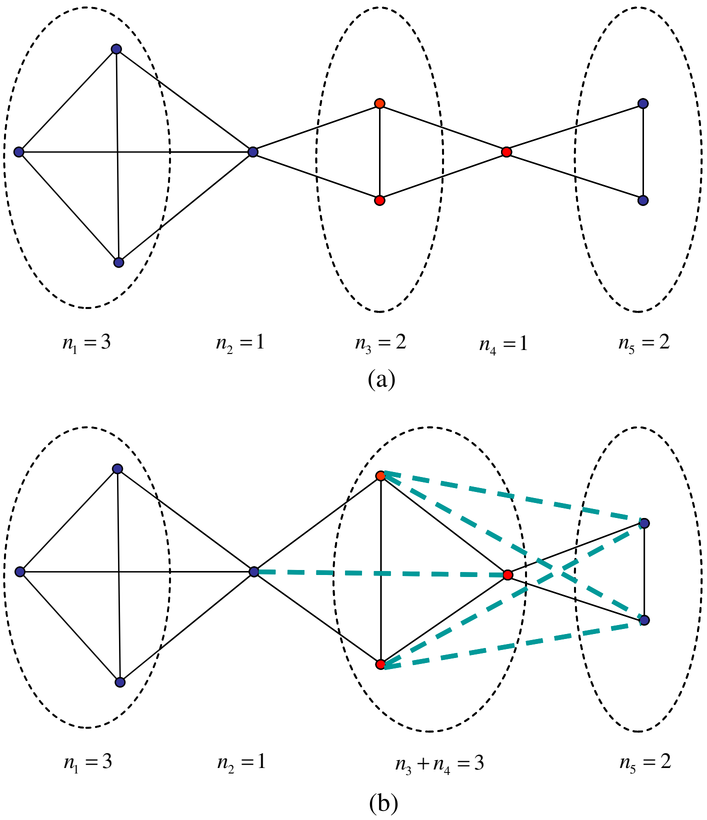

Fig. 4. (b) $G^*_{D=4}(n_1 = 3, n_2 = 1, n_3 + n_4 = 3, n_5 = 2)$ is obtained by merging clique K_{n_3} and K_{n_4} in (a) $G^*_{D=3}(n_1 = 3, n_2 = 1, n_3 = 2, n_4 = 1, n_5 = 2)$ via adding the blue dotted links.

$$D \leqslant \left\lfloor \frac{\cosh^{-1}(N-1)}{\cosh^{-1}\left(\frac{\mu_1+a}{\mu_1-a}\right)} \right\rfloor + 1$$

given by Chung et al. [6], where μ_1 is the largest eigenvalue of the Laplacian Q and a is the algebraic connectivity, Lin and Zhan [16] obtain an upper bound on $\frac{a}{\mu_1}$

$$\frac{a}{\mu_1} \leqslant \frac{\cosh\left(\frac{\cosh^{-1}(N-1)}{D-1}\right) - 1}{\cosh\left(\frac{\cosh^{-1}(N-1)}{D-1}\right) + 1}.$$

Combining a simple upper bound on μ_1

$$\mu_1 \leqslant N. \tag{4}$$

Lin and Zhan [16] arrive at an upper bound of the algebraic connectivity in relation to D and N

$$a(G(N,D)) \leqslant a_{up}(N,D) = N\frac{\cosh\left(\frac{\cosh^{-1}(N-1)}{D-1}\right) - 1}{\cosh\left(\frac{\cosh^{-1}(N-1)}{D-1}\right) + 1}. \tag{5}$$

For $D = 2$, $a_{\max}(N, D = 2) = N - 2$, which is equal to the upper bound (5).

