Asymptotic Bounds on the Maximum Number of Minimal Separators in a Graph

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Abstract

For a graph $G = (V, E)$ and two nodes $a, b \in V$, a set $S \subseteq V \backslash \{a, b\}$ is a separator if there exists no path between a and b that does not pass through any nodes in S. Such a separator is minimal if it does not contain another separator for a and b as a proper subset. This paper is concerned with finding the asymptotic growth of the maximum number of minimal separators in any graph with respect to $|V|$. We refute the lower bound $\Omega(1.4521^{|V|})$ claimed in [1], by presenting a flaw in the constructed family of graphs with supposedly more than $\Omega(1.4521^{|V|})$ minimal separators. Instead, we conjecture that there exists no graph with more than $O(3^{\frac{|V|}{3}}) \subset O(1.4422^n)$ minimal separators, and provide some proofs supporting this conjecture.

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Contents

1 Preliminaries

1.1 Graph Theory

A *graph* consists of nodes and edges, and is denoted as $G = (V, E)$, where V is the set of nodes and E is the set of edges. The edge connecting nodes a and b is typically written as (a, b). Throughout this paper, only undirected graphs are considered, meaning $(a, b) = (b, a)$. An *induced subgraph* $G' = (V', E')$ is a graph that consists of a subset $V' \subset V$ of the nodes, where $(a, b) \in E'$ if and only if $(a, b) \in E$ and $a, b \in V'$. We use $G_{V \setminus P}$ to denote the induced subgraph of $G = (V, E)$ where all nodes $v \in P$ have been removed from V. A *path* between two nodes v_1, v_m is an ordered collection of nodes $(v_1, v_2, ..., v_{m-1}, v_m)$ such that $(v_i, v_{i+1}) \in E$ for all $i \in \{1, 2, ..., m-1\}$. The notation $(v_1, v_2, ..., v_m) \in E$ is defined to be equivalent with $(v_1, v_2), (v_2, v_3), ..., (v_{m-1}, v_m) \in E$. Figure 1 shows an example of a graph.

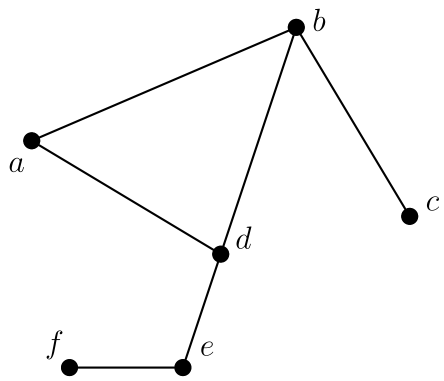

Figure 1: A graph $G = (V, E)$ with $V = \{a, b, c, d, e, f\}$ and $E = \{(a, b), (a, d), (b, c), (b, d), (d, e), (e, f)\}$ One possible path in G between f and a is (f, e, d, a).

1.1.1 Minimal Separators

For a graph $G = (V, E)$ and nodes $a, b \in V$, a set $S \subseteq V \setminus \{a, b\}$ is an *(a, b)-separator* if and only if there is no path between a and b in the induced subgraph $G_{V \setminus S}$. Such a separator is *minimal* if there exists no node $v \in S$ such that $S \setminus \{v\}$ is also an (a, b)-separator. The number of minimal separators of a graph $G = (V, E)$ is the number of distinct sets $S \subseteq V$ that are minimal (a,b)-separators for some pair $a,b \in V$. Figure 2 illustrates the concept of minimal separators. Henceforth $\text{sep}(G)$ is used to refer to the number of distinct minimal separators in graph G, and $\mathbb{G}[n]$ denotes the set of all graphs with $|V| = n$. In order to refer to the maximum number of minimal separators in any graph with n nodes, we use $\xi_n = \max_{G \in \mathbb{G}[n]} [\text{sep}(G)]$.

Figure 2: Two (a,b)-separators (colored white) of the same graph. Only the rightmost one is minimal. The black nodes and edges represent the induced subgraph $G_{V \setminus S}$.

1.1.2 Melon Graphs

Intuitively, a melon graph is a graph where two nodes a and b are connected by exactly ℓ disjoint paths of lengths $k_1, k_2, ..., k_\ell$. Figure 3 shows an example of a melon graph. Currently, the graph known to have the highest number of minimal separators with respect to $|V|$ is a melon graph. We use $[X]$ to denote the set $\{1, 2, ..., X\}$, where $X \in \mathbb{N}$.

