Graphs with the second signless Laplacian eigenvalue $\leq 4$

Abstract: We discuss the question of classifying the connected simple graphs $H$ for which the second largest eigenvalue of the signless Laplacian $Q(H)$ is $\leq 4$. We discover that the question is inextricably linked to a knapsack problem with infinitely many allowed weights. We take the first few steps towards the general solution. We prove that this class of graphs is minor closed.

Keywords: Signless Laplacian, eigenvalues of a graph, Signless Laplacian matrix, $Q$-eigenvalue, Second largest eigenvalue

MSC: 05C50

1 Notations and Definitions

The symbol $I$ will denote the identity matrix of suitable size for the context. For a square matrix $M$ and $k$ a positive integer we denote $\lambda_k(M)$ the $k^{th}$ largest eigenvalue of $M$. We denote $E_{p,q}$ the matrix of appropriate shape with 1 in the $(p, q)$ entry and zeros elsewhere. We also by $J_{p,q}$ the $p \times q$ matrix in which every entry is 1 and $J_p = J_p,p$.

For a graph $G$ and a vertex $v$ of $G$ we denote by $d_v(G)$ (or $d_v$ if the context is clear) the degree of the vertex $v$ in $G$. We denote by $C_n$ a cycle with $n$ vertices, $P_n$ a path with $n$ vertices (and length $n - 1$).

If $G_j$ ($j = 1, \ldots, m$) are rooted graphs on disjoint vertex sets $V_j$ ($j = 1, \ldots, m$) with root vertices $v_j \in V_j$ ($j = 1, \ldots, m$), we consider a graph $G$ on the vertex set $\bigcup_{j=1}^m V_j$ with the $v_j$ identified, obtained by the replacement of all the $v_j$ ($j = 1, \ldots, m$) by a new vertex $v$ adjacent to all of the neighbors of $v_j$ in $G_j$ for all $j$ ($j = 1, \ldots, m$). We consider $G$ as a rooted graph with root vertex $v$. Such a graph $G$ (or an isomorphic copy of it) will be referred to as the graph obtained from the $G_j$ by identifying the roots.

Example 1.1. Let $G_1$ be a rooted $C_3$, $G_2$ a rooted $P_2$ and $G_3$ a $P_3$ rooted at an end vertex. Then the graph $G$ would be the graph depicted in Figure 1.

2 Introduction

Let $\kappa_k(G)$ or simply $\kappa_k$ be the $k^{th}$ largest eigenvalue of the signless Laplacian $Q(G) = D(G) + A(G)$ of a finite simple graph $G$, i.e. $\kappa_k(G) = \lambda_k(Q(G))$. Here $A(G)$ is the adjacency matrix of $G$ and $D(G)$ is the diagonal matrix of vertex degrees. In [1] the connected graphs $G$ such that $\kappa_2(G) \leq 3$ are classified and in [8] the same is achieved for $\kappa_2(G) \leq 2 + \sqrt{2}$. We will call a connected graph $\alpha$-compliant if $\kappa_2(G) \leq \alpha$. 

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The classifications given in these articles follow a similar pattern. In each classification, there is a family of graphs of unlimited degree at a particular root vertex satisfying the required spectral property which we will call $G$-graphs (depending on $\alpha$) and there is another family of exceptional graphs which also satisfy the spectral property. For a connected rooted graph $G$, we denote by $Q_{\text{root}}(G)$ the matrix $Q(G)$ with the row and column corresponding to the root vertex deleted. A graph of the family of $G$-graphs is obtained by taking any set of connected rooted graphs with $\rho(Q_{\text{root}}(G)) \leq \alpha$ and identifying all the roots to a single vertex. For $\alpha = \sqrt{2}$, the connected rooted graphs that satisfy this condition are $C_3$, $P_2$, and $P_3$ rooted at an end vertex. For $\alpha = 2 + \sqrt{2}$, the relevant connected rooted graphs are $C_3$, $C_4$ and $P_2$, $P_3$ and $P_4$ rooted at an end vertex. For $\alpha = 3$, there are 4 exceptional graphs and for $\alpha = 2 + \sqrt{2}$ there are 17 exceptional graphs.

The authors of [8] suggest that the same should be done for $\kappa_2(G) \leq 4$ and this is the subject of these notes. There are two known results that explain the significance of $\kappa_2(G) \leq 4$. We denote by $P_n$ the path with $n$ vertices and by $C_n$ the cycle with $n$ vertices.

**Lemma 2.1.** Let $H$ be an order $n$ subgraph of a graph $G$. Then $\kappa_k(H) \leq \kappa_k(G)$ for $k = 1, 2, \ldots, n$.

For the proof see [4, Theorem 2.1]. The underlying reason is that $Q(G) = X(G)X(G)'$ where $X(G)$ is the incidence matrix of $G$. If we define $Z(G) = X(G)'X(G)$, then $Q(G)$ and $Z(G)$ have the same non-zero eigenvalues and $Z(H)$ is a principal submatrix of $Z(G)$. It follows that the eigenvalues of $Z(H)$ interlace those of $Z(G)$ by the standard interlacing inequality [2, Corollary 2.5.2].

**Lemma 2.2.** The eigenvalues of $Q(C_n)$ are $4 \left( \cos \left( \frac{k\pi}{n} \right) \right)^2$ for $k = 0, 1, \ldots, n - 1$. 
From these lemmas we find that $\kappa_2(P_n) \leq \kappa_2(C_n) = 4 \left( \cos \left( \frac{\pi}{n} \right) \right)^2 < 4$. In the classifications of [1, 8] already graphs with unlimited maximal degree appear and it now becomes clear that in the $\kappa_2 \leq 4$ problem we will also need to handle graphs with unlimited diameter.

The method used in [8] is to produce a list of 29 minimal forbidden graphs (the authors do not say how they were obtained) and then using involved and delicate arguments they establish the classification.

**Definition 2.3.** An emergent graph is a graph that is not a $\mathcal{S}$-graph, but can be obtained from a $\mathcal{S}$-graph by adding either an edge between existing vertices or by adding a pendent edge and vertex.

**Definition 2.4.** A minimal emergent graph is an emergent graph which does not have another emergent graph as a subgraph.

There is an easier method, one that is open to computer calculation. It is based on the fact that every connected graph can be built from a single vertex by successively adding pendent vertices and edges.

In our thought experiment we start from a single vertex and successively add pendent vertices and edges. At each step we may possibly remain within the family of $\mathcal{S}$-graphs indefinitely or we may exit the family of $\mathcal{S}$-graphs.

The ways of exiting the family of $\mathcal{S}$-graphs are limited in such a way that it is easy to determine the collection $\mathcal{E}$ of minimal emergent graphs. Fortunately $\mathcal{E}$ is finite. A key observation is that every subgraph of a $\mathcal{S}$-graph is again a $\mathcal{S}$-graph so that by restarting the process from the graphs in $\mathcal{E}$ we can never reenter the $\mathcal{S}$-graphs. We place the graphs of $\mathcal{E}$ in a queue from which we successively remove graphs. For each such graph $G$ removed, we throw it away if it is not 2- or $\sqrt{2}$-compliant. Otherwise we add pendent and edges in all possible ways to produce graphs $H$. If $\kappa_1(H) \leq 2 + \sqrt{2}$ then we insert $H$ into the queue if it is not already there. If for any $\mathcal{S}$-graph $G$ removed, all augmented graphs $H$ have $\kappa_1(H) > 2 + \sqrt{2}$, then we recognize that $G$ is a maximal graph with $\kappa_2(G) \leq 2 + \sqrt{2}$ and we print it. In this way the queue eventually becomes empty and we find that we have printed a list of 17 graphs, namely the ones described in [8]. Then every connected graph $G$ with $\kappa_2(G) \leq 2 + \sqrt{2}$ is either a $\mathcal{S}$-graph or a subgraph of one of the 17 graphs listed.

The plan in the current article is to apply a similar strategy for 4-compliant graphs. We will not succeed, but we do hope to make some progress in this direction. For the balance of this article we take $\alpha = 4$.

### 3 Attachments and $\mathcal{S}$-graphs

For the remainder of this article we are concerned with graphs $G$ such that $\kappa_2(G) \leq 4$ which we call compliant.

**Definition 3.1.** An abstract $\mathcal{S}$-graph is a connected graph such that by taking some vertex as root, $\lambda_1(Q_{\text{root}}(G)) \leq 4$.