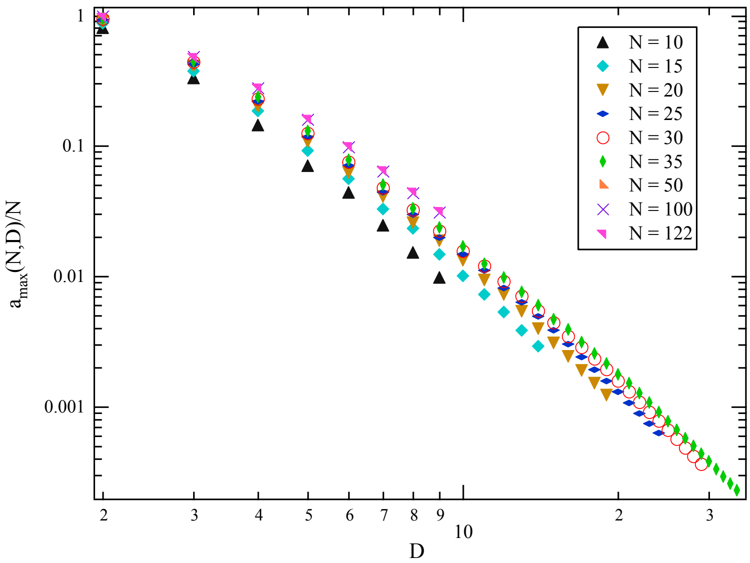

Fig. 5. The scaled maximal algebraic connectivity $a_{max}(G(N, D))/N$ (marker) as a function of the diameter D in log-log scale.

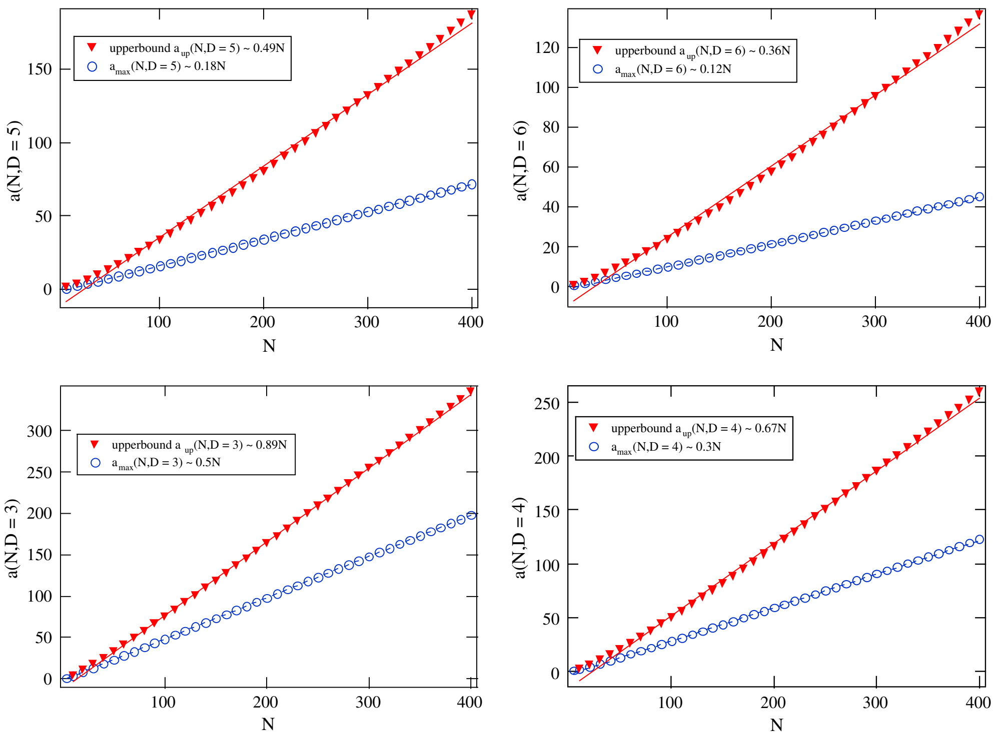

Fig. 6. Comparison of $a_{max}(N, D)$ and the upper bound of $a(N, D)$ when $3 \leqslant D \leqslant 6$.

Fig. 6 illustrates that $a_{up}(N, D)$ loosely bounds the largest possible algebraic connectivity $a_{\max}(N, D)$. The upper bound $a_{up}(N, D)$ increases approximately linearly with N for $3 \leqslant D \leqslant 6$ and the corresponding slope is much higher than that of $a_{\max}(N, D)$. When $D = 3$, each node in clique K_{n_2} and K_{n_3} of $G^*_{D=3}(1, n_2, n_3, 1)$ possesses the maximum degree $d_{\max} = N - 2$. When $D = 4$, the maximum degree of $G^*_{D=4}(1, n_2, n_3, n_4, 1)$ is $d_{\max} = N - 3$, which corresponds to a node in clique K_{n_3}. Since, $\mu_1 \geqslant d_{\max} + 1$ [12,11], the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ has $\mu_1 \approx N$, for $D = 3, 4$. Therefore, the relative loose bound of (5) is not introduced by the $\mu_1 \approx N$ approximation of (4), when $D = 3, 4$.