Definition. Given $\ell \in \mathbb{N}$ and numbers $k_1, k_2, ..., k_\ell \in \mathbb{N}$, a *melon graph* $M = (V, E)$ is defined as follows:

- The nodes a and b are in V.
- For every $i \in [\ell]$, node $v_{i,j} \in V$ for all $j \in [k_i]$
- Path $(a, v_{i,1}, v_{i,2}, ..., v_{i,k_i}, b) \in E$ for every $i \in [\ell]$.
- Nothing else is in E or V.

A *layer* in a melon graph is defined as the set of nodes $\{v_{i,1}, v_{i,2}, ..., v_{i,k_i}\}$ for some $i \in [\ell]$. The graph $M_{x,\ell}$ is defined to be the melon graph with ℓ layers and $k_i = x$ for all i.

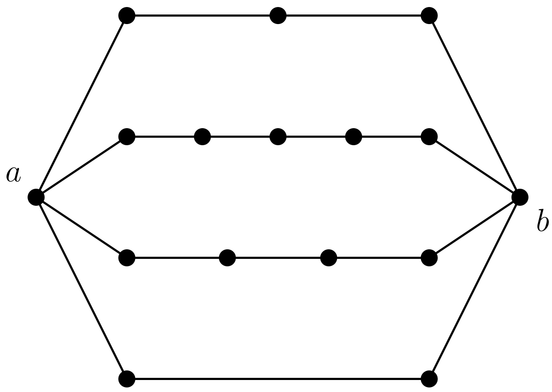

Figure 3: Melon graph with $\ell = 4,\ k_1 = 3, k_2 = 5, k_3 = 4, k_4 = 2$.

1.2 Computational Complexity Theory

Computational complexity theory is the area of mathematics concerned with classifying different computational problems, usually with respect to their asymptotic behaviour.

In order to study the asymptotic behaviour of a function $f\colon \mathbb{N} \to \mathbb{R}$, the notations O, Ω and Θ are used. Intuitively, O is an upper bound of $f(n)$. Formally, $f(n)$ is $O(g(n))$ if there exists some values $n_0, c > 0$ such that $f(n) \leq c \cdot g(n)$ for all $n \geq n_0$. Conversely, Ω is a lower bound. The function $f(n)$ is $\Omega(g(n))$ if there exists some $n_0, c > 0$ such that $f(n) \geq c \cdot g(n)$ for all $n > n_0$. A function $f(n)$ is $\Theta(g(n))$ if it is both $O(g(n))$ and $\Omega(g(n))$.

2 Introduction

This paper concerns studying ξ_n, the maximum number of minimal separators across all graphs with $n = |V|$. It does this through refuting a previously believed lower bound, and conjecturing what the tight bound might be.

An example of a practical application of minimal separators is finding the most efficient way of stopping *something* from reaching *something else*. This can include stopping an infectious disease spreading from person A to person B (where the nodes are people, and the edges represent whether two people interact), or stopping an army at point A from reaching point B (in which case the graph would represent a map of the terrain).

Bounding the maximum number of possible minimal separators in a graph is useful for developing algorithms which find and compare such separators. One possible such comparison is finding the lowest cost minimal separator, if different costs are assigned to nodes. It is furthermore used in the study of exact algorithms whose aim is to optimally solve hard problems exponentially faster than the brute force search [2, 3, 4, 5, 6].

A well-known lower bound on ξ_n is $\Omega(3^{\frac{n}{3}}) \subset \Omega(1.4422^n)$ [3]. This bound is attained in the melon graph $M_{3,\ell}$ shown in Figure 4. Intuitively, to create a minimal (a, b)-separator, one node is picked from each layer. There are three choices per layer, and $\frac{n-2}{3}$ layers, resulting in at least $3^{\frac{n-2}{3}} \in \Omega(3^{\frac{n}{3}})$ minimal separators.

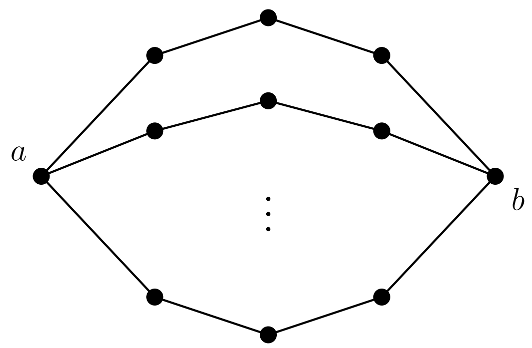

Figure 4: Melon graph $M_{3,\ell}$ with $\Omega(3^{\frac{n}{3}})$ minimal separators.