**Definition 3.2.** A rooted $\mathcal{S}$-graph is a connected rooted graph $G$ such that $\lambda_1(Q_{\text{root}}(G)) \leq 4$.

We need the following lemma

**Lemma 3.3.** Let $H$ be a subgraph of a rooted graph $G$ that has the root of $G$ as a vertex and consider this vertex to be the root of $H$. Then $\lambda_1(Q_{\text{root}}(H)) \leq \lambda_1(Q_{\text{root}}(G))$.

**Proof.** The matrix $Q_{\text{root}}(H)$ is entrywise dominated by $Q_{\text{root}}(G)$ or by some principal submatrix of $Q_{\text{root}}(G)$. □

**Definition 3.4.** A $\mathcal{C}$-attachment is a connected rooted graph $G$ of order at least 2 for which $\lambda_1(Q_{\text{root}}(G)) \leq 4$ and such that deleting the root (and any edges incident on the root) does not disconnect the graph.

**Lemma 3.5.** Every $\mathcal{S}$-graph is compliant.
Proof. This follows from standard interlacing inequalities [2, Corollary 2.5.2] that $\kappa_2(G) = \lambda_2(Q(G)) \leq 4$ since $Q_{\text{root}}(G)$ is the submatrix of $Q(G)$ obtained by deleting the single row and corresponding column corresponding to the root.

\[ \text{Proposition 3.6.} \quad \text{The } \mathcal{C}\text{-attachments may be classified as follows:} \]

- A path of length at least one with the root at an end.
- A cycle of length at least 3 with the root anywhere.
- $K_{3,1}$ with the root at a pendent (AC1).
- AC1 with a pendent added at a pendent vertex which is not the root (AC2).
- A rooted $C_3$ but with a pendent added not at the root (AC3).
- A rooted $C_n$ with an edge added from the root to the far vertex (AC4).
- A rooted $C_n$ with a pendent added at a vertex adjacent to the root (AC5).

\[ \text{Figure 2: The forbidden rooted graph.} \]
has a Perron root strictly larger than $4$, the rooted graph depicted above cannot occur in an attachment. It is impossible to have a degree three vertex at distance 2 from the root. Similarly degree three vertices cannot occur at a distance greater than 2.

We proceed by placing a rooted $P_2$ in a queue. Then, we continually remove rooted graphs from the queue and record their appearance. For each rooted graph so removed, we build further attachments in one of the following ways:

- We attach a pendent at any vertex except the root.
- We add an edge to two nonadjacent vertices (one of which may be the root).

If the resulting rooted graph is a $C$-attachment we enqueue it unless
- it is already present in the queue,
- it is a path or cycle with 4 vertices.

This algorithm will eventually record all $C$-attachments except for rooted paths and cycles.

To see this, consider a $C$-attachment $G$. If every neighbour of the root has degree $\leq 2$ then $G$ is a path or a cycle. Otherwise choose an edge that leads from the root to a vertex $v$ of degree $\geq 3$. Remove all the other edges incident with the root to obtain a rooted graph $H$. Note that $H$ has to be connected. Let $K$ be the tree consisting of all the edges incident with $v$. Then $K$ is a subgraph of $H$ and can be extended to a spanning tree $T$ of $H$. Let $C$ denote the current graph as it passes through the algorithm. The algorithm starts with $C$ the rooted $P_2$ with $v$ and the root as vertices. Successively adding pendent edges to $C$ at $v$ we can obtain $K$. Then by successively adding pendent edges to $C$ we can obtain $T$. Then by successively adding edges to $C$ we can obtain $H$. Finally we successively add back to $C$ the edges of $G$ removed in constructing $H$. As soon as $C$ has at least 4 vertices it possess a degree 3 vertex and can never be a path or cycle with 4 vertices. The current graph $C$ is always a $C$-attachment since it is a subgraph of $G$.

![Figure 3: The five attachments AC1, AC2, AC3, AC4, AC5 from left to right.](image)

We now have the structure theorem for $\mathcal{G}$-graphs.

**Theorem 3.7.** Every rooted $\mathcal{G}$-graph $G$ can be obtained by taking a finite union of $C$-attachments and identifying all the roots to a single vertex which is then the root of $G$.

**Proof.** Consider the graph $H$ obtained by deleting the root from $G$. Then split $H$ into connected components and to each component add back the root. It is clear that the resulting graphs $G_j$ are $C$-attachments and that $G$ can be reconstructed from the union of these attachments by identifying all the roots to a single vertex — the root of $G$.

Note that $Q_{\text{root}}(G) = \bigoplus_j Q_{\text{root}}(G_j)$.

An important point is that the largest vertex degree in a $C$-attachment is three.

**Corollary 3.8.** If a $\mathcal{G}$-graph has a vertex of degree four or more, then $G$ is a rooted $\mathcal{G}$-graph at that vertex. A $\mathcal{G}$-graph cannot have two distinct vertices of degree four or more.

The corollary follows from Proposition 3.6 and Theorem 3.7.
Corollary 3.9. Every cycle in a rooted $\mathcal{G}$-graph passes through the root.

4 Effective matrices

We now discuss the effect of adding $k$ vertices in the form of a path or a cycle to a graph $G$. Although in some circumstances the graph $G$ may be arbitrary, usually it will not be a $\mathcal{G}$-graph. Initially for convenience we will suppose that $G$ has order $n$ and that the attachment will be made at the $n$th vertex.

Definition 4.1. For $k$ a positive integer we define the effective matrix $F_k = Q(G) + \frac{6k}{2k+1} E_{n,n}$. We define the effective matrix $F = Q(G) + 4E_{n,n}$.

Proposition 4.2. Let $G$ be a graph of order $n$, the degree of the $n$th vertex being $a$. Let $G_k$ be the graph obtained by attaching a path of length $k$ (with $k \geq 1$) to the $n$th vertex. Then $\kappa_2(G_k) > 4$ (respectively $\kappa_2(G_k) = 4$) according as $\lambda_2(F_k) > 4$ (respectively $\lambda_2(F_k) = 4$).

Proof. We find

$$Q(G_k) = \begin{pmatrix} ? & \cdots & \cdots & ? & 0 & \cdots & 0 \\ \vdots & \ddots & \cdots & \vdots & \vdots \\ \vdots & \vdots & ? & ? & 0 & \vdots \\ ? & \cdots & ? & a + 1 & 1 & \ddots & 0 \\ 0 & \cdots & 1 & 2 & \ddots & \ddots \\ 0 & \cdots & \ddots & \ddots & 2 & 1 \\ 0 & \cdots & \cdots & 0 & 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} R & X' \\ X & Y \end{pmatrix}$$

where $R$ is $n \times n$, $X$ is $k \times n$ and $Y$ is $k \times k$. Using Schur complements, we find that the congruent matrices

$$\begin{pmatrix} 4I - R - X'(4I - Y)^{-1}X & 0 \\ 0 & 4I - Y \end{pmatrix}$$

have the same number of positive, negative and zero eigenvalues. A calculation shows that the matrix $X'(4I - Y)^{-1}X$ has $\frac{2k-1}{2k+1}$ as its $(n, n)$ entry and zeroes elsewhere. Hence the effective matrix

$$F_k = R + \frac{2k-1}{2k+1} E_{n,n}$$

has the same number of eigenvalues $> 4$ and $= 4$ as $Q(G_k)$. Note that all the eigenvalues of $4I - Y$ are strictly positive. This is a consequence of the fact that $4I - Y$ is irreducibly diagonally dominant [7, Theorem 1.11]. We have $\det(4I - Y) = 2k + 1$. For example in case $k = 5$

$$X = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad 4I - Y = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 3 \end{pmatrix}, \quad (4I - Y)^{-1} = \frac{1}{11} \begin{pmatrix} 9 & 7 & 5 & 3 & 1 \\ 7 & 14 & 10 & 6 & 2 \\ 5 & 10 & 15 & 9 & 3 \\ 3 & 6 & 9 & 12 & 4 \\ 1 & 2 & 3 & 4 & 5 \end{pmatrix}$$

We will say that the cost of attaching a path of length $k$ at a single vertex is $\frac{6k}{2k+1}$ at that vertex. The cost of attaching a path of infinite length (whatever that means) is 2.