Alon and Milman [17] present another upper bound of the algebraic connectivity in relation to diameter D and the maximum degree $d_{\max}$

$$a(G) \leqslant \frac{2d_{\max}}{D^2}\left(\log_2 N^2\right)^2. \tag{6}$$

Hence,

$$G^*_{D=3}(1, n_2, n_3, 1) \leqslant \frac{2(N-2)}{9}(\log_2 N^2)^2,$$

$$G^*_{D=4}(1, n_2, n_3, n_4, 1) \leqslant \frac{2(N-3)}{16}(\log_2 N^2)^2,$$

which bounds the $a_{\max}(N, D)$ even loser, especially for large N.

However, we should mention that the two upper bounds (5) and (6) may be tight in other cases. In view of the relative loose upper bounds, at least for smaller diameter $D \leqslant 6$, the largest possible algebraic connectivity $a_{\max}(N, D)$ or its approximations derived from data fitting is of great interest. We refer to [15], where $a_{\max}(N, D)$ as well as its the corresponding topology are presented for a wide range of diameter D and size N.

6. Conclusion

We propose a class of graphs $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$, within which the largest number of links, the minimum average hopcount, and more interestingly, the maximum of any Laplacian eigenvalue among all graphs with N nodes and diameter D can be achieved. The largest possible algebraic connectivity $a_{\max}(N, D)$ is rigorously determined for diameter $D = 2, 3, 4$ and $D = N - 1$. For other diameters, the maximum of any Laplacian eigenvalue can be searched within $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$, which is feasible due to the reduction in size of the Laplacian from a $N \times N$ to a $(D + 1) \times (D + 1)$ matrix.

Combining both the theoretical and numerical results, we have (1) illustrated the different topological features of graphs that maximize different Laplacian eigenvalues, which provides an extra motivation to investigate graphs maximizing the algebraic connectivity; (2) presented the relation between the maximum algebraic connectivity $a_{\max}(N, D)$ and the size N as well as the diameter D; (3) compared two upper bounds of the algebraic connectivity proposed in literature with the largest possible $a_{\max}(N, D)$ for small diameter. This is a first step to explore the application of these maximal possible Laplacian eigenvalues via the class $G^*_D(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$. Rich mathematical results related to the characteristic polynomial of both the Laplacian and adjacency matrix are documented in [9], which is, however, still far from being able to analytically determine the graph optimizing a given eigenvalue. More numerical results about the $a_{\max}(N, D)$ as well as the corresponding graph are being collected and updated in [15].

A. The graph that maximizes the algebraic connectivity

	$a_{\max}(G(N=26,D))$	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}
$D=2$	24	1	24	1							
$D=3$	11.1345	1	12	12	1						
$D=4$	5.6834	1	7	10	7	1					
$D=5$	3.1264	1	5	7	7	5	1				
$D=6$	1.8566	1	3	6	6	6	3	1			
$D=7$	1.1555	1	2	5	5	5	5	2	1		
$D=8$	0.781781	1	2	3	5	4	5	3	2	1	
$D=9$	0.517162	1	1	3	4	4	4	4	3	1	1

	$a_{\max}(G(N=50,D))$	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}
$D=2$	48	1	48	1							
$D=3$	23.074278	1	24	24	1						
$D=4$	12.641101	1	15	18	15	1					
$D=5$	7.080889	1	9	15	15	9	1				
$D=6$	4.290025	1	6	11	14	11	6	1			
$D=7$	2.764758	1	5	8	11	11	8	5	1		
$D=8$	1.859022	1	3	7	9	10	9	7	3	1	
$D=9$	1.320825	1	3	5	7	9	9	7	5	3	1

	$a_{\max}(G(N=100,D))$	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}
$D=2$	98	1	98	1							
$D=3$	48.0385	1	49	49	1						
$D=4$	27.6754	1	31	36	31	1					
$D=5$	15.8799	1	19	30	30	19	1				
$D=6$	9.7886	1	13	22	28	22	13	1			
$D=7$	6.3833	1	9	17	23	23	17	9	1		
$D=8$	4.358863	1	7	13	19	20	19	13	7	1	
$D=9$	3.098801	1	5	10	16	18	18	16	10	5	1