Note that only the (a, b)-separators of $M_{3,\ell}$ are counted in $\Omega(3^{\frac{n}{3}})$. Including minimal separators for all pairs of nodes will not increase the bound asymptotically, since for any other pair of nodes, there exists only polynomially many separators which are not (a, b)-separators.

The upper bound $\xi_n \in O(n\phi^n)$ was shown by Fomin and Villanger in [5], where $\phi = \frac{1+\sqrt{5}}{2}$, the golden ratio. Gaspers and Mackenzie claimed that $\xi_n \in \Omega(1.4521^n)$ [1]. However, this paper presents an error in their proof of this lower bound.

3 Refuting the Previously Held Best Lower Bound

The intention of the proof in [1] is to construct a family of graphs that have $\Omega(1.4521^n)$ minimal separators. One of these graphs is shown in Figure 5. The fault in the proof lies in the assumption that all sets described as separators will actually remove every path from a to b. In fact, a majority of the sets that are claimed to be separators are not. The following is the proof directly quoted from [1]:

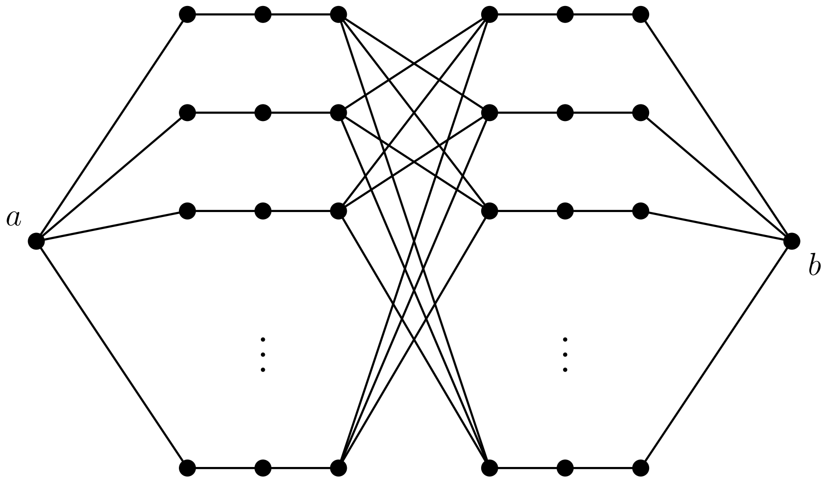

Figure 5: G_1, as constructed in the proof. Nodes $v_{i,j}$ are omitted for $j \in \{4, 5, ..., 23\}$. This is the graph claimed to have $\Omega(1.4521^n)$ separators.

Theorem. $\xi_n \in \Omega(1.4521^n)$ [1]

Proof. We prove the theorem by exhibiting a family of graphs $\{G_1, G_2, ...\}$ and lower bounding their number of minimal separators. Let $I = \{1, ..., 6\}$ and $J = \{1, ..., 24\}$. The graph G_1 is constructed as follows (see 5). It has vertex set $V = \{a, b\} \cup \{v_{i,j} : i \in I, j \in J\}$. We denote by V_i the vertex set $\{v_{i,j} : j \in J\}$. The edge set E of G_1 is obtained by first adding the paths $(a, v_{1,j}, v_{2,j}, v_{3,j})$ and $(v_{4,j}, v_{5,j}, v_{6,j}, b)$ for all $j \in J$, and then adding the edges $\{(v_{3,j}, v_{4,k}) : j, k \in J \text{ and } j \neq k\}$. The graph $G_\ell, \ell \geq 2$, is obtained from ℓ disjoint copies of G_1, merging the copies of a, and merging the copies of b.

