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Graphs of given order and size and minimum algebraic connectivity

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Abstract

The structure of connected graphs of given size and order that have minimal algebraic connectivity is investigated. It is shown that they must consist of a chain of cliques. Moreover, an upper bound for the number of maximal cliques of size 2 or larger is derived.

Key words: algebraic connectivity, graph Laplacian, Fiedler vector, AutoGraphiX
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1. Introduction

Let $G = (V, E)$ be a simple (finite) undirected graph with vertex set V and edge set E. Let $n = |V(G)|$ and $m = |E(G)|$ denote the number of vertices and edges of G, respectively. The *Laplacian* of G is the matrix

$$L(G) = D(G) - A(G) , \tag{1}$$

where $A(G)$ denotes the adjacency matrix of the graph and $D(G)$ is the diagonal matrix whose entries are the vertex degrees, i.e., $D_{vv} = d(v)$. We write L for short if there is no risk of confusion.

The Laplacian L is symmetric and all its eigenvalues are nonnegative. The first eigenvalue is always 0. The second smallest eigenvalue, denoted by $\alpha(G)$ in the following, has become quite popular and is called the *algebraic connectivity* of G by Fiedler [12]. It allows some conclusions about the connectedness of the graph. A graph G is connected if and only if $\alpha(G) \neq 0$. Moreover, $\alpha(G)$ is a lower bound for the vertex and edge

connectivities of G. Hence properties of the algebraic connectivity has been investigated in the literature. In particular many upper and lower bounds have been shown. We refer to the recent survey by de Abreu [10] and the references cited therein. An eigenvector corresponding to the algebraic connectivity is called a *Fiedler vector* of the graph.

In this contribution we are interested in the following question: *"Which graph has minimum algebraic connectivity among all connected graphs of given order and size?"* More formally: Given the class

$$\mathcal{C}_{n,m} = \{G \text{ is a connected graph with } |V(G)| = n \text{ and } |E(G)| = m\}. \tag{2}$$

Characterize the graph $G \in \mathcal{C}_{n,m}$ that has least algebraic connectivity. Belhaiza et al. [3] used the AGX-system which raised the conjecture that such extremal graphs belong to a family called path-complete graphs by Šoltés [17]. These are defined as follows: they consist of a complete graph, an isolated vertex or a path and one or several edges joining one end vertex of the path (or the isolated vertex) to one or several vertices of the clique, see [3] for more details. Godsil and Royle [15] assume that *"graphs with small values of $\alpha(G)$ tend to be elongated graphs of large diameter with bridges"*. For example, for trees on n vertices with a fixed diameter the algebraic connectivity is minimized for paths with stars of (almost) equal size attached to both ends, see [11]. Cubic graphs with minimal algebraic connectivity look like a "string of pearls" [7] and trees with a given degree sequence are caterpillars with its highest degrees at its ends [5].

Starting with Brualdi and Solheid [8] there exist a lot of literature that characterize extremal graphs with respect to the spectral radius of the adjacency matrix (often called the *index* of the graph). In contrast there are much fewer results on extremal graphs with respect to the algebraic connectivity [10]. The reason might be that Fiedler vectors change sign and thus tools that are based on graph perturbations are difficult to apply. In this paper we show that the concept of *geometric nodal domain* that we have already used in [5] is also suited for the problem given above. Thus we are able to do a step towards a proof of the conjecture that graphs with prescribed order and size that have minimal algrebraic connectivity are path-complete graphs.

The paper is organized as follows: Section 2 collects well-known facts that we need for our investigations. In Section 3 we show that level sets of any Fiedler vector for an extremal graph are always connected and induce cliques. In Section 4 we give conditions on the number of cliques of size 2 or larger. We show that there are not more than 8 such cliques when there is at most one characteristic edge (where the Fielder vector changes sign). Notice that path-complete graphs have at most two such cliques.

2. Preliminary Results

2.1. Basic Properties

We write $e = uv$ for an edge with end vertices u and v and use the symbol $u \sim v$ to indicate that these vertices are adjacent. For technical reasons we also have to deal with weighted graphs. Let $w(e)$ denote the weight of edge $e \in E$. Then the Laplacian is defined analogously as $L(G) = D(G) - A(G)$, where the adjacency matrix contains the edge weights and the diagonal entries of $D(G)$ are the sums of the weights of the edges incident to the vertices of G, i.e. $D_{vv} = \sum_{u \sim v} w(vu)$.

Obviously every eigenvector f corresponding to some eigenvalue λ must satisfy the eigenvalue equation

$$(Lf)(v) = \sum_{uv \in E} w(uv)(f(v) - f(u)) = \lambda f(v) . \tag{3}$$

Proposition 1 ([6]). *Let f be an eigenvector corresponding to an eigenvalue $\lambda \neq 0$ of L. Then the following holds:*

(i) *If $f(x) > 0$, then there exists a neighbor $y \sim x$ with $f(y) < f(x)$.*

(ii) *Every local maximum v_m of f (i.e., $f(v_m) \geq f(u)$ for all neighbors $u \sim v_m$) has strictly positive evaluation, i.e., $f(v_m) > 0$.*

(iii) *If z is a zero vertex of f (i.e., $f(z) = 0$), then either all neighbors of z are also zero vertices, or there exist positive and negative vertices of f (i.e., vertices with positive and negative valuation) that are adjacent to z.*

The Rayleigh quotient associated to the Laplacian matrix L is defined by

$$\mathcal{R}_L(f) = \frac{\langle f, Lf \rangle}{\langle f, f \rangle} = \frac{\sum_{uv \in E} w(uv)(f(u) - f(v))^2}{\sum_{v \in V} f(v)^2} . \tag{4}$$

The following results characterize the algebraic connectivity $\alpha(G)$. It is an immediately corollary of the Courant-Fischer Theorem.