	$a_{\max}(G(N=122,D))$	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	n_{10}
$D=2$	120	1	120	1							
$D=3$	59.031762	1	60	60	1						
$D=4$	34.442561	1	39	42	39	1					
$D=5$	19.858188	1	24	36	36	24	1				
$D=6$	12.266200	1	16	27	34	27	16	1			
$D=7$	8.021537	1	11	20	29	28	21	11	1		
$D=8$	5.499296	1	8	16	23	26	23	16	8	1	
$D=9$	3.910465	1	6	13	18	23	22	19	13	6	1

B. Proofs

B.1. Proof of Theorem 8

First, according to Theorem 4 and the fact that adding links can always reduce the average hopcount, the minimum average hopcount in graphs with given size N and diameter D can be only be achieved within the class $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$. Second, within the set $G_D^*(n_1 = 1, n_2, \ldots,$

$n_D, n_{D+1} = 1)$, any graph can be transformed into $G_D^*(1, \ldots, 1, n_{\frac{D}{2}+1} = N - D, 1, \ldots, 1)$ for even D, or into $G_D^*(1, \ldots, 1, n_{\lfloor \frac{D}{2} \rfloor+1} \geqslant 1, n_{\lceil \frac{D}{2} \rceil+1} \geqslant 1, 1, \ldots, 1)$ for odd D via the following node shifting, where the average hopcount can always be reduced. We consider first the case that D is odd. We repeat the node shifting process (a) and (b) in the proof of Theorem 7 for $r \leqslant \left\lfloor \frac{D}{2} \right\rfloor$, until $n_i = 1$ for $i < \left\lfloor \frac{D}{2} \right\rfloor + 1$ and all the remaining nodes are shifted into clique $\left\lfloor \frac{D}{2} \right\rfloor + 1$. When a node is shifted from K_{n_r} to $K_{n_{r+1}}$, its distance to any node in clique $i < r$ is increased by one, while its distance to any node in clique $i > r + 1$ is reduced by one. Hence, via such a node shifting operation, the sum of the hopcounts between all nodes pairs is reduced by $\sum_{j=r+2}^{D+1} n_j - \sum_{j=1}^{r-1} n_j \geqslant \sum_{j=\lceil \frac{D}{2} \rceil+1}^{D+1} n_j - \sum_{j=1}^{\lfloor \frac{D}{2} \rfloor-1} 1 > 0$, because $r \leqslant \left\lfloor \frac{D}{2} \right\rfloor$ and $n_j \geqslant 1$ for $j \in [1, D+1]$. Similarly, from clique K_{n_D} to clique $K_{\lceil \frac{D}{2} \rceil+2}$, we denote the first encountered clique that has size larger than one as K_{n_r}. The $n_r - 1$ nodes in clique K_{n_r} are shifted to clique K_{n_r-1}. This shifting process is recursively carried out until $n_i = 1$ for $i > \left\lceil \frac{D}{2} \right\rceil + 1$ and all other nodes are shifted to the clique $K_{\lceil \frac{D}{2} \rceil+1}$. Shifting one node from clique K_{n_r} to clique $K_{n_{r-1}}$, where $\left\lceil \frac{D}{2} \right\rceil + 1 < r \leqslant D$, reduces the sum of the hopcounts between all node pairs by $\sum_{j=1}^{r-2} n_j - \sum_{j=r+1}^{D+1} n_j \geqslant \sum_{j=1}^{\lceil \frac{D}{2} \rceil} n_j - \sum_{j=\lceil \frac{D}{2} \rceil+2}^{D+1} 1 > 0$. The average hopcount can always be reduced as long as a node is shifted. Therefore, $G_D^*(1, \ldots, 1, n_{\lfloor \frac{D}{2} \rfloor+1} \geqslant 1, n_{\lceil \frac{D}{2} \rceil+1} \geqslant 1, 1, \ldots, 1)$ has the minimum average hopcount. The size of clique $\left\lfloor \frac{D}{2} \right\rfloor + 1$ and clique $\left\lceil \frac{D}{2} \right\rceil + 1$ have no effect on the average hopcount due to the symmetry of G_D^*. Taking $n_{\lfloor \frac{D}{2} \rfloor+1} = N - D$ and $n_{\lceil \frac{D}{2} \rceil+1} = 1$, we have