Let us now lower bound the minimal (a, b)-separators S_j in G_1 that do not contain any vertex from $\{v_{1,j}, v_{2,j}, v_{3,j}, v_{4,j}, v_{5,j}, v_{6,j}\}$ for some $j \in J$. Each such separator contains a vertex from $\{v_{1,k}, v_{2,k}, v_{3,k}\}$, for $k \in J \setminus \{j\}$, since $(a, v_{1,k}, v_{2,k}, v_{3,k}, v_{4,j}, v_{5,j}, v_{6,j}, b)$ is a path in G_1, and it contains a vertex from $\{v_{4,k}, v_{5,k}, v_{6,k}\}$, for $k \in J \setminus \{j\}$, since $(a, v_{1,j}, v_{2,j}, v_{3,j}, v_{4,k}, v_{5,k}, v_{6,k}, b)$ is a path in G_1.

Due to minimality, the separators in S_j contain no other vertices. Thus, we have that $|S_j| = 3^{2(|J|-1)}$. We also note that $S_j \cap S_k = \varnothing$ if $j \neq k$. Therefore, the number of minimal separators of G_1 is at least $|J| \cdot 3^{2(|J|-1)} > 2.1271 \cdot 10^{23}$. Minimal (a, b)-separators for G_ℓ are obtained by taking the union of minimal separators for the different copies of G_1.

Their number is therefore at least $(|J| \cdot 3^{2(|J|-1)})^{\ell} = (|J| \cdot 3^{2(|J|-1)})^{\frac{n-2}{6|J|}} \in \Omega(1.4521^n)$, where $n = \ell \cdot 6 \cdot |J| + 2$ is the number of vertices of G_ℓ. $\square$

As an example of a set claimed to be a separator, consider $P = \{v_{2,k} \mid \forall k \neq 1\} \cup \{v_{5,k} \mid \forall k \neq 1\}$. According to the proof, $P \in S_1$. But P is not a separator. The path $(a, v_{1,1}, v_{2,1} v_{3,1}, v_{4,2}, v_{3,3}, v_{4,1}, v_{5,1}, v_{6,1}, b)$ is still in $G_{V \setminus P}$. Actually, we can decide exactly which of the presumed minimal separators actually are separators:

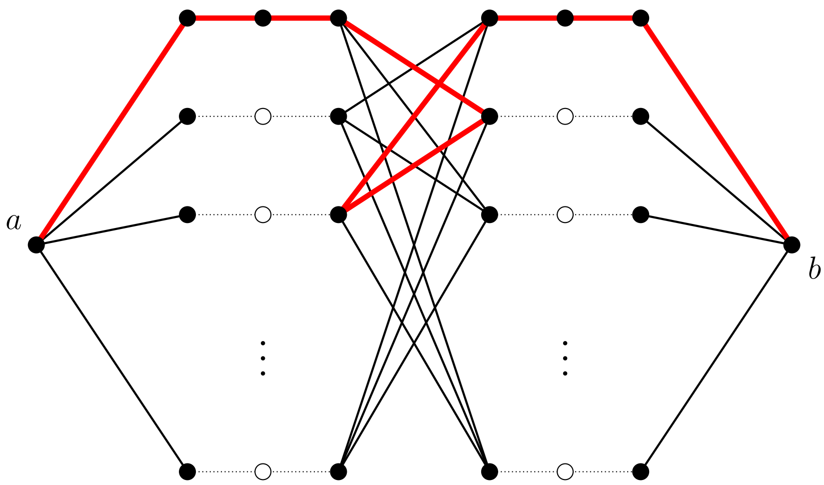

Figure 6: The induced subgraph $G_{V \setminus P}$, with one possible path between a and b marked.

Lemma 3.1. *Using the same construction as the proof, for any $S \in S_j$ to be an (a,b)-separator, it needs to contain either $\{v_{3,k} \mid \forall k \neq j\}$, $\{v_{4,k} \mid \forall k \neq j\}$ or $\{v_{3,k}, v_{4,k} \mid \forall k \neq j, k \neq t$ for some $t \neq j\}$ as a subset.*

Proof. Assume, for sake of contradiction, that we have a set $S \in S_j$ that does not have any of the described subsets. This means that there exists some $z \neq q$ such that $v_{z,3}, v_{4,q} \in S$ where $z, q \neq j$. Then the path $(a, v_{1,j}, v_{2,j}, v_{3,j}, v_{4,q}, v_{3,z}, v_{4,j}, v_{5,j}, v_{6,j}, b)$ is in $G_{V \setminus S}$, which means S is not an (a,b)-separator. $\square$

A consequence of Lemma 3.1 is that $|\{s \mid s \in S_j,\ s \text{ is a separator}\}| \leq 2 \cdot 3^{|J|-1} + (|J| - 1) \cdot 2^2$. Thus, the total amount of such separators is $(2|J| \cdot 3^{|J|-1} + |J|(|J|-1) \cdot 2^2)^{\frac{n}{6|J|}}$. This expression is maximized at $|J| = 2$, where it is less than $1.2836^n < 3^{\frac{n}{3}}$. This inequality implies that the construction of the family of graphs G_ℓ does not change the bounds of ξ_n.