Proposition 2. *For a graph $G = (V, E)$ we have*

$$\alpha(G) = \min_{f \neq 0 \in \mathbb{R}^{|V|}, \sum f(v) = 0} \mathcal{R}_L(f) . \tag{5}$$

Moreover, $f \neq 0$ is a Fiedler vector if and only if $\sum_{v \in V} f(v) = 0$ and $\mathcal{R}_L(f) = \alpha(G)$.

2.2. Nodal Domains and Dirichlet Matrix

Fiedler [13] has shown that the subgraph induced by all non-positive vertices of any Fiedler vector and the subgraph induced by all non-negative vertices are both connected. Such connected subgraphs are called *weak nodal domains* [6, 9] or *Perron components* [16].

For further investigations we use the notion of a *graph with boundary* $G(V_0 \cup \partial V, E_0 \cup \partial E)$ introduced by Friedman [14]. Thus the vertex set V of a graph is partitioned into a non-empty set V_0 of so called *interior vertices* and a set of ∂V of so called *boundary vertices*. Edges that join interior vertices are then called *interior edges* and edges that join an interior vertex with a boundary vertex is called *boundary edge*. The respective sets are denoted by E_0 and ∂E. There are no edges between boundary vertices. Figure 1 shows a graph with one boundary vertex.

The *Dirichlet matrix* L_0 is the matrix obtained from graph Laplacian L by deleting all rows and columns that correspond to boundary vertices. The first Dirichlet eigenvalue $\nu(G)$ of L_0 is strictly positive. If the graph induced by the interior vertices is connected, then $\nu(G)$ is simple and there exists an eigenvector which is strictly positive at all interior vertices.
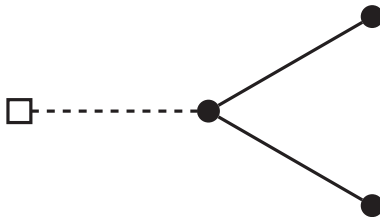
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Figure 1: Graph with one boundary vertex (□) and three interior vertices (●). There are one boundary edge (dashed line) and two interior edges.

Proposition 3. *For a graph with boundary $G(V_0 \cup \partial V, E_0 \cup \partial E)$ we have*

$$\nu(G) = \min_{f \neq 0 \in \mathbb{R}^{|V_0|}} \mathcal{R}_{L_0}(f) \tag{6}$$

Moreover, $f \neq 0$ is an eigenvector affording the first Dirichlet eigenvalue $\nu(G)$ if and only if $\mathcal{R}_{L_0}(f) = \nu(G)$.

Analogously to [5] we introduce the concept of a *geometric nodal domain* of a (Fiedler) eigenvector f. Following Fiedler [13] we call all vertices where f vanishes the *characteristic vertices* of G and all edges where f changes sign the *characteristic edges* of G. Now we subdivide every characteristic edge $e = xy \in E(G)$ into edges $e_1 = xv_0$ and $e_2 = v_0 y$ with weights $w_1 = |f(y) - f(x)|/|f(x)|$ and $w_2 = |f(y) - f(x)|/|f(y)|$, respectively, by inserting a new vertex v_0. By this procedure we obtain a new (weighted) graph G' with the same algebraic connectivity $\alpha(G)$ and a corresponding Fiedler vector f' with $f'(v) = f(v)$ for all $v \in G$ and $f(v_0) = 0$ for all new vertices v_0. Thus the connected graph G^+ (G^-) introduced by the non-negative (non-positive) vertices of G' can be seen as a graph with the zero vertices (where f' vanishes) as its boundary vertices. Its first Dirichlet eigenvalue coincide with $\alpha(G)$ with f' restricted to G^+ as the corresponding eigenvector, i.e., $\alpha(G) = \nu(G^+)$, see [5, 6] for further details. We call the graph G^+ a *geometric nodal domains* of G. Figure 2 illustrates the situation for the Fiedler vector of a tree.

Now we do the opposite and *glue* two graphs with boundary together along their boundary vertices. Let $G_1 = (V_1, E_2)$ and $G_2 = (V_2, E_2)$ be two connected graphs with boundary with the same number of boundary vertices, $|\partial V_1| = |\partial V_2|$. Then we construct a new graph G without boundary by identifying boundary vertices of G_1 with those of G_2 pairwise and turning these into interior vertices. If such a new interior vertices v_0 has degree 2 we may (but need not) replace this vertex and its incident edges of weights $1/c_1$ and $1/c_2$ by a new edge of weight $1/(c_1 + c_2)$. The latter procedure is necessary if we want to revert the decomposition of the graph in its geometric nodal domains. So let us call this *mending* an edge. The following result provides us an estimate on the algebraic connectectivity whem mending an edge in terms of the first Dirichlet eigenvalues of the corresponding components.