Using essentially the same method of proof, we have the following.
Proposition 4.3. Let $G$ be a graph of order $n$, the degree of the $n^{th}$ vertex being $a$. Let $G_k$ be the graph obtained by taking a cycle of length $k + 1$ (with $k \geq 2$) and identifying a vertex of the cycle to the $n^{th}$ vertex. Then $\kappa_2(G_k) > 4$ (respectively $\kappa_3(G_k) = 4$) according as $\lambda_2(F) > 4$ (respectively $\lambda_3(F) = 4$).

We will say that the cost of attaching a cycle of any length at a single vertex is 4 at that vertex. In exactly the same way, we can find the costs of the attachments from AC1 to AC5. The cost of AC1 is 4, the cost of AC2 and AC3 is 16 and the cost of AC4 and AC5 is infinite, for AC4 and AC5, the matrix $Y$ already has 4 as an eigenvalue.

Let us be more specific here. Consider for example the case of attaching AC4 to a non-$\mathcal{C}$-graph $G$ at a vertex $v$ of $G$ of degree $d_v$. We denote the resulting graph by $H$. Considering $G$ as a graph rooted at $v$ we see that $Q_{\text{root}}(G) > 4$. Then $Q(H)$ has as principal submatrix the matrix $Q_{\text{root}}(G) \oplus M$ where

$$M = \begin{pmatrix}
a & 1 & 1 & 1 \\
1 & 2 & 0 & 1 \\
1 & 0 & 2 & 1 \\
1 & 1 & 1 & 3
\end{pmatrix}$$

where $a = 3 + d_v \geq 4$. Then both $Q_{\text{root}}(G)$ and $M$ have spectral radius $> 4$ and it follows that $\kappa_2(H) > 4$.

We work a couple of examples to show how costs are calculated. This process follows the proof of Proposition 4.2 with $X$ and $Y$ replaced by analogous matrices. Note that $X$ has shape $k \times 1$ and $Y$ shape $k \times k$ where $k$ is the number of non-root vertices in the attachment.

Example 4.4. If the attachment is a rooted $C_4$, then we may take

$$X = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad Y = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$$

Then $X'(4I - Y)^{-1}X = (2)$ and the cost is 2 plus the degree of the attachment at its root. The cost is 4.

Example 4.5. If the attachment is a rooted AC2, then we may take

$$X = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 3 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

Then $X'(4I - Y)^{-1}X = (15)$ and the cost is 15 plus the degree of the attachment at its root. The cost is 16.

Proposition 4.6. Costs are additive. Specifically let $G$ be a rooted $\mathcal{C}$-graph built from $\mathcal{C}$-attachments $G_j$ for $j = 1, \ldots, m$. Then the cost of $G$ at its root is the sum of the costs of the attachments $G_j$.

Proof. For each $G_j$, let the corresponding matrices be $X_j$ and $Y_j$. Then the corresponding matrices for $G$ are the partitioned matrices

$$X = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_m \end{pmatrix}, \quad Y = \begin{pmatrix} Y_1 & 0 & \cdots & 0 \\ 0 & Y_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & Y_m \end{pmatrix}$$

and a calculation shows that $X'(4I - Y)^{-1}X = \sum_{j=1}^{m} X_j'(4I - Y_j)^{-1}X_j$. The result now follows since $d_{\text{root}}(G) = \sum_{j=1}^{m} d_{\text{root}}(G_j)$. ⊓⊔

We leave the proof of the following proposition to the reader.

Proposition 4.7. Let $G$ be a graph of order $n$. Let $G_j$ be rooted $\mathcal{C}$-graphs for $j = 1, \ldots, n$ rooted at vertices $v_j$. Let $H$ be the graph obtained by attaching each $G_j$ to the $j^{th}$ vertex of $G$ at the vertex $v_j$ of $G_j$. Let $F = Q(G) +$
We see that the examples 5.2 through 5.4 below make use of the Propositions 4.6 and 4.7.

\[ \sum_{j=1}^{n}(\text{cost}(G_j) - d_j(G_j))E_{j,i} \] where \( \text{cost}(G_j) \) is the cost of attaching \( G_j \) at \( v_j \). Then \( \kappa_2(H) > 4 \) (respectively \( \kappa_3(H) = 4 \)) according as \( \lambda_2(\bar{F}) > 4 \) (respectively \( \lambda_2(\bar{F}) = 4 \)).

5 Capacities

Let \( H \) be a compliant rooted graph (typically a non \( \bar{G} \)-graph). We wish to consider which combinations of \( \bar{G} \)-attachments can be attached to the root and maintain compliancy. We define the capacity of the graph at the root to be the greatest value of \( t \) such that \( \lambda_2(Q(H) + tE_{\text{root,root}}) \leq 4 \). It is now clear that the problem of deciding which \( \bar{G} \)-graphs can be attached root to root with \( G \) and produce a compliant graph is essentially a knapsack problem.

The knapsack problem derives its name from the problem faced by someone who possesses a knapsack and must fill it with the most valuable items. Given a set of items, each with a given weight (or cost in our case), which items should be selected for inclusion so that the total weight is less than or equal to the given weight limit (capacity) of the knapsack. Solving the knapsack problem is difficult computationally and was once used in a system of public key encryption.

In our case, the available weights (costs) are the quantities \( \frac{4k}{2k+1} \) for \( k = 1, 2, 3, \ldots \) together with 4 and 16. If one wishes to include the possibility of attaching paths of infinite length, then one should also allow 2 among the possible weights. Note that the additive semigroup generated by these numbers is complicated and has infinitely many points of accumulation.

Note that a capacity of 4 can be satisfied by appending a cycle of length three or more, an AC1 or three pendants.

Computing the capacity is not always easy. In case \( \kappa_1(H) > 4 \), \( \kappa_2(H) < 4 \) and \( \text{det}(4I - Q_{\text{root}}(H)) < 0 \) we may consider \( Q(H) + tE_{\text{root,root}} \) as \( t \) increases from zero. Certainly \( \lambda_1(Q + tE_{\text{root,root}}) \) increases and \( \text{det}(4I - Q(H)) < 0 \). We see that \( \lambda_2(Q(H) + tE_{\text{root,root}}) = 4 \) when \( t = \text{det}(4I - Q(H))/\text{det}(4I - Q_{\text{root}}(H)) \). Then \( t \) is the capacity of the root.

If \( \kappa_1(H) > 4 \), \( \kappa_2(H) = 4 \) and \( \text{det}(4I - Q_{\text{root}}(H)) < 0 \), then the capacity of \( H \) at the root is zero. However, it can also happen that \( \kappa_1(H) > 4 \), \( \kappa_2(H) = 4 \) and \( \text{det}(4I - Q_{\text{root}}(H)) = 0 \) and then we get no information about the capacity. It may be strictly positive even though \( \kappa_2(H) = 4 \).

Example 5.1. Let \( H \) be the rooted graph in Figure 6. Then

\[
Q(H) = \begin{pmatrix}
2 & 1 & 1 & 0 & 0 \\
1 & 2 & 1 & 0 & 0 \\
1 & 1 & 4 & 1 & 1 \\
0 & 0 & 1 & 1 & 0 \\
0 & 0 & 1 & 0 & 1
\end{pmatrix}
\quad \text{and} \quad
Q_{\text{root}}(H) = \begin{pmatrix}
2 & 1 & 0 & 0 \\
1 & 4 & 1 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & 0 & 1
\end{pmatrix}
\]

Then \( \kappa_1(H) = 5.323404276 \) and \( \kappa_2(H) = 2.357926368 \) and \( \text{det}(4I - Q_{\text{root}}(H)) = -21 \). The capacity of the knapsack is

\[
\frac{\text{det}(4I - Q(H))}{\text{det}(4I - Q_{\text{root}}(H))}
\]

which is \( \frac{32}{21} = \frac{24}{17} \) in this example. The cost of a rooted \( P_2 \) is \( \frac{3}{7} \) and the cost of a rooted \( P_3 \) is \( \frac{8}{7} \) from Proposition 4.2. We will obtain a compliant graph by adding two rooted \( P_2 \) total cost \( \frac{3}{7} < \frac{24}{17} \) or one rooted \( P_3 \) cost \( \frac{8}{7} < \frac{24}{17} \), but not by adding a rooted \( C_3 \) cost 4 since \( 4 > \frac{24}{17} \). The result is compliant if the total cost is \( \leq \) the capacity of the knapsack.