4 Melon Graphs

We conjecture that the melon graph $M_{3,\frac{n-2}{3}}$ is the graph with the most minimal separators across all graphs $G \in \mathbb{G}[n]$. This is equivalent to the following:

Conjecture. *The bound $\xi_n \in \Theta(3^{\frac{n}{3}})$ holds.*

4.1 Optimal Melon Graph

We begin by showing $M_{3,\frac{n-2}{3}}$ is the graph with the most minimal separators among all melon graphs in $\mathbb{G}[n]$.

Lemma 4.1. *The number of minimal separators in a melon graph $M = (V, E)$ with ℓ layers and values $k_1, k_2, ..., k_\ell$ satisfies*

$$\operatorname{sep}(M) \in \Theta(\prod_{i\in[\ell]} k_i) \tag{1}$$

when $\prod_{i\in[\ell]} k_i$ is asymptotically larger than or equal to $|V|^2$.

Proof. We begin by considering the lower bound. In order to create a minimal (a, b)-separator, one node $v_{i,j}$ is picked for each $i \in [\ell]$. This is a separator, since for each path $(a, v_{i,1}, ..., v_{i,k_i}, b) \in E$, one node is in the separator. It is minimal, since the removal of some node $v_{i,j}$ from the separator makes it possible to traverse the path $(a, v_{i,1}, ..., v_{i,k_i}, b)$ from a to b. Thus, $\operatorname{sep}(M) \in \Omega(\prod_{i\in[\ell]} k_i)$.

To show that the same holds for the upper bound, we consider the different natures of minimal separators in M for any pair $u, v \in V$. The cases of separators S we consider are:

- At most one node from each layer is in S.
- Exactly two nodes from some layer are in S.
- Three or more nodes from some layer are in S.

- At least one of a and b is in S.

Note that these cases are exhaustive, i.e., every subset $S \subseteq V$ that is a potential minimal separator is considered in at least one case.

Case 1. Firstly, we show that there exists no minimal separator with at most one node in each layer that is not already counted as a minimal (a, b)-separator. We show this through contradiction. Assume there exists some minimal separator $S = \{v_{i_1,j_1}, v_{i_2,j_2}, ..., v_{i_m,j_m}\}$ for distinct values $i_1, i_2, ..., i_m$, and $m < \ell$. Let z be an index such that $v_{z,j} \notin S$ for all $j \in \{1, 2, ..., k_z\}$. For any pair $v_{x,y}, v_{u,v} \in V \backslash S$, at least one of the following paths must be in $G_{V \backslash S}$:

- $(v_{x,y}, v_{x,y+1}, ..., v_{x,k_x}, b, v_{u,k_u}, ..., v_{u,v})$
- $(v_{x,y}, v_{x,y-1}, ..., v_{x,1}, a, v_{u,1}, ..., v_{u,v})$
- $(v_{x,y}, v_{x,y+1}, ..., v_{x,k_x}, b, v_{z,k_z}, ..., v_{z,1}, a, v_{u,1}, ..., v_{u,v})$
- $(v_{x,y}, v_{x,y-1}, ..., v_{x,1}, a, v_{z,1}, ..., v_{z,k_z}, b, v_{u,k_u}, ..., v_{u,v})$

See Figure 7 for an example of such a set S. Note that this implies that there also exists a path between a or b and any node $v_{x,y} \in V \backslash S$. Thus, S is not a separator if S does not contain a node from every layer, in which case it is already counted as an (a, b)-separator.

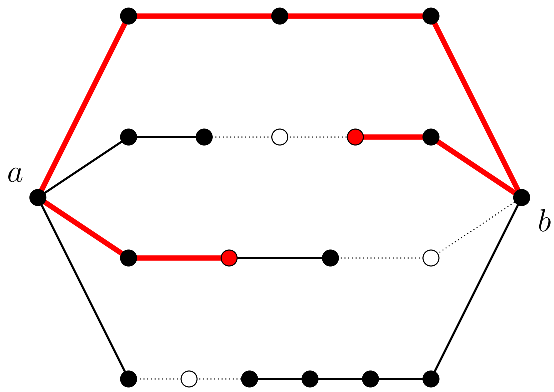

Figure 7: An example of a set S considered in *Case* 1. Two nodes and the path between them are marked in red.