Proposition 4 ([1, Lemma 2]). *Let G be a connected graph and D any diagonal matrix. Let μ denote the second smallest eigenvalue of $L(G) = D - A(G)$. Let W be a set of G such that $G - W$ is disconnected and L_1, L_2 be the principal submatrices of $L(G)$*
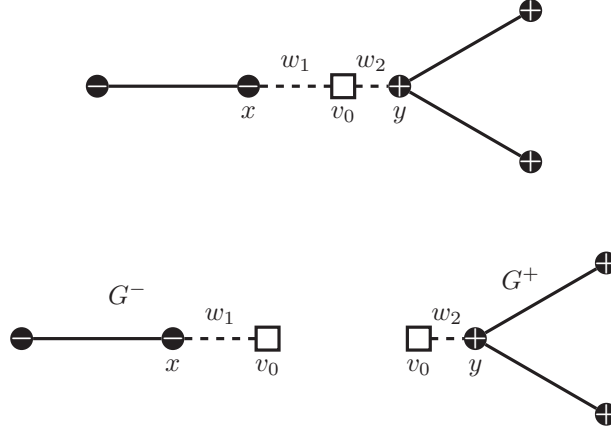
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Figure 2: Construction of the positive and negative geometric nodal domain of Fiedler vector f of a tree. We first split a (possible) characteristic edge xy by a new vertex v_0 with weights $w_1 = |f(y) - f(x)|/|f(x)|$ and $w_2 = |f(y) - f(x)|/|f(y)|$ for the respective edges xv_0 and v_0y. We set $f(v_0) = 0$, i.e., v_0 is then a characteristic vertex of f. The negative (positive) geometric nodal domain is the subgraph G^- (G^+) of all vertices with non-positive (non-negative) evaluation.

corresponding the components G_1 and G_2. Suppose $\tau(L_1) \leq \tau(L_2)$, where $\tau(M)$ denotes the smallest eigenvalue of matrix M. Then either $\tau(L_2) > \mu$ or $\tau(L_1) = \tau(L_2) = \mu$.

Lemma 5. *Let $G_1 = (V_1, E_2)$ and $G_2 = (V_2, E_2)$ be two connected graphs with boundary. Let G be a graph obtained by glueing G_1 and G_2 together. Then $\alpha(G) \leq \max(\nu(G_1), \nu(G_2))$ where the inequality is strict if $\nu(G_1) \neq \nu(G_2)$.*

PROOF. Let W be the set of vertices in G that are obtained by the identifying the boundary vertices in G_1 and G_2. Then Lemma 2 of [1] implies the result. Notice that we get the Dirichlet matrices $L_0(G_1)$ and $L_0(G_1)$ are just the respective principle submatrices of the Laplacian $L(G)$. $\square$

Corollary 6. *For a graph $G \in \mathcal{C}_{n,m}$ let G_1 and G_2 denote the two geometric nodal domains of a Fiedler vector f. If G_1 or G_2 does not have minimum first Dirichlet eigenvalue among all graphs with the same number of boundary vertices, interior vertices and edges, then G cannot have minimum algebraic connectivity in class $\mathcal{C}_{n,m}$.*

2.3. Graph Perturbations

Assume we have an edge $xu \in E(G)$ but $xv \notin E(G)$. Then we get a new graph G' by replacing edges xu by xv. This graph perturbation is called *shifting* in [4]. If G belongs to class $\mathcal{C}_{n,m}$ then $G' \in \mathcal{C}_{n,m}$ whenever G' remains connected.

Lemma 7 (*Shifting* [2, 4]). *Let f be a Fiedler vector of G and let G' be a graph obtained from G by shifting edge xu to xv. If $f(x) \leq f(v) \leq f(u)$ or $f(x) \geq f(v) \geq f(u)$, then $\alpha(G') \leq \alpha(G)$. If at least one of these inequalities is strict, then $\alpha(G') < \alpha(G)$.*

PROOF. Without loss of generality we assume $||f||_2 = 1$. Then a straightforward computation gives $\mathcal{R}_{L(G')}(f) - \mathcal{R}_{L(G)}(f) = ((f(x) - f(u)) + (f(x) - f(v))) \cdot (f(u) - f(v)) \leq 0$.

Hence $\alpha(G') \le \mathcal{R}_{L(G')}(f) \le \mathcal{R}_{L(G)}(f) = \alpha(G)$. The first inequality must be strict if $f(x) \ne f(v)$ or $f(v) \ne f(u)$, since otherwise f would be a Fielder vector on G' by Proposition 2 but violates eigenvalue equation (3) for one of the vertices x, v, u on G', a contradiction. $\qquad\square$

The following lemma describes the (well-known) effect of adding or removing edges.

Lemma 8. *Let f be a Fiedler vector of G.*

  (i) *Let G' be a graph obtained from G by removing an edge $xy \in E(G)$. Then $\alpha(G') \le \alpha(G)$, where the equality holds if and only if $f(x) = f(y)$.*

  (ii) *Assume that $x, y \in V(G)$ with $xy \notin E(G)$. Let G' be a graph obtained from G by adding edge xy. If $f(x) = f(y)$, then $\alpha(G') = \alpha(G)$.*

For a graph with boundary $G(V_0 \cup \partial V, E_0 \cup \partial E)$ an analogous result holds for an eigenvector to the first Dirichlet eigenvalue $\nu(G)$.