The examples 5.2 through 5.4 below make use of the Propositions 4.6 and 4.7.
Example 5.2. Consider adding attachments to the ends of a single edge. Although $P_2$ is a $\bar{S}$-graph this does make sense. If the weights at the vertices are $a$ and $b$, then the effective matrix

\[ \bar{F} = \begin{pmatrix} 1 + a & 1 \\ 1 & 1 + b \end{pmatrix} \]

has its smaller eigenvalue $\leq 4$ if $8 - 3(a + b) + ab \geq 0$ and $a + b \geq 6$. Now attach a single pendent and a path of length 8 to the first vertex. Then $a = \frac{4}{3} + \frac{16}{9} = \frac{28}{9}$, $b = \frac{8}{3} + \frac{8}{5} + \frac{20}{11} + \frac{88}{45} + \frac{100}{51} + \frac{3364}{1683} = 12$. The eigenvalues of the effective matrix are then $\frac{4966}{561}$ and 4. The corresponding graph is a compliant graph with 612 vertices.

Example 5.3. With the same setup as in the previous example, attach to the first vertex a pendent and a path of length 4. To the second vertex attach two pendants, a path of length 2, a path of length 5, a path of length 22, a path of length 25 and a path of length 841. Then

\[ a = \frac{4}{3} + \frac{16}{9} = \frac{28}{9}, \quad b = \frac{8}{3} + \frac{8}{5} + \frac{20}{11} + \frac{88}{45} + \frac{100}{51} + \frac{3364}{1683} = 12 \]

The eigenvalues of the effective matrix are $\frac{118}{9}$ and 4. The corresponding graph is a compliant graph with 904 vertices.

Example 5.4. We may also take a triangle and add attachments at the vertices. In this case, the effective matrix is

\[ \bar{F} = \begin{pmatrix} 2 + a & 1 & 1 \\ 1 & 2 + b & 1 \\ 1 & 1 & 2 + c \end{pmatrix} \]

The locus of $\lambda_2(\bar{F}) = 4$ is shown in Figure 4. The locus of $\lambda_1(\bar{F}) = 4$ lies behind this surface and that of $\lambda_3(\bar{F}) = 4$ lies in front and is connected to the surface at the point $(a, b, c) = (3, 3, 3)$. We remark that the line segments joining $(3, 3, 3)$ to each of the three points $(0, 3, 3)$, $(3, 0, 3)$ and $(3, 3, 0)$ all lie in the surface.

We attach a path of length 3 to the first vertex giving $a = \frac{12}{7}$. To the second vertex we add two pendants, a path of length 2, a path of length 4, a path of length 23 a path of length 529 and a path of length 373297 so that $b = \frac{7}{4} + \frac{8}{7} + \frac{92}{57} + \frac{2116}{1059} + \frac{1493188}{726599} = 12$. We attach nothing to the third vertex, so $c = 0$. Then

\[ \det(\lambda I - \bar{F}) = \frac{1}{7}(\lambda - 4) \left( 7\lambda^2 - 110\lambda + 151 \right) \]

and the resulting graph of order 373863 is a compliant graph.

Example 5.5. Let $H$ be a rooted graph with 9 vertices such that

\[
Q(H) = \begin{bmatrix}
3 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 3 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 3 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 3 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 6 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
\end{bmatrix}
\]
Then $\kappa_1(H) = 7.4040$, $\kappa_2(H) = 4$, $\kappa_3(H) = 4$, $\kappa_4(H) = 3.8176$ and $\det(4I - Q_{\text{root}}(H)) = 0$. Since

$$\det(\lambda I - (Q(H) + tE_{\text{root,root}})) = (\lambda - 2)(\lambda - 3)(\lambda - 4)^2(\lambda - 1)^3(\lambda^4 - 12\lambda^3 + 37\lambda^2 - 22\lambda - t(\lambda^3 - 6\lambda^2 + 7\lambda - 2))$$

we see that as $t$ increases from zero, it is the root $\kappa_4$ that increases, while $\kappa_2$ and $\kappa_3$ remain at $4$. Thus, the capacity at the root is strictly positive (actually $\frac{4}{3}$) in spite of $\kappa_2(H) = 4$.

6 Effective matrices for attaching paths between vertices

**Definition 6.1.** For $k$ a positive integer we define the effective matrix $F'_k$ by

$$F'_k = Q(G) + \frac{2k + 1}{k + 1} (E_{n-1,n-1} + E_{n,n}) + \frac{1}{k + 1} (E_{n-1,n} + E_{n,n-1})$$
Proposition 6.2. Let \( G \) be a graph of order \( n \). Let \( G_k \) be the graph obtained by adding a path of length \( k + 1 \) (with \( k \geq 0 \)) between the \( n - 1 \)th vertex and the \( n \)th vertex. Then \( \kappa_2(G_k) > 4 \) (respectively \( \kappa_2(G_k) = 4 \)) according as \( \lambda_2(F_k') > 4 \) (respectively \( \lambda_2(F_k') = 4 \)). Note that the case \( k = 0 \) corresponds to adding an edge when none was previously present. If these vertices are adjacent then we insist that \( k \geq 1 \) so as not to produce a multiple edge.

Again the method of proof is as for Proposition 4.2. However, to make things clearer we give the following example.

Example 6.3. Consider the complete graph on 4 vertices and we wish to consider attaching a path of length 3 between the last two vertices (i.e. 2 vertices added). The signless Laplacian of the resulting graph is

\[
Q = \begin{pmatrix}
3 & 1 & 1 & 1 & 0 & 0 \\
1 & 3 & 1 & 1 & 0 & 0 \\
1 & 1 & 4 & 1 & 1 & 0 \\
1 & 1 & 1 & 4 & 0 & 1 \\
0 & 0 & 1 & 0 & 2 & 1 \\
0 & 0 & 0 & 1 & 1 & 2 \\
\end{pmatrix}
\]

giving

\[
X = \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix}
\]

and \( Y = \begin{pmatrix} 2 & 1 \\
1 & 2 \end{pmatrix} \)

Then we find

\[
X'(4I - Y)^{-1}X = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 2 & 1 & \frac{1}{2} \\
0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\end{pmatrix}
\]

and note that

\[
\begin{pmatrix}
3 & 1 & 1 & 1 \\
1 & 3 & 1 & 1 \\
1 & 1 & 3 + \frac{5}{2} & 1 + \frac{5}{2} \\
1 & 1 & 1 + \frac{5}{2} & 3 + \frac{5}{2} \\
\end{pmatrix} = \begin{pmatrix}
3 & 1 & 1 & 1 \\
1 & 3 & 1 & 1 \\
1 & 1 & 4 + \frac{5}{2} & 1 + \frac{5}{2} \\
1 & 1 & 1 + \frac{5}{2} & 4 + \frac{5}{2} \\
\end{pmatrix} = \begin{pmatrix}
3 & 1 & 1 & 1 \\
1 & 3 & 1 & 1 \\
1 & 1 & 4 & 1 \\
1 & 1 & 1 & 4 \\
\end{pmatrix} + \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 2 & 1 & \frac{1}{2} \\
0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\end{pmatrix}
\]

Corollary 6.4. In the context of Proposition 6.2, let \( F'_\infty = \lim_{k \to \infty} F'_k \). If \( \lambda_2(F'_\infty) \leq 4 \) then for every positive integer \( k \) adding any path with \( k \) new vertices between the vertices \( n - 1 \) and \( n \) yields a graph \( G_k \) with \( \kappa_2(G_k) \leq 4 \), i.e. a compliant graph.

Proof. If any number \( k \) of added vertices yields a compliant graph, then \( \lambda_2(F'_k) \leq 4 \) and it suffices to let \( k \to \infty \). Conversely if \( \lambda_2(F'_\infty) \leq 4 \), then necessarily \( \lambda_2(F'_k) \leq 4 \) since in every case \( F'_\infty - F'_k \) is positive semidefinite. \( \square \)

A subdivision of a graph \( H \) is a graph obtained from a graph isomorphic to \( H \) by replacing some of its edges by internally vertex disjoint paths.

Corollary 6.5. Let \( G \) be a graph and let \( H \) be subdivision of \( G \). If \( H \) is compliant, then so is \( G \).