$$\min_{\mathcal{G} \in G(N,D)} E[H(\mathcal{G})] = \frac{(N - D - 1)\left(\sum_{i=1}^{\lfloor \frac{D}{2} \rfloor} i + \sum_{i=1}^{\lceil \frac{D}{2} \rceil} i\right) + \binom{N-D}{2} + \sum_{i=1}^{D} i(D - i + 1)}{\binom{N}{2}}$$
$$= \frac{N - D - 1}{N(N-1)} \left(2 \left\lfloor \frac{D}{2} \right\rfloor^2 + N + D\right) + \frac{\sum_{i=1}^{D} i(D - i + 1)}{\binom{N}{2}}.$$

When D is even, the clique $K_{\lfloor \frac{D}{2} \rfloor+1} = K_{\lceil \frac{D}{2} \rceil+1}$ are the same. Similarly, any other graph $G_D^*(n_1 = 1, n_2, \ldots, n_D, n_{D+1} = 1)$ can be transformed into $G_D^*(1, \ldots, 1, n_{\frac{D}{2}+1} = N - D, 1, \ldots, 1)$ by nodes shifting, which can only decrease the average hopcount. When D is even, we have

$$\min_{\mathcal{G} \in G(N,D)} E[H(\mathcal{G})] = \frac{2\,(N - D - 1) \sum_{i=1}^{\frac{D}{2}} i + \binom{N-D}{2} + \sum_{i=1}^{D} i(D - i + 1)}{\binom{N}{2}}$$
$$= \frac{N - D - 1}{N(N-1)} \left(\frac{D^2}{2} + N\right) + \frac{\sum_{i=1}^{D} i(D - i + 1)}{\binom{N}{2}}.$$

B.2. Proof of Theorem 10

Theorem 9 shows that the characteristic polynomial of the corresponding Laplacian matrix of $G_{D=3}^*(n_1 = 1, n_2, n_3, n_4 = 1)$ satisfies (1). The algebraic connectivity of $G_{D=3}^*(n_1 = 1, n_2, n_3, n_4 = 1)$ is the smallest zero z_3 of the polynomial,

$$q_3(\mu) = p_3(\mu)/\mu = \mu^3 - (2N - n_1 - n_4)\,\mu^2$$
$$+ \left(n_2^2 + n_3^2 + n_1 n_2 + n_1 n_3 + n_1 n_4 + 3 n_2 n_3 + n_2 n_4 + n_3 n_4\right) \mu - N n_2 n_3$$

that, here with $n_1 = n_4 = 1$, $n_2 = m$ and $n_3 = N - 2 - m$ reduces to

$$q_3(\mu) = \mu^3 - 2(N-1)\mu^2 + ((N-2)(N+1) + (m-1)(N-m-3))\mu \\ -Nm(N-m-2). \tag{7}$$

Second, we only need to consider the case $m \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$because the $m > \left\lfloor \frac{N-2}{2} \right\rfloor$ can be reduced to the case $m \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$by swapping the clique K_{n_1} and K_{n_4}. We will now show that, for $m \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$, the smallest zero z_3 of (7) satisfies $m - 1 < z_3 < m$.

All zeros of the orthogonal polynomial $p_D(\mu)$ are simple and non-negative. The sign of $q_3(\mu)$ for $\mu = m$, $\mu = N - 1$ and for $\mu = N$ follows from

$$q_3(m) = -m < 0, \tag{8}$$

$$q_3(N-1) = m(N-2-m) > 0, \tag{9}$$

$$q_3(N) = -N < 0. \tag{10}$$

Likewise, we find that

$$q_3(m-1) = -2m + 2m^2 - 3Nm + N^2, \tag{11}$$

which obtains, as a function of m, a minimum at $m_0 = \frac{2+3N}{4}$. Thus, for $0 \leqslant m \leqslant m_0$, the function $q_3(m-1)$ is decreasing in m. Because $m \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$, it follows $m \leqslant \frac{N-2}{2} = m^*$ and that $q_3(m^* - 1) = 4$. Finally, because $m \leqslant m^* < m_0$ it follows that