PROOF. The statements immediately follow from the Courant-Fisher Theorem (Propositions 2 and 3) and eigenvalue equation (3). $\qquad\square$

3. Level Sets and Cliques

In the following let G be an *extremal graph* in $\mathcal{C}_{n,m}$ and let f be a Fiedler vector. We define induced subgraphs

$$G_\beta^+ = G[\{v \in V(G) \colon f(v) \ge \beta\}] \quad \text{and} \quad G_\beta^- = G[\{v \in V(G) \colon f(v) \le \beta\}] \,.$$

Then the following generalization of Fiedler's nodal domain result holds for extremal graphs.

Theorem 1. *Let G be an* extremal graph *in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. Then G_β^+ and G_β^- are connected (or empty) for all $\beta \in \mathbb{R}$.*

PROOF. G_0^+ is connected by Fiedler's Theorem [13]. Thus G_β^+ is connected for all $\beta \le 0$ as otherwise we had a strictly negative local maximum in f, a contradiction to Proposition 1. Now suppose we find a $\beta > 0$ such that G_β^+ is disconnected with (at least) two components G_1 and G_2. Let v_m be the maximum of f in G_1 and assume $f(u) \le f(v_m)$ for all $u \in V(G_2)$ (otherwise exchange the rôles of G_1 and G_2). Then there exist vertices $x \in G_2$ that are adjacent to vertices y with $f(y) < \beta$, since otherwise G would not be connected. Now we shift all these edges xy to xv_m and get a new connected graph $G' \in \mathcal{C}_{n,m}$. Construct a vector f' on G' by $f'(w) = f(v_m)$ for all $w \in V(G_2)$ and $f'(w) = f(w)$ otherwise. Thus by Lemma 7, $\mathcal{R}_{L_0(G^+)}(f) \ge \mathcal{R}_{L_0(G'^+)}(f') > \nu(G'^+)$ where the last inequality must be strict since the eigenvalue equation (3) is violated for x on G'^+. As G_β^+ is subgraph of the positive geometric nodal domain G^+, f restricted to G^+ is an eigenvector corresponding to $\nu(G^+)$ and thus $\alpha(G) = \nu(G^+) = \mathcal{R}_{L_0(G^+)}(f) > \nu(G'^+)$. Thus by Corollary 6, $\alpha(G') < \alpha(G)$, a contradiction to the extremality of G. The statement follows for G_β^- by looking at $-f$ instead of f. $\qquad\square$

Lemma 9 (Triangle argument). *Let u, v, and w be three vertices with $f(u) \leq f(v) \leq f(w)$ where at least one of these inequalities is strict. If $u \sim w$ then also $u \sim v$ and $v \sim w$.*

PROOF. Suppose $u \nsim v$. Then we shift uw to uv and get graph G' with smaller algebraic connectivity by Lemma 7. By Theorem 1, G_β^+ is connected for $\beta = f(v)$ and thus there exists a path from v to w in G_β^+. Hence G' remains connected and consequently $G' \in \mathcal{C}_{n,m}$, a contradiction to the extremality of G. The analogous argument applies if $v \nsim w$. $\qquad\square$

Corollary 10. *Every edge $e = uv$ with $f(u) \neq f(v)$ is either a cut edge or it is contained in a triangle.*

Definition 1. We create a partition $\mathcal{S}_f = \{S_0, \ldots, S_k\}$ of $V(G)$ as follows:

- Let S_0 be the set of all vertices of G where f assumes its maximum.

- Let S_i be the set of vertices in $G \setminus \bigcup\limits_{j=0}^{i-1} S_j$ which are adjacent to vertices in S_{i-1}.

We call the sets S_i the levels of G with respect to f.

It is obvious from this definition that there are no edges between levels S_i and S_j whenever $|i - j| > 1$. Moreover, there must be at least two levels, since f changes sign.

Remark 11. By construction S_i contains all vertices that have distance i from a maximum of f. Thus the size of this partition $|\mathcal{S}_f| = k + 1$ is just the 1 plus the shortest distance between a maximum and a minimum of f.

Lemma 12. *For any two vertices $v_i \in S_i$ and $v_{i+1} \in S_{i+1}$ we find $f(v_i) > f(v_{i+1})$.*

PROOF. By construction the statement holds for S_0 and S_1 and thus for $i = 0$. Now assume it holds for all $j < i$. Let v_m be the minimum of f in S_i and let $u_m \in S_{i-1}$ with $u_m \sim v_m$. Assume that there exists a vertex w with $f(w) \geq f(v_m)$ and $w \notin \bigcup_{j=0}^{i-1} S_j$. By our induction hypothesis $f(v_m) \leq f(w) < f(u_m)$. Then by Lemma 9, $w \sim u_m$ and consequently $w \in S_i$. Thus the proposition follows by induction. $\qquad\square$