Proof. It suffices to prove the result in case \( H \) is obtained from \( G \) by subdividing a single edge of \( G \) once only. The effective matrix of \( H \) minus the effective matrix of \( G \) is \( F'_1 - F'_0 \) which is seen to be positive definite. \( \square \)
It is worth noting that in the situation of Corollary 6.5 it is in general false that \( \kappa_2(G) \leq \kappa_2(H) \) in case \( H \) is not compliant. For certain graphs we have

\[
Q(G) = \begin{pmatrix}
4 & 0 & 0 & 1 & 1 & 1 & 1 \\
0 & 4 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 4 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 4 & 0 & 0 & 1 \\
1 & 1 & 1 & 0 & 5 & 1 & 1 \\
1 & 1 & 1 & 0 & 1 & 5 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 6
\end{pmatrix}
\quad \text{and} \quad
Q(H) = \begin{pmatrix}
4 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\
0 & 4 & 0 & 1 & 1 & 1 & 1 & 0 \\
0 & 0 & 4 & 1 & 1 & 1 & 1 & 0 \\
1 & 1 & 1 & 4 & 0 & 0 & 1 & 0 \\
1 & 1 & 1 & 0 & 5 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 & 1 & 5 & 1 & 0 \\
1 & 1 & 1 & 0 & 1 & 1 & 6 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 2
\end{pmatrix}
\]

and indeed we find that \( \kappa_2(G) = 5 \) and \( \kappa_2(H) = 4.875 \) even though \( H \) is a subdivision of \( G \).

The reader may consult [9] for other results on edge subdivision.

**Lemma 6.6.** Any subdivision of a non-\( \mathcal{G} \)-graph is again a non-\( \mathcal{G} \)-graph.

**Proof.** Again, it suffices to establish this in the case of a single subdivision of a single edge.

If this is false then an unsubdivison of a \( \mathcal{G} \)-graph would be a non-\( \mathcal{G} \)-graph. We investigate where a vertex of degree two might occur in a \( \mathcal{G} \)-graph. If it occurs in a path or cycle attachment, then the unsubdivision would yield a shortened path or cycle attachment. If it occurs in AC2, then the unsubdivison would yield AC1. The degree two vertices of AC3 and AC4 cannot be subdivided. Either unsubdivision of AC5 yields AC3. The only other possibility is that the root might be of degree two. If the graph is a single attachment then it can only be a cycle or AC3 or AC5. The root in AC3 cannot be subdivided. Unsubdividing the root of AC5 gives AC3. The remaining case is that the \( \mathcal{G} \)-graph has exactly two attachments. They must be either paths or AC1 or AC2. It is clear that each of the nine possible combinations yields a \( \mathcal{G} \)-graph on unsubdividing the root. \( \square \)

We may extend Proposition 6.2 with the following.

**Proposition 6.7.** Let \( p_1, \ldots, p_m, q_1, \ldots, q_m \) be vertices of a graph \( G \) with \( p_j \neq q_j \) for \( j = 1, \ldots, m \). Let \( k_1, \ldots, k_m \) be nonnegative integers with \( k_j \geq 1 \) in case \( p_j \) and \( q_j \) are adjacent \( (j = 1, \ldots, m) \). Let \( F' \) be the matrix defined by

\[
F' = Q(G) + \sum_{j=1}^{m} \left( \frac{2k_j}{k_j + 1} (E_{p_j, p_j} + E_{q_j, q_j}) + \frac{1}{k_j + 1} (E_{p_j, q_j} + E_{q_j, p_j}) \right)
\]

Let \( H \) be the graph in which for each \( j = 1, \ldots, m \) a path of length \( k_j \) has been added between \( p_j \) and \( q_j \). Then \( \kappa_2(H) > 4 \) (respectively \( \kappa_2(H) = 4 \) according as \( \lambda_2(F') > 4 \) (respectively \( \lambda_2(F') = 4 \)).

In this proposition, the vertices \( p_1, \ldots, p_m, q_1, \ldots, q_m \) do not have to be distinct. The proof is left to the reader.

Consider the graph below.

The capacity at every vertex is 2. Thus, one can attach a path of arbitrary length to any vertex and obtain a compliant graph. One may not however join any two vertices with a path of arbitrary length and obtain a
compliant graph. Consider joining vertices \( a \) and \( b \) with a path of length \( k \). Then the effective matrix is

\[
\begin{pmatrix}
3 + \frac{2k+1}{k+1} & 1 + \frac{1}{k+1} & 1 & 1 & 0 \\
1 + \frac{1}{k+1} & 4 + \frac{2k+1}{k+1} & 1 & 1 & 1 \\
1 & 1 & 4 & 1 & 1 \\
1 & 1 & 1 & 3 & 0 \\
0 & 1 & 1 & 0 & 2
\end{pmatrix}
\]

and calculations show that this has \( \kappa_2 \leq 4 \) for \( k \leq 2 \) but not for \( k > 2 \).

Now consider the graph \( K_4 \) with vertex set \( \{a, b, c, d\} \). The capacity at each vertex is \( \frac{1}{4} \). In fact, we may attach a cycle of arbitrary length at every vertex and maintain compliancy. We can also add paths of arbitrary length between \( a \) and \( b \) and simultaneously between \( c \) and \( d \) and maintain compliancy. However, we cannot add paths of arbitrary length between \( a \) and \( b \) and simultaneously between \( a \) and \( c \) and maintain compliancy. Already, the graph

is not compliant.

## 7 Graph minors and compliancy

By contraction of an edge \( uv \) in a graph \( G \) we mean identification of \( u \) and \( v \), specifically the replacement of \( u \) and \( v \) by a new vertex \( w \) adjacent to all of the neighbors of \( u \) and \( v \). A graph \( H \) is a minor of a graph \( G \) if \( H \) can be obtained from \( G \) by repeatedly deleting vertices and edges and contracting edges. We say that \( G \) contains \( H \) as a minor if a graph isomorphic to \( H \) is a minor of \( G \). It is easy to see that the minor relation is transitive.

A class \( \mathcal{C} \) of graphs is said to be minor closed if \( G \in \mathcal{C} \) and \( H \) is a minor of \( G \) implies that \( H \in \mathcal{C} \).

It is easy to see that if a graph \( G \) is a subdivision of a graph \( H \), then \( H \) is a minor of \( G \). Hence the next result extends Corollary 6.5.

**Theorem 7.1.** Compliant graphs are minor closed.

**Proof.** As defined above graph minors are obtained by repeatedly performing three types of operation.

1. Removing an edge.
2. Removing a vertex and all its edges.
3. Collapsing an edge.

Let \( G \) be a compliant graph. If \( H \) is obtained by dropping a vertex or an edge, then it is clear that \( H \) is also compliant since it is a subgraph of \( G \) and consequently has fewer edges. We only need to consider the case when \( H \) is obtained from \( G \) by collapsing an edge. Let this edge be \( z = uv \). Incident with vertex \( u \), we have edges \( e_j \) for \( j = 1, \ldots, p \). Incident with vertex \( v \), we have edges \( e_j \) for \( j = 1, \ldots, r \). There may also be additional edges \( g_j = uw_j \) and \( h_j = vw_j \) for \( j = 1, \ldots, q \) that occur in pairs. When the edge \( z \) collapses, the edges of each pair merge into a single edge \( y_j \) for \( j = 1, \ldots, q \). We may write the matrix

\[
Z(G) = \begin{pmatrix}
Y_{11} & Y_{12} & 0 \\
Y_{12}' & Y_{22} & 1 \\
0 & 1' & 2
\end{pmatrix}
\]
where the first block refers to edges not mentioned, the last block to the single edge \( z \) and the second block to the edges \( e_i (i = 1, \ldots, p), g_j (j = 1, \ldots, q), h_j (j = 1, \ldots, q), f_k, (k = 1, \ldots, r) \) taken in that order. We have

\[
Y_{22} = \begin{pmatrix}
I_p + J_p & J_{p,q} & 0_{p,q} & 0_{p,r} \\
J_{q,p} & I_q + J_q & I_q & 0_{q,r} \\
0_{q,p} & I_q & I_q + J_q & J_{q,r} \\
0_{r,p} & 0_{r,q} & J_{r,q} & I_r + J_r
\end{pmatrix}.
\]

Note that the edge \( g_j \) touches exactly the same unmentioned edges as \( h_j \) for each specific \( j \). After collapse we have

\[
Z(H) = \begin{pmatrix}
Y_{11} & Z_{12} \\
Z_{12} & Z_{22}
\end{pmatrix}
\]

where using the ordering \( e_i (i = 1, \ldots, p), y_j (j = 1, \ldots, q), f_k, (k = 1, \ldots, r) \), we have

\[
Z_{22} = \begin{pmatrix}
I_p + J_p & J_{p,q} & J_{p,r} \\
J_{q,p} & I_q + J_q & J_{q,r} \\
J_{r,p} & J_{r,q} & I_r + J_r
\end{pmatrix}.
\]