$$q_3(m-1) > 0. \tag{12}$$

From (8), (12), (9) and (10), it follows that $q_3(\mu)$ has simple zeros $z_3 < z_2 < z_1$ satisfying $m - 1 < z_3 < m$, $m < z_2 < N - 1$ and $N - 1 < z_1 < N$. Hence, among the class $G^*_D(1, n_2, n_3, 1)$, the largest algebraic connectivity can be obtained by $G^*_{D=3}\left(1, \left\lfloor \frac{N-2}{2} \right\rfloor, N - 2 - \left\lfloor \frac{N-2}{2} \right\rfloor, 1\right)$, where m is maximized.

Finally, according to Corollary 5, the algebraic connectivity of $G^*_{D=3}\left(1, \left\lfloor \frac{N-2}{2} \right\rfloor, N - 2 - \left\lfloor \frac{N-2}{2} \right\rfloor, 1\right)$ is also the maximum $a_{\max}(N, D = 3)$ of all the graphs with N nodes and diameter $D = 3$, and $\left\lfloor \frac{N-2}{2} \right\rfloor - 1 \leqslant a_{\max}(N, D = 3) \leqslant \left\lfloor \frac{N-2}{2} \right\rfloor$.

B.3. Proof of Theorem 11

Note that the graph $G^*_{D=4}(1, m, N - 2m - 2, m, 1)$ represents the symmetric case $n_2 = n_4 = m$, where m satisfies $m \leqslant \frac{N-3}{2}$, which follows from the assumption that $n_3 \geqslant 1$. If follows from Theorem 9 that the algebraic connectivity of $G^*_{D=4}(1, m, N - 2m - 2, m, 1)$ corresponds to the smallest zero z_4 of the following polynomial:

$$q_4(\mu) = (\mu^2 + (1 + m - N)\,\mu + Nm - 2m^2 - 2m)(\mu^2 + (1 - m - N)\,\mu + Nm).$$

A straightforward calculation reveals that z_4 is the smallest root of the first quadratic factor in $q_4(\mu)$, i.e.

$$z_4 = \frac{N-1-m}{2} - \frac{1}{2}\sqrt{N^2 - 2N - 6Nm + 1 + 10m + 9m^2}.$$

In addition, it is easy to verify that z_4 is maximized for $m = \frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N-8}$. Finally, because z_4 is a concave function of m, it follows that, for integer values of m, z_4 is maximized for either $m = \left\lfloor \frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N-8} \right\rfloor$ or $m = \left\lceil \frac{N}{3} - \frac{5}{9} - \frac{1}{18}\sqrt{6N-8} \right\rceil$.

Because $q_4(0) = Nm^2(N - 2 - 2m) > 0$ and $q_4(m) = -m^2$, the following inequality, which will be used later on, holds

$$z_4 < m. \tag{13}$$

B.4. Proof of Theorem 12

Note that the graph $G^*_{D=4}(1, m+a, N-2m-2, m-a, 1)$ represents the non-symmetric case $n_2 = m+a, n_4 = m-a$, where m satisfies $m \leqslant \frac{N-3}{2}$. For the time being we will treat both m and a as real numbers. We can restrict ourselves to the case $a > 0$ because the case $a < 0$ can be changed to the case $a > 0$ by swapping the order of the five cliques.

If follows from Theorem 9 that the algebraic connectivity of $G^*_{D=4}(1, m+a, N-2m-2, m-a, 1)$ corresponds to the smallest zero w_4 of the following polynomial:

$$\begin{aligned} p_a(\mu) = {} & \mu^4 - (2N-2)\mu^3 + (1 + N^2 - a^2 - 2N + 2Nm - 2m - 3m^2)\mu^2 \\ & + (2m^3 + 2Nm^2 - 2N^2m - 4a^2 + 2Na^2 - 2ma^2 + 4Nm - 2m)\mu \\ & + N(m^2 - a^2)(N - 2 - 2m). \end{aligned}$$

For $a = 0$ the polynomial $p_0(\mu)$ reduces to $q_4(\mu)$ which has smallest root $z_4 = \frac{N-1-m}{2} - \frac{1}{2}\sqrt{N^2 - 2N - 6Nm + 1 + 10m + 9m^2}$ according to Theorem 11. We will now show that for $0 < a \leqslant m - 1$, the inequality $p_a(z_4) < 0$ holds.