Corollary 13 (Level separation argument). *Each two levels S_i and S_{i+1} are separated by some cutting plane, i.e., there exist two numbers $\beta_1 > \beta_2$ such that $S_i \subseteq G_{\beta_1}^+$ and $S_{i+1} \subseteq G_{\beta_2}^-$.*

Theorem 2. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. Then each level S_i induces a clique.*

PROOF. If $|S_i| = 1$, then there is nothing to show. Otherwise, let v and u be two different vertices in S_i. Assume without loss of generality $f(v) \leq f(u)$. If $i = 0$, then there exists a vertex $w \in S_1$ with $w \sim u$. By Lemma 12, $f(w) < f(v) = f(u)$ and thus $u \sim v$ by Lemma 9. If $i > 0$, then by construction there exists a vertex $w \in S_{i-1}$ with $w \sim v$. Again $f(v) \leq f(u) < f(w)$ and $u \sim v$. Thus any two vertices in S_i must be adjacent. $\square$

By the same arguments we can describe how adjacent cliques are connected.

Theorem 3. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. If $x_i \in S_i$ and $x_{i+1} \in S_{i+1}$ are adjacent, then $y_i \in S_i$ and $y_{i+1} \in S_{i+1}$ are also adjacent whenever $f(y_i) \leq f(x_i)$ and $f(y_{i+1}) \geq f(x_{i+1})$.*

We have two immediate corollaries for this theorem.

Lemma 14. *Let v_i° denote a minimum of f in S_i. Then $S_{i+1} \cup \{v_i^\circ\}$ induces a clique.*

Theorem 4. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. Then $S_0 \cup S_1$ induces a clique.*

Theorem 5. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. If $f(v) > 0$ for all $v \in S_1$ then each vertex $v \in S_1$ is adjacent to a vertex in S_2.*

PROOF. Suppose we find a $v \in S_1$ that is not adjacent to some vertex in S_2. Let $w \in S_0$. By construction, $f(w) > f(v)$. By Theorem 4, v and w have the same neighbors except v and w, respectively. Thus a straightforward computation using (3) gives $(d - \alpha(G) + 1)(f(v) - f(w)) = 0$ and consequently $\alpha(G) = d + 1$ where d denotes the degree of v and w. However, the algebraic connectivity is bounded from above by the minimum degree of G, a contradiction. $\qquad\square$

4. Counting Cliques

In the previous section we have shown that an extremal graph G consists of a chain of cliques. Using our notation we can describe path-complete graphs and formulate the conjecture of Belhaiza et al. [3] in the following way:

Conjecture 1. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G. Let S_i be as in Definition 1. Then $S_{i-1} \cup S_i$ induces a clique for all $i = 1, \ldots, |\mathcal{S}_f|$ and $|S_j| = 1$ for all $j \geq 2$ or all $j \leq |\mathcal{S}_f| - 1$.*

Thus we have to count the number of cliques S_j of size larger than 1. Let us call such cliques *proper*. Furthermore, we say that (proper) cliques build a chain if their union induces a connected graph.

Now let us look at the positive nodal domain G^+ of G. Assume first that there is only one characteristic edge or vertex. Thus all levels consist of vertices with nonnegative valuation. Let ℓ be the index of the lowest level in G^+ and let $n_i = |S_i|$ be the number of vertices in S_i. Let v° be the boundary vertex of the geometric nodal domain and let P be a shortest path from a vertex in level S_0 to v°. Obviously $P \cap S_i = \{v_i^\circ\}$ consists of a single vertex. Let $S_i^\circ = S_i \setminus \{v_i^\circ\}$ (which might be $\emptyset$). By Lemma 14 we choose v_i° such that it minimizes Fiedler vector f in S_i.

Suppose that there is some proper clique S_p with $p \geq 2$. Then we might try to construct a new positive nodal domain G^* and a function f^* in the following way (see Fig. 3):
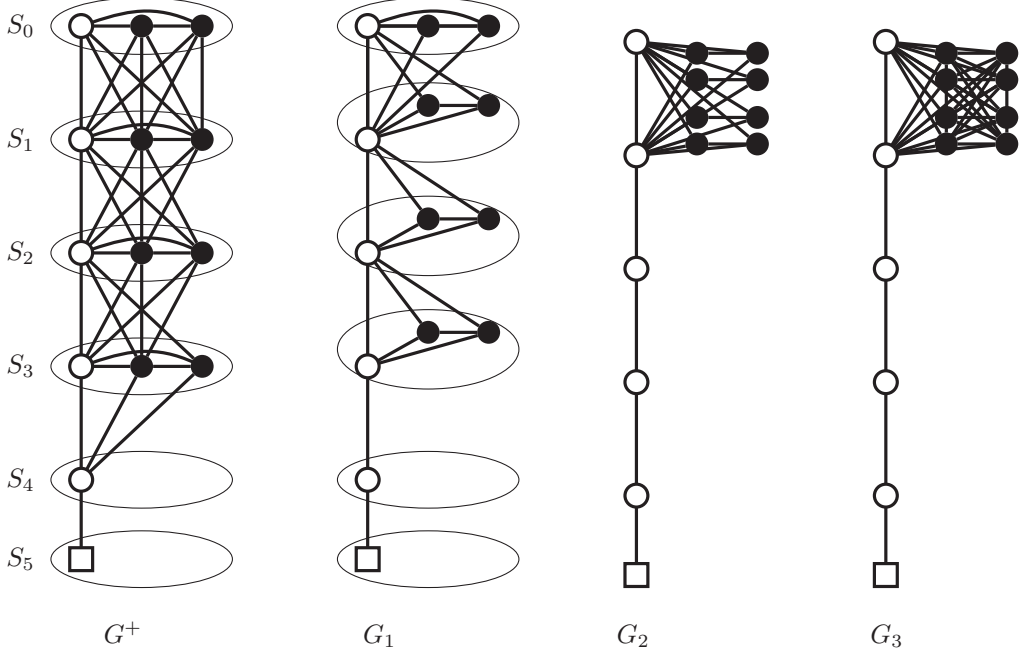
Figure 3: Graphs with boundary from Steps 1–4
($\square$ ... boundary vertex, $\circ$ ... vertices $v_0^\circ, \ldots, v_\ell^\circ$ in path P, $\bullet$ ... vertices in $S_0^\circ \cup \cdots \cup S_\ell^\circ$, $\ell = 5$)