There is a surjective map \( \mu \) which takes each edge of \( G \) to the corresponding edge of \( H \). We have \( \mu(g_j) = \mu(h_j) = y_j \) for each \( j \). It will be clear that \( Z(H) \) is a principal submatrix of the matrix

\[
W = \begin{pmatrix}
Y_{11} & Y_{12} \\
Y_{12} & W_{22}
\end{pmatrix}
\]

where in the same ordering as for \( Y_{22} \) we have

\[
W_{22} = \begin{pmatrix}
I_p + J_p & J_{p,q} & J_{p,q} & J_{p,r} \\
J_{q,p} & I_q + J_q & I_q + J_q & J_{q,r} \\
J_{q,p} & I_q + J_q & I_q + J_q & J_{q,r} \\
J_{r,p} & J_{r,q} & J_{r,q} & I_r + J_r
\end{pmatrix}.
\]

Now the matrix

\[
4I - Z(G) = \begin{pmatrix}
4I - Y_{11} & -Y_{12} & 0 \\
-Y_{12} & 4I - Y_{22} & -1 \\
0 & -1' & 2
\end{pmatrix}
\]

has the same number of positive, zero and negative eigenvalues as

\[
\begin{pmatrix}
4I - Y_{11} & -Y_{12} & 0 \\
-Y_{12} & 4I - Y_{22} & -1 \\
0 & -1' & 2
\end{pmatrix}.
\]

This matrix therefore has at most one negative eigenvalue since \( G \) is compliant. Now a calculation shows that

\[
2Y_{22} + f - 2W_{22} = \begin{pmatrix}
J_p & J_{p,q} & -J_{p,q} & -J_{p,r} \\
J_{q,p} & I_q & -J_q & -J_{q,r} \\
-J_{q,p} & -J_q & I_q & J_{q,r} \\
-J_{r,p} & -J_{r,q} & J_{r,q} & I_r
\end{pmatrix},
\]

which is a positive semidefinite rank one matrix. Therefore the matrix

\[
4I - W = \begin{pmatrix}
4I - Y_{11} & -Y_{12} \\
-Y_{12}' & 4I - W_{22}
\end{pmatrix}
\]

also has at most one negative eigenvalue, \( W \) has at most one eigenvalue greater than 4 and the same is also true of \( Z(H) \).
Graphs with the second signless Laplacian eigenvalue $\leq 4$

Figure 5: Graph for which a minor has a larger $\kappa_2$.

However taking a minor does not always decrease $\kappa_2$ as the following example shows.

**Example 7.2.** Let $H$ be the graph in Figure 5. Let $K$ be the graph with the edge $(e, f)$ collapsed. Then $\kappa_2(H) = 4.170086$, $\kappa_2(K) = 4.181305$.

**Conjecture 7.3.** Let $G$ be a graph and $H$ a minor of $G$ with $n$ vertices. Then for $k = 1, \ldots, n$ if $\kappa_k(G) \leq 4$ the inequality $\kappa_k(H) \leq \kappa_k(G)$ holds.

## 8 Computation of the minimal emergent graphs

We start by making a small change to the thought experiment of the Introduction. We rewrite Definition 2.3 as

**Definition 8.1.** An emergent graph is a graph that is not a $\mathcal{G}$-graph, but can be obtained from a $\mathcal{G}$-graph by adding either an edge between existing vertices or by adding a pendent edge and vertex or by subdividing an existing edge.

This is consistent by virtue of Corollary 6.5 and Lemma 6.6. We will use the expression *operation* to mean any of the three operations in Definition 8.1.

In this section we will show how to compute the finite family $E$ of minimal emergent graphs.

As explained in the Introduction the purpose of determining such a family $E$ is to classify all connected compliant graphs. That objective now appears to be hopeless, but one might still wish to classify connected compliant graphs of sufficiently small order. This reduced objective makes the computation of the emergent graphs worthwhile.

**Definition 8.2.** A minimal emergent graph is an emergent graph with the property that it cannot be obtained from another emergent graph by applying an operation.

### 8.1 A first look at the problem

Let $H'$ be a minimal emergent graph and suppose that $H$ is a $\mathcal{G}$-graph rooted at a vertex $r$ from which it was obtained by one of the operations in Definition 8.1. Then if $H'$ was produced by the addition of a pendent, it was certainly not at the root. It was at a non-root vertex of a single attachment. If an edge was added it may have been added within a single attachment (and may have been incident with the root) or the edge may have been added between two non-root vertices of two different attachments. If an edge was subdivided, then this took place within an attachment. There may well be other $\mathcal{C}$-attachments of $H$ apart from the one or two just mentioned, but nevertheless, it is the fact that the change stems from at most two attachments that makes the calculations feasible.
Let $K'$ be the graph $H'$ with the unmentioned attachments removed, $K$ the graph $H$ with the unmentioned attachments removed and $S$ the graph obtained from the unmentioned attachments by identifying the root vertices all of which will be denoted $r$. Then $H$ is obtained from $K$ and $S$ by identifying the roots and $H'$ is obtained from $K'$ and $S$ by identifying the roots. Furthermore $H$, $K$ and $S$ are all $\mathcal{G}$-graphs.

It cannot be that $K'$ is a $\mathcal{G}$-graph rooted at $r$ for then $H'$ is a $\mathcal{G}$-graph and not emergent. In the case that $K'$ is a non $\mathcal{G}$-graph, then $K'$ is an emergent graph. In the case that $K'$ is a $\mathcal{G}$-graph, then it must be a $\mathcal{G}$-graph rooted at a vertex different from $r$ and it is the unmentioned attachments comprising $S$ that account for $H'$ being a non $\mathcal{G}$-graph.

To enumerate the minimal emergent graphs (using a digital computer) we first enumerate the graphs $K'$ that can occur. If such a $K'$ is a non $\mathcal{G}$-graph, then we include $K'$ in $\mathcal{E}$ and we are done. If not, then we have to discuss which $\mathcal{G}$-graphs $S$ attached to $K'$ at the original root would yield an emergent graph $H'$.

**Example 8.3.** Let $K'$ be the graph shown in Figure 6. It is obtained by adding a pendent edge to $K = AC3$. Note that $K'$ is not a $\mathcal{G}$-graph at the original root shown with a heavy dot, but it is still a $\mathcal{G}$-graph rooted at the vertex where the pendent was added, consisting of a rooted $C_3$ and two rooted $P_2$. We need to figure out which $\mathcal{G}$-graphs $S$ attached to $K'$ at the original root would yield an emergent graph $H'$. Taking $S$ to be a rooted $P_2$ would not be sufficient since the graph created would still be a $\mathcal{G}$-graph built from $AC3$ and two rooted $P_2$s. In this case, the possibilities for $S$ are two rooted $P_2$s or a single rooted $P_3$. Both would yield a possible $H'$.

![Figure 6: AC3 with a pendent attached](image)

To figure this out for every possible $K'$ looks difficult, so we employ a subterfuge.

### 8.2 Division of labour

In order to simplify the calculations, we divide the problem into two separate tasks. The first task is to find a family $\mathcal{F}$ of graphs with the property that for every emergent graph $H'$ there is a graph $H''$ in $\mathcal{F}$ obtained by applying a (possibly empty) sequence of operations to $H'$. The second task is to determine the family $\mathcal{E}$ by finding all minimal emergent graphs that can be obtained from a graph in $\mathcal{F}$ by applying a sequence of edge deletions, vertex deletions and unsubdivisions (i.e. by reversing the operations).

The second task is routine. The first task is more complicated. The advantage of this approach is that it avoids very detailed discussion of individual cases.

### 8.3 A key observation

The algorithm will proceed by enumerating all possible graphs $K$ and then all possible graphs $K'$ and then by considering which graphs $H'$ can occur. There is a problem at the first step since path and cycle attachments may have large order.
Roughly speaking, we use the fact that if \( K \) has long cycle or path attachments, then \( H' \) will also have long trails of degree two vertices.