Plugging $\mu = z_4$ into $p_a(\mu)$ we obtain

$$p_a(z_4) = -\frac{1}{2}a^2\left(N^2 - 4Nm + 3m^2 - 3 + (N - m - 3)\sqrt{N^2 - 2N - 6Nm + 1 + 10m + 9m^2}\right).$$

Because $N \geqslant 2m + 3$ it follows that $N - m - 3 > 0$. Therefore, if $N^2 - 4Nm + 3m^2 - 3 \geqslant 0$ then if follows directly that $p_a(z_4) < 0$ for $a > 0$. Next we consider the case $N^2 - 4Nm + 3m^2 - 3 < 0$. Note that this condition implies that $N < 4m$. Let us first rewrite $p_a(z_4)$ as follows:

$$p_4(z_4; a) = -\frac{1}{2}a^2\left(r_1 + r_2\sqrt{r_3}\right)$$

with $r_1 = N^2 - 4Nm + 3m^2 - 3 < 0, r_2 = N - m - 3 > 0$ and $r_3 = N^2 - 2N - 6Nm + 1 + 10m + 9m^2 > 0$. Then it readily can be verified that

$$p_a(z_4)(-r_1 + r_2\sqrt{r_3}) = \frac{1}{2}a^2(r_1^2 - r_2^2 r_3) = 2a^2(2N - 2m - 3)(N - 2m - 2)(N - 4m) < 0.$$

Therefore, also for the case $N^2 - 4Nm + 3m^2 - 3 < 0$ it follows that $p_a(z_4) < 0$ for $a > 0$. Because $p_a(0) > 0$ it follows from $p_a(z_4) < 0$ that the smallest root w_4 of $p_a(\mu)$ always satisfies $w_4 < z_4$. This completes the proof of Theorem 12.

B.5. Proof of Theorem 14

We only need to consider the case $n_2 \geqslant n_4$ because the $n_2 \leqslant n_4$ can be reduced to the case $n_2 \geqslant n_4$ by swapping the order of the five cliques. First consider the points $(n_2, n_4) = (\lfloor m \rfloor + k, \lfloor m \rfloor - k)$, with $k = 1, \ldots, \lfloor m \rfloor - 1$. Then the algebraic connectivity of the corresponding graph $G^*_{D=4}(1, n_2, N - n_2 - n_4 - 2, n_4, 1)$ is smaller than that of $G^*_{D=4}(1, \lfloor m \rfloor, N - 2\lfloor m \rfloor - 2, \lfloor m \rfloor, 1)$ according to Theorem 12 with $a = k$. Note that the points $(n_2, n_4) = (\lfloor m \rfloor + k, \lfloor m \rfloor - k)$, with $k = 1, \ldots, \lfloor m \rfloor - 1$ are situated on the line $n_2 + n_4 = 2\lfloor m \rfloor$. All grid points (n_2, n_4) situated below this line also have a corresponding graph $G^*_{D=4}(1, n_2, N - n_2 - n_4 - 2, n_4, 1)$ with algebraic connectivity smaller than that of $G^*_{D=4}(1, \lfloor m \rfloor, N - 2\lfloor m \rfloor - 2, \lfloor m \rfloor, 1)$. This follows from applying Theorems 12 and 11.

The same reasoning holds for the points $(n_2, n_4) = (\lceil m \rceil + k, \lceil m \rceil - k)$, with $k = 1, \ldots, \lceil m \rceil - 1$, and grid points above the line that contains these points. The only points on the grid that we have not covered yet are those satisfying $\Gamma : (n_2, n_4) = (\lceil m \rceil + k, \lfloor m \rfloor - k)$, with $k = 0, \ldots, \lfloor m \rfloor - 1$. We will now show that among the graphs $G^*_{D=4}(1, n_2, N - n_2 - n_4 - 2, n_4, 1)$, where (n_2, n_4) belongs to Γ, the highest algebraic connectivity is achieved for $k = 0$.

According to Theorem 12 the algebraic connectivity of the graph $G^*_{D=4}(1, m + a, N - 2m - 2, m - a, 1)$ corresponds to the smallest root of $p_a(\mu)$.