Step 1. For $i = 1, \ldots, \ell$, remove all edges between cliques S_{i-1} and S_i that are not incident to v_{i-1}° or v_1°. By Lemma 14 we get a new connected graph G_1 with boundary. Let f_1 be an eigenvector corresponding to the first Dirichlet eigenvalue. Then by Lemmata 8 and 12 we have $\nu(G_1) \leq \nu(G^+)$ where the inequality is strict whenever we remove at least one edge. Notice that in G_1 the vertices of clique S_i° are only adjacent to vertices in $S_i^\circ \cup \{v_{i-1}^\circ, v_i^\circ\}$. Moreover, f_1 is constant on S_i° by symmetry, since otherwise $\nu(G_1)$ were not a simple eigenvalue. By Proposition 1 we find $f_1(v_i^\circ) < f_1(y)$ for all $y \in S_i^\circ$. (We do not know yet, whether we also have $f_1(y) \leq f_1(v_{i-1}^\circ)$.)

Step 2. Let k be such that $f_1(v_{k-1}^\circ) - f_1(v_k^\circ) \leq f_1(v_{j-1}^\circ) - f_1(v_j^\circ)$ for all $j = 1, \ldots, \ell$, that is, k minimizes $f_1(v_{j-1}^\circ) - f_1(v_j^\circ)$. Let $\varepsilon = (f_1(v_0^\circ) - f_1(v_1^\circ)) - (f_1(v_{k-1}^\circ) - f_1(v_k^\circ)) \geq 0$. Define f_2 by

$$f_2(x) = \begin{cases} \max\{f_1(x) + \varepsilon, \, f_1(v_0^\circ)\}, & \text{for } x \in \{v_0^\circ, \ldots, v_{k-1}^\circ\}, \\ \max\{f_1(v_1^\circ) + f_1(x) - f_1(v_j^\circ), f_1(v_0^\circ)\}, & \text{for } x \in S_j^\circ \text{ and } j = 2, \ldots, \ell, \quad (7) \\ f_1(x), & \text{otherwise.} \end{cases}$$

Then we find for all $j = 1, \ldots, \ell$, $f_2(v_j^\circ) \geq f_1(v_j^\circ)$ and $f_1(v_1^\circ) \leq f_2(v_1^\circ) < f_2(x) \leq f_2(v_0^\circ)$ for all $x \notin \{v_0^\circ, \ldots, v_\ell^\circ\}$. Consequently $(f_2(x))^2 \geq (f_1(x))^2$ for all $x \in G_1$ where the inequality is strict for every $x \in S_j^\circ$ with $j \geq 2$.

For edges $v_{j-1}^\circ v_j^\circ$ we have $f_2(v_0^\circ) - f_2(v_1^\circ) = f_1(v_0^\circ) - (f_1(v_1^\circ) + \varepsilon) = f_1(v_{k-1}^\circ) - f_2(v_k^\circ)$, $f_2(v_{k-1}^\circ) - f_2(v_k^\circ) = f_1(v_{k-1}^\circ) + \varepsilon - f_1(v_k^\circ) = f_1(v_0^\circ) - f_1(v_1^\circ)$, and $f_2(v_{j-1}^\circ) - $

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$f_2(v_j^\circ) = f_1(v_{j-1}^\circ) - f_2(v_j^\circ)$ for $j \notin \{1, k\}$. Consequently, $\sum_{j=1}^{\ell} (f_2(v_{j-1}^\circ) - f_2(v_j^\circ))^2 = \sum_{j=1}^{\ell} (f_1(v_{j-1}^\circ) - f_1(v_j^\circ))^2$. Notice that we have constructed f_2 such that $j = 1$ minimizes $f_2(v_{j-1}^\circ) - f_2(v_j^\circ)$.