Suppose that \( K \) has a \( C_k \) or \( P_k \) with \( k \geq 7 \) as an attachment. We claim without proof that there is a \( K_1 \) obtained by replacing the \( C_k \) or \( P_k \) with a corresponding \( C_{k-1} \) or \( P_{k-1} \) and corresponding graphs \( K'_1 \) and \( H'_1 \) such that \( H'_1 \) is emergent and \( H' \) can be obtained from \( H'_1 \) by a single edge subdivision. This means that so long as we consider \( H'_1 \), we need not consider \( H' \).

The consequence is that we need only consider \( \mathcal{G} \)-graphs \( K \) built out of one or two \( \mathcal{C} \)-attachments from the list \( P_k \) \((k = 2, \ldots, 6)\), \( C_k \) \((k = 3, \ldots, 6)\), AC1, AC2, AC3, AC4, AC5. Hence, all possible \( K \) and \( K' \) can be enumerated.

### 8.4 The algorithm

If \( K' \) is not a \( \mathcal{G} \)-graph, then it is emergent and we append it to \( \mathcal{F} \). If \( K' \) is a \( \mathcal{G} \)-graph at its root \( r \) then \( H' \) is a \( \mathcal{G} \)-graph and not emergent, so we throw \( K' \) away. The objective is to find for every other \( \mathcal{G} \)-graph \( K' \) and every possible emergent \( H' \) a suitable \( H'' \).

**Algorithm 8.4.** Let \( d = d_r(K') \). From the description above it is clear that \( d \in \{1, 2, 3, 4\} \). For each value of \( d \), we provide a list of lists of \( \mathcal{C} \)-attachments. For each item in the list, each of the attachments in the contained list must be attached to \( K' \) at \( r \) to produce a graph \( H'' \) which must then be appended to \( \mathcal{F} \).

- \( d = 4 \), \( \{0\} \). (i.e. append \( K' \) to \( \mathcal{F} \)).
- \( d = 3 \), \( \{P_2\} \). (i.e. let \( H'' \) be \( K' \) with a pendent attached at \( r \). Append \( H'' \) to \( \mathcal{F} \)).
- \( d = 2 \), \( \{P_2, P_2\} \), \( \{AC2\} \).
- \( d = 1 \), \( \{P_2, P_2, P_2\} \), \( \{AC2, AC2\} \), \( \{C_3\} \).

**Proposition 8.5.** In all cases Algorithm 8.4 will produce a suitable \( H'' \).

**Proof.** We prove the result by examining various cases. After the first two cases have been eliminated, we have \( d_r(S) + d \leq 3 \) and the only options are (i) \( d_r(S) = 2 \) and \( d = 1 \) and (ii) \( d_r(S) = 1 \) and \( 1 \leq d \leq 2 \).

**Case** \( d = 4 \).

If \( d = 4 \) and \( K' \) is a \( \mathcal{G} \)-graph, then by Corollary 3.8 it is a \( \mathcal{G} \)-graph rooted at \( r \). Such \( K' \) have been excluded. Hence \( K' \) is a non \( \mathcal{G} \)-graph. It suffices to take \( H'' = K' \).

**Case** \( d_r(S) + d = 4 \).

Then let \( k = 4 - d \leq d_r(S) \). We observe that identifying the roots of \( k \) rooted \( P_2 \) and \( K' \) (rooted at \( r \)) yields a subgraph \( L \) of \( H' \) that has degree 4 at \( r \). But \( L \) cannot be a \( \mathcal{G} \)-graph rooted at a vertex different from \( r \) by Corollary 3.8. It cannot be a \( \mathcal{G} \)-graph rooted at \( r \) since \( K' \) is not. Hence \( L \) is a non \( \mathcal{G} \)-graph and we may take \( H'' = L \) since \( H' \) was minimal.

**Case** \( d_r(S) + d = 2 \) and \( S \) is a single \( \mathcal{C} \)-attachment rooted at \( r \).

Then \( S \) is AC3, AC5 or a cycle. Then \( S \) can be obtained from a rooted \( C_3 \) by a possibly empty sequence of operations. Let \( L \) be the graph obtained by replacing \( S \) in \( H' \) by \( C_3 \). Then \( L \) cannot be a \( \mathcal{G} \)-graph rooted at \( r \) since \( K' \) is not. It cannot be a \( \mathcal{G} \)-graph rooted at some other vertex of \( K' \) by Corollary 3.9. Since \( K' \) is not \( P(2) \) it cannot be a \( \mathcal{G} \)-graph rooted at a vertex of \( C_3 \) different from \( r \). Hence \( L \) is a non \( \mathcal{G} \)-graph and we may take \( H'' = L \) since \( H' \) was minimal.

**Case** \( d_r(S) = 1 \) and \( d \in \{1, 2\} \).

Then \( S \) is AC1, AC2 or a path.

In case \( S \) is AC1 or AC2, then we take \( H'' = H' \). In case \( S \) is a path, we show that we can replace it by a \( P_3 \) and hence also by AC2.

Consider such an attachment \( S \) that is a path that runs from \( r \) to a pendent vertex \( v \). Suppose that its length is \( \geq 3 \). Let \( L \) be the result of replacing \( S \) by a path \( P \) of length 3 in \( H' \). Let \( w \) be the pendent vertex of \( P \) not equal to \( r \).
As before \(L\) is not a \(\mathcal{G}\)-graph rooted at \(r\) since \(K'\) is not.

We claim that \(L\) is not a \(\mathcal{G}\)-graph rooted at a vertex \(t\) of \(P\) different from \(r\). To see this, we assume the contrary. Then \(t\) is the neighbour of \(r\) in \(P\) since \(K'\) surely possesses a degree 3 vertex and otherwise \(L\) would have a forbidden graph rooted at \(t\) (as shown in Figure 2). This forces the \(\mathcal{C}\)-attachment of \(L\) rooted at \(t\) containing \(r\) to be AC1 or AC2 which is not possible since it forces either \(d_t(S) \geq 3\) or that \(L\) is a \(\mathcal{G}\)-graph rooted at \(r\). This proves the claim.

Hence \(L\) is a \(\mathcal{G}\)-graph rooted at a vertex \(s\) of \(K'\) different from \(r\). But now there is a \(\mathcal{C}\)-attachment \(T\) rooted at \(s\) that reaches the pendent vertex \(w\) of \(P\). Hence \(T\) must be either a path or one of AC1, AC2, AC3, AC4 or AC5 rooted at \(s\) and have \(w\) as a pendent vertex. Since the length of \(P\) is 3, this is only possible if \(T\) is a path. But then we can recover \(H'\) by replacing \(T\) with a longer path. Hence \(H'\) is a \(\mathcal{G}\)-graph rooted at \(s\) contradicting the assumption that \(H'\) is emergent.

**Case \(d = 1, d_r(S) = 2\) and \(S\) is not a single \(\mathcal{C}\)-attachment rooted at \(r\)**

Then both \(R\) and the degree one attachments in \(S\) are either paths or AC1 or AC2 rooted at \(r\). We claim that we can take \(H''\) to be the graph in which both degree one attachments of \(S\) are replaced by rooted \(P_3\)'s. This can be checked by examining all possible cases or visually from Figure 7 which shows a graph \(L\) built from \(K'\) attached to two paths \(rba\) and \(rcd\) at the root vertex \(r\). One can see (with a little imagination) that \(L\) cannot be a \(\mathcal{G}\)-graph rooted at a vertex different from \(r\). Since (as before) it is not a \(\mathcal{G}\)-graph rooted at \(r\) it is a non \(\mathcal{G}\)-graph. We may take \(H'' = L\).

![Figure 7: Graph used in fourth case of the proof of Proposition 8.5](image_url)

### 8.5 Results

The results of applying Algorithm 8.4 are shown in Figure 8. There are 25 minimal emergent graphs labelled ME1 ... ME25. In fact, it is true that all these graphs are compliant.

Returning to Example 5.2, we see that a single edge with weights of 4 at each vertex is compliant. The weight of 4 can be replaced by a cycle, three pendants or an AC1. This accounts for ME3, ME13, ME14, ME17, ME18 and ME24.