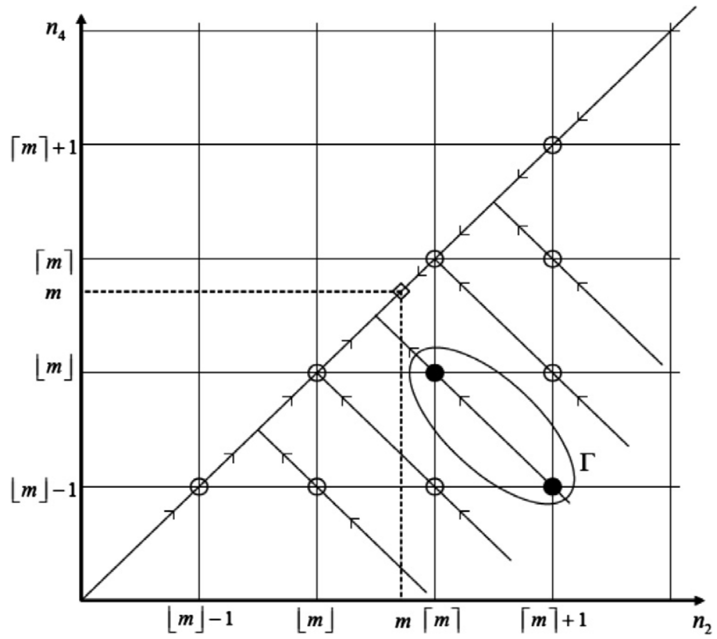

Fig. 7. Sketch of the proof of Theorem 14.

Then $p_{a+1}(z_4) < p_a(z_4) < 0$ because $p_{a+1}(z_4) - p_a(z_4) = \frac{2a+1}{a^2} p_a(z_4) < 0$, where the latter inequality follows from the proof of Theorem 12. In the same manner we can show that $0 < p_{a+1}(0) < p_a(0)$. Denote the smallest root of $p_a(\mu)$by μ_a and the smallest root of $p_{a+1}(\mu)$by μ_{a+1}. Assume that $\mu_{a+1} > \mu_a$, then $p_a(\mu)$ and $p_{a+1}(\mu)$ intersect at least twice on the interval $[0, z_4]$. This implies that the function $h(\mu) = p_a(\mu) - p_{a+1}(\mu)$ has at least two zeros on the interval $[0, z_4]$. Because $h(\mu) = (1 + 2a)(\mu^2 - 2(N - m - 2)\mu + N(N - 2m - 2)$ it follows that the zeros of $h(\mu)$ will be situated around $\mu^* = N - m - 2$. However, because $N \geqslant 2m + 3$ and $z_4 < m$ (according to (13)) it follows $\mu^* > m > z_4$. Therefore only one zero of $h(\mu)$ could be situated in $[0, z_4]$. Therefore we conclude that $\mu_{a+1} \leqslant \mu_a$.

The possibility that $\mu_{a+1} = \mu_a$ can be excluded in the same way. Therefore it follows that $\mu_{a+1} < \mu_a$.

This implies that the algebraic connectivity of $G^*_{D=4}(1, \lceil m \rceil, N - \lceil m \rceil - \lfloor m \rfloor - 2, \lfloor m \rfloor, 1)$ is larger than that of $G^*_{D=4}(1, \lceil m \rceil + 1, N - \lceil m \rceil - \lfloor m \rfloor - 2, \lfloor m \rfloor - 1, 1)$, which itself has a larger algebraic connectivity than $G^*_{D=4}(1, \lceil m \rceil + 2, N - \lceil m \rceil - \lfloor m \rfloor - 2, \lfloor m \rfloor - 2, 1)$. Repeating this argument, until the graph $G^*_{D=4}(1, \lceil m \rceil + \lfloor m \rfloor - 1, N - \lceil m \rceil - \lfloor m \rfloor - 2, 1, 1)$, shows that for (n_2, n_4) in Γ, the highest algebraic connectivity is achieved for $G^*_{D=4}(1, \lceil m \rceil, N - \lceil m \rceil - \lfloor m \rfloor - 2, \lfloor m \rfloor, 1)$.

This completes the proof of the first part of the theorem. The used argumentation is visualized in Fig. 7. The upperbound on $a_{\max}(N, D = 4)$ follows from Corollary 13.

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