Step 3. For $j = 2, \ldots, \ell$, replace all edges in G_1 between $\{v_{j-1}^\circ, v_j^\circ\}$ and S_j° by corresponding edges between $\{v_0^\circ, v_1^\circ\}$ and S_j°. Thus we obtain a new graph G_2 with boundary. Furthermore, we find for all replaced edges, $|f_2(v_0^\circ) - f_2(x)| \le |f_1(v_{j-1}^\circ) - f_1(x)|$ and $|f_2(v_1^\circ) - f_2(x)| \le |f_1(v_j^\circ) - f_1(x)|$ for $x \in S_j^\circ$. Thus $\sum_{xy \in E(G_2)} (f_2(x) - f_2(y))^2 \le \sum_{xy \in E(G_1)} (f_1(x) - f_1(y))^2$ and consequently $\nu(G_2) \le \mathcal{R}_{L_0(G_2)}(f_2) \le \mathcal{R}_{L_0(G_1)}(f_1) = \nu(G_1) \le \nu(G^+) = \alpha(G)$, where at least one inequality is strict.

Step 4. Notice that G_2 consists of path P and a couple of cliques S_j° such that $S_j^\circ \cup \{v_0^\circ, v_1^\circ\}$ induces a clique for all $j = 0, \ldots, \ell$. Let f_3 be an eigenvector affording the first Dirichlet eigenvalue for G_2. By symmetry f_3 must be constant on all S_j°. Now if $x_i \in S_i^\circ$ and $x_j \in S_j^\circ$, then eigenvalue equation (3) implies that $(2 - \nu(G_2)) f_3(x_i) = f_3(v_0^\circ) + f_3(v_1^\circ) = (2 - \nu(G_2)) f_3(x_j)$. Since $f_3(v_0^\circ) + f_3(v_1^\circ) > 0$ we must have $\nu(G_2) \ne 2$ and $f_3(x_i) = f_3(x_j)$. Thus f_3 is constant on $\bigcup_{i=0}^{\ell} S_i^\circ$. Now construct G_3 by inserting new edges between vertices in $\bigcup_{i=0}^{\ell} S_i^\circ$ (if possible). By Lemma 8 we have $\nu(G_3) = \nu(G_2) < \nu(G^+) = \alpha(G)$.

If we are able to insert all those edges that we have removed during Step 1 we obtain a new graph with boundary $G^* = G_3$ which belongs to the same class as G^+. If we find that $G_3 \not\cong G^+$, then G cannot have smallest algebraic connectivity by Corollary 6.

Theorem 6. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G with one characteristic edge or vertex. Let S_i be as in Definition 1, $n_i = |S_i|$, and ℓ be the index of the lowest level in G^+. Let q denote the number of "missing" edges between adjacent cliques, i.e., the number of tuples $(x_{i-1}, x_i) \in S_{i-1} \times S_i$ with $x_{i-1} x_i \notin E(G)$ for $i = 1, \ldots, \ell$. Then*

$$\delta + q = \sum_{i=0}^{\ell-2} \sum_{j=i+2}^{\ell} (n_i - 1)(n_j - 1) - \sum_{i=1}^{\ell-1} (n_i - 1) + q < 0 \tag{8}$$

where

$$\delta = \sum_{i=0}^{\ell-2} \sum_{j=i+2}^{\ell} (n_i - 1)(n_j - 1) - \sum_{i=1}^{\ell-1} (n_i - 1) . \tag{9}$$

PROOF. Step 4 can only be performed if there are sufficiently many "slots" open where we can insert all the edges that we have removed in Step 1. When we insert all possible edges then G_3 consists of a clique with all vertices from $\cup_{i=0}^{\ell} S_i^\circ \cup \{v_0^\circ, v_1^\circ\}$ and the path $v_1^\circ v_2^\circ \ldots v_\ell^\circ$. Hence the maximal number of edges in the new graph G_3 (without characteristic edge) is given by

$$\frac{1}{2} \left(2 + \sum_{i=0}^{\ell} (n_i - 1) \right) \left(1 + \sum_{i=0}^{\ell} (n_i - 1) \right) + (\ell - 1) . \tag{10}$$

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When G is an extremal graph then G^+ consists of cliques S_i and edges between adjacent cliques S_i and S_{i+1}. Thus the maximal number of edges in the original graph G^+ (without characteristic edge) is given by

$$\frac{1}{2} \sum_{i=0}^{\ell} n_i(n_i - 1) + \sum_{i=0}^{\ell-1} n_i n_{i+1} .\tag{11}$$

The difference δ between (10) and (11) can be simplified as follows:

$$
\begin{aligned}
\delta &= \frac{1}{2}\left(2 + \sum_{i=0}^{\ell}(n_i - 1)\right)\left(1 + \sum_{i=0}^{\ell}(n_i - 1)\right) + (\ell - 1) \\
&\quad - \left(\frac{1}{2}\sum_{i=0}^{\ell} n_i(n_i - 1) + \sum_{i=0}^{\ell-1} n_i n_{i+1}\right) \\
&= \ell + \frac{1}{2}\left(\sum_{i=0}^{\ell}(n_i - 1)\right)^2 - \frac{1}{2}\sum_{i=0}^{\ell}(n_i - 1)^2 + \sum_{i=0}^{\ell}(n_i - 1) - \sum_{i=0}^{\ell-1} n_i n_{i+1} \\
&= \ell + \sum_{i=0}^{\ell-1}\sum_{j=i+1}^{\ell}(n_i - 1)(n_j - 1) + \sum_{i=0}^{\ell}(n_i - 1) - \sum_{i=0}^{\ell-1} n_i n_{i+1} .
\end{aligned}
$$