The following edges are individually infinitely subdivisible (while maintaining compliancy):

- ME1: \(\{a, d\}, \{b, e\}, \{c, f\}\),
- ME2: \(\{a, f\}, \{d, f\}, \{b, g\}, \{c, g\}\),
- ME3: none
- ME4: \(\{d, g\}, \{f, g\}, \{a, i\}, \{f, i\}\),
- ME5: \(\{d, g\}, \{e, g\}, \{c, h\}, \{f, h\}, \{b, i\}, \{e, i\}, \{a, j\}, \{f, j\}\),
- ME6: \(\{a, d\}, \{b, d\}, \{c, d\}, \{a, e\}, \{b, e\}, \{c, e\}\),
- ME7: \(\{c, d\}, \{c, e\}, \{a, f\}, \{d, f\}, \{b, g\}, \{e, g\}\),
- ME8: \(\{c, d\}, \{a, e\}, \{b, f\}, \{c, g\}, \{d, g\}, \{e, h\}, \{f, h\}\),
- ME9: \(\{c, f\}, \{d, g\}, \{f, i\}, \{g, i\}\),
- ME10: \(\{b, e\}, \{c, f\}, \{d, g\}, \{g, h\}, \{a, i\}, \{h, i\}, \{e, j\}, \{f, j\}\),
- ME11: \(\{b, c\}, \{b, d\}, \{c, d\}, \{a, e\}\),
- ME12: \(\{a, d\}, \{b, e\}, \{c, f\}, \{d, f\}, \{c, g\}, \{e, g\}\),
- ME13: none
- ME14: none
- ME15: none
- ME16: none
- ME17: none
- ME18: none
- ME19: none
- ME20: none
- ME21: none
- ME22: none
- ME23: none
- ME24: none
- ME25: none

\[\square\]
9 Small compliant graphs

The reader may consult http://math.mcgill.ca/drury/research/compliant/index.html for a list of all 554 maximal compliant simple graphs with 26 or fewer vertices. Here maximal means that the graph cannot
be realized as a minor of another compliant graph. They were generated by the method suggested in the Introduction starting from the list of 25 emergent graphs listed above.

We mention a very few specific compliant graphs that may be of interest.

- $K_6$. This is maximal compliant.
- The following 7 vertex graph.

![Graph 1](image1)

- The following 7 vertex graph.

![Graph 2](image2)

- The 7 vertex wheel with a cycle attached at the hub vertex.
- The Petersen graph.
- $K_{4,4}$. Note that $K_{4,4}$ has ME3 as a subgraph. Both of these and every graph in between has $\kappa_2$ equal to 4.
- The graph $K_{3,2}$ with a cycle attached at a degree three vertex.
- The triangle graph $T_6$ with a path of arbitrary length attached at all the degree two vertices.
- The join of a single vertex to $P_4$ (i.e. 5 vertex fan) with two arbitrary cycles attached at the degree four vertex. In fact, the five vertex fan has a capacity of 8 at the degree 4 vertex. This can be satisfied for example with 6 pendants and that graph is maximal. It can also be satisfied with two AC1, but this graph is not maximal.

## 10 $S$-graphs

**Definition 10.1.** An $S$-graph is a simple graph with possible multiple loops. The number of loops at a given vertex is called the loop number or path number of the vertex. The degree of a vertex in an $S$-graph is the number of edges attached to the vertex plus twice the number of loops (according to Diestel’s book on Graph Theory, [5, page 28]). The signless Laplacian of an $S$-graph $G$ is $Q(G) = A(G) + D(G)$ as before where $D(G)$ denotes the diagonal matrix of vertex degrees.

The incidence matrix of an $S$-graph is as usual for normal edges and vertices, but the entry is $\sqrt{2}$ for a loop and vertex. Loops are counted separately. Thus, for a triangle $T$ with two loops at vertex 1, one at vertex 2 and none at vertex 3 the incidence matrix would be

$$X = \begin{pmatrix}
0 & 1 & 1 & \sqrt{2} & \sqrt{2} & 0 \\
1 & 0 & 1 & 0 & 0 & \sqrt{2} \\
1 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}$$
and we would have

\[
Q = XX' = \begin{pmatrix} 6 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 2 \end{pmatrix} \quad \text{and} \quad Z = X'X = \begin{pmatrix} 2 & 1 & 1 & 0 & 0 & \sqrt{2} \\ 1 & 2 & 1 & \sqrt{2} & \sqrt{2} & 0 \\ 1 & 1 & 2 & \sqrt{2} & \sqrt{2} & \sqrt{2} \\ 0 & \sqrt{2} & \sqrt{2} & 2 & 2 & 0 \\ 0 & \sqrt{2} & \sqrt{2} & 2 & 2 & 0 \\ \sqrt{2} & 0 & \sqrt{2} & 0 & 0 & 2 \end{pmatrix}.
\]

We denote by \( n(G) \) the order of an \( S \)-graph and \( m(G) \) the total number of edges and loops.

**Lemma 10.2.** For any \( S \)-graph \( G \), we have \( Q(G) = X(G)X(G)' \). If \( H \) is a \( S \)-subgraph of a \( S \)-graph \( G \), then \( \kappa_k(H) \leq \kappa_k(G) \) for \( 1 \leq k \leq \min(m(H), n(H)) \).

**Proof.** The first statement is obvious. For the second, if an edge or a loop is removed, then the resulting \( Z(H) = X(H)'X(H) \) matrix is a principal submatrix of the original \( Z(G) = X(G)'X(G) \). Since \( Q(G) \) and \( Z(G) \) have the same non-zero eigenvalues and similarly for \( Q(H) \) and \( Z(H) \), the claim follows by standard interlacing inequalities [2, Corollary 2.5.2].

Each \( S \)-graph has a collection of simple graphs that it represents. These simple graphs are obtained by repeatedly carrying out the following operations.

- For a vertex with loop number at least one, decrease the loop number by 1 and add a path of length at least one at the vertex. There is no limit on the length of the path.
- For two vertices, both with loop number at least one, decrease each loop number by one and add a path of arbitrary length between the two vertices (at least one added vertex if the vertices are adjacent).
- For a vertex with loop number at least two, decrease the loop number by two and add a path between the vertex and itself, so that at least two vertices are added (i.e. attach a cycle).

Of course, if we take a simple graph and view it as an \( S \)-graph (with all the loop numbers zero) then it represents itself (and only itself).

Thus, for the triangle \( S \)-graph \( T \) described above, a represented simple graph might be a triangle with additionally a path of arbitrary length between vertex 1 and vertex 2 and a path of arbitrary length also attached at vertex 1.

**Proposition 10.3.** If an \( S \)-graph is compliant, then all the simple graphs that it represents are also compliant.

We leave the proof to the reader.

Some lists of compliant \( S \)-graphs graphs can also be downloaded from http://math.mcgill.ca/drury/research/compliant/index.html.

**Acknowledgements:** The author thanks the referees for their suggestions and comments which substantially improved this article.

He also thanks Brendan McKay for making publically available his Nauty program and in particular the coding of his canonical graph concept which allows isomorphism classes of graphs to be stored in a binary search tree.

**Data availability statement:** The data related to this article is partially deposited on 17 November 2021 and available until at least 17 November 2023 on: https://www.math.mcgill.ca/drury/research/compliant/index.html
References

[1] M. Aouchiche, P. Hansen, C. Lucas, On the extremal values of the second largest Q-eigenvalue, Linear Algebra Appl. 435 (2011) 2591-2606.
[2] A.E. Brouwer, W.H. Haemers, Spectra of Graphs, Springer, New York, 2012.
[3] D. Cvetković, S.K. Simić, On graphs whose second largest eigenvalue does not exceed \( \sqrt{\frac{\lambda_1 + \lambda_2}{2}} \), Discrete Math. 138 (1995).
[4] D. Cvetković, P. Rowlinson, S.K. Simić, Eigenvalue bounds for the signless Laplacian, Publ. Inst. Math. (Beograd) (N.S.) 81 (95) (2007) 11–27.
[5] R. Diestel, Graph Theory, Graduate Texts in Mathematics 173, Springer, 5th edition.
[6] R.A. Horn and C.J. Johnson, Matrix Analysis, Cambridge University Press, 2012.
[7] R.S. Varga, Geršgorin and His Circles, Springer, 2004.
[8] Xingyu Lei, Jianfeng Wang & Maurizio Brunetti, Graphs whose second largest signless Laplacian eigenvalue does not exceed \( 2 + \sqrt{3} \), Linear Algebra and its Applications 603 (2020) 242-264.
[9] Guilherme Porto, Luiz Emilio Allem, Eigenvalue Interlacing in Graphs, Proceeding Series of the Brazilian Society of Applied and Computational Mathematics, Vol. 5, N. 1, 2017.