Using $\sum_{i=0}^{\ell-1} n_i n_{i+1} = \sum_{i=0}^{\ell-1}(n_i - 1)(n_{i+1} - 1) + \sum_{i=0}^{\ell-1} n_i + \sum_{i=0}^{\ell-1} n_{i+1} - \ell$ we arrive at

$$\delta = \sum_{i=0}^{\ell-2}\sum_{j=i+2}^{\ell}(n_i - 1)(n_j - 1) - \sum_{i=1}^{\ell-1}(n_i - 1)$$

The number of free "slots" is $\delta + q$. Notice that we can perform Steps 1–4 whenever the number of edges in the original graph G^+ does not exceed (10). Consequently, G cannot be extremal if $\delta + q \geq 0$. $\qquad\square$

Theorem 6 gives a necessary condition for extremal graphs. We can deduce a few structural elements. In particular we can easily derive that there must not be too many proper cliques.

Theorem 7. *Let G be an extremal graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G with one characteristic edge or vertex. Let S_i be as in Definition 1, $n_i = |S_i|$, and ℓ the index of the lowest level in G^+. Then the following holds:*

(i) If $n_0 \geq 2$, then there are at most three proper cliques, which are $\{S_0\}$, $\{S_0, S_1\}$, or $\{S_0, S_1, S_2\}$.

(ii) If $n_0 = 1$, then there are at most four proper cliques. If there are four proper cliques, then they must build a chain.

PROOF. δ as defined in (9) can be seen as a quadratic function in $n_0, \ldots, n_\ell$. Its partial derivatives are given by

$$\frac{\partial \delta}{\partial n_k} = \sum_{\substack{j=0 \\ j \notin \{k-1, k, k+1\}}}^{\ell}(n_j - 1) - \begin{cases} 0 & \text{if } k \in \{0, \ell\}, \\ 1 & \text{otherwise.} \end{cases}$$

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We want to characterize extremal graphs. Thus by Theorem 6 we have to find minimal forbidden configurations where $\delta \geq -q$ and where all partial derivatives are nonnegative. The latter is satisfied when there is at least one proper clique which is not adjacent to S_k.

Case $n_0 \geq 2$: If $n_0 = n_j = 2$ for some $j \geq 2$ and $n_k = 1$ otherwise, then $\delta = 0$. Moreover, $\frac{\partial \delta}{\partial n_i} \geq 0$ except when $i = 1$ and $j = 2$. Thus (i) holds.

Case $n_0 = 1$: Let $J = \{j, j+1, j+2, j+3, j+4\}$ such that $n_j = 2$ for all $j \in J$ and $n_k = 1$ for all $k \notin J$. Then $\delta = 1$ and $\frac{\partial \delta}{\partial n_i} \geq 2$. Hence there cannot be more than four proper cliques. If these four cliques do not build a chain we again find $\delta \geq 0$. Thus (2) holds. $\qquad \square$

Remark 15. It is obvious that Theorems 6 and 7 hold completely analogously for the negative nodal domain G^-.

Remark 16. One can deduce more rules when there are at most three proper cliques for the case $n_0 = 1$.

What can be done when there is more than one characteristic edge (where the Fiedler vector f changes sign)? Assume there is a clique S_c that contains both vertices with positive and negative valuation. Then we can proceed as follows: Remove all but one characteristic edges. Denote its number by m_c. Then construct a graph with boundary for the positive (and negative) geometric nodal domain. Every vertex where f vanishes is assigned to one of the two nodal domains (not necessarily the same for each of these vertices). Then we can rearrange the two nodal domains as for the proof of Theorem 6. However, we have insert the characteristic edges again to obtain the same total number of edges for the resulting graph. Thus we can partition this set of edges for both nodal domains in any way that is appropriate. Thus we arrive at the following result.

Theorem 8. *Let G be an* extremal *graph in $\mathcal{C}_{n,m}$ and f a Fiedler vector of G with one characteristic edge or vertex. Let S_i be as in Definition 1, $n_i = |S_i|$, and ℓ^+ the index of the lowest level in G^+ and ℓ^- the index of the highest level in G^-. Let $\ell = |\mathcal{S}_f| = \ell^+ + \ell^-$. Then at least one of the following inequalities must hold for every choice of $m_c^+ \geq 0$ and $m_c^- \geq 0$ such that $m_c^+ + m_c^- + 1$ is the number of characteristic edges.*

$$\delta^+ = \sum_{i=0}^{\ell^+-2} \sum_{j=i+2}^{\ell^+} (n_i - 1)(n_j - 1) - \sum_{i=1}^{\ell^+-1} (n_i - 1) + q^+ - m_c^+ < 0 \,,$$

$$\delta^- = \sum_{i=\ell^-}^{\ell-2} \sum_{j=i+2}^{\ell} (n_i - 1)(n_j - 1) - \sum_{i=\ell^-+1}^{\ell-1} (n_i - 1) + q^- - m_c^- < 0 \,.$$

q^+ and q^- denote the number of "missing" edges between adjacent cliques in the positive and negative nodal domain, respectively.

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