Case 2. If a minimal separator S includes exactly two nodes $v_{i,x}, v_{i,y}$ where $x < y$ in the same layer i, it must be the case that exactly one of the nodes it separates is $v_{i,u}$ for some $u \in \{x+1, x+2, ..., y-1\}$. Otherwise, the separator is not minimal. It must also be the case that no other node is in the separator, since $v_{i,u}$ is already separated from all other nodes (except other nodes of the form $v_{i,q}$ for some $q \in \{x+1, x+2, ..., y-1\}$, but a $(v_{i,q}, v_{i,u})$-separator containing $v_{i,x}$ and $v_{i,y}$ would need to contain three nodes in layer i). Thus, there are less than $|V|^2$ separators of this form.

Case 3. In the case where a minimal separator includes at least three nodes $v_{i,x}, v_{i,y}, v_{i,z}$, where $x < y < z$, in the same layer i, it must be the case that it separates nodes $v_{i,u}, v_{i,q}$ for some $x < u < y < v < z$. But in this case, one of $v_{i,x}$ or $v_{i,z}$ can be removed, which means the separator is not minimal.

Case 4. If either a and b are in some minimal separator, it can by the same reasoning include at most one other node. Thus, there can be no more than $|V|$ such separators. Figure 8 shows an example of such a minimal separator. Finally, if both a or b is in a minimal separator S, no other node can be in the separator for it to remain minimal. Thus there is only one such separator.

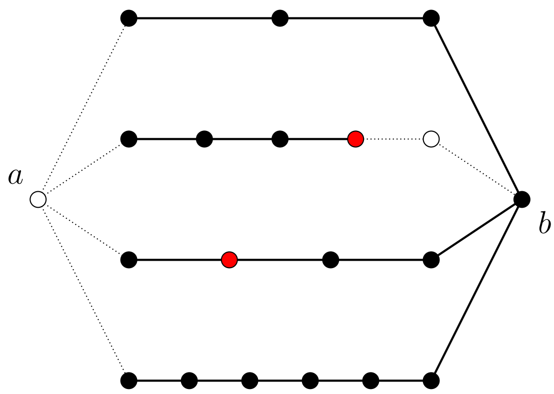

Figure 8: An example of a set S considered in *Case* 4. Two nodes separated are marked in red.

Thus, we have that $\text{sep}(M) \leq \prod_{i \in [\ell]} k_i + |V|^2 + 1 \in O(\prod_{i \in [\ell]} k_i)$, which proves the lemma. □

Theorem 4.2. *For two melon graphs* $M_{3,\frac{n-2}{3}}$ *and* $M \in \mathbb{G}[n]$*, the inequality* $\operatorname{sep}(M_{3,y}) \geq \operatorname{sep}(M)$ *is satisfied.*

Proof. Note that (1) implies that $\operatorname{sep}(M_{x,\frac{n-2}{x}}) \in \Omega(x^{\frac{n}{x}})$. Thus, $\operatorname{sep}(M_{x,\frac{n-2}{x}})$ is asymptotically larger than n^3, which means we only need to consider graphs where (1) holds.

Consider the values $k_1, k_2, ..., k_\ell$ of M. By (1), the theorem is true if and only if

$$3^{\frac{n-2}{3}} \geq \prod_{i \in [\ell]} k_i.$$

Note that $n - 2 = \sum_{i \in [\ell]} k_i$. The inequality is thus equivalent to

$$\sum_{i \in [\ell]} k_i \cdot \frac{\ln(3)}{3} \geq \sum_{i \in [\ell]} \ln(k_i),$$

which is true if

$$\frac{\ln(3)}{3} \geq \frac{\ln(k_i)}{k_i} \text{ for all } i \in [\ell].$$

The function $\frac{\ln(x)}{x}$ has its only maximum at $x = e$, and is strictly increasing for $x < e$ and strictly decreasing for $x > e$. This, combined with noting that $\frac{\ln(3)}{3} > \frac{\ln(2)}{2}$, shows that the inequality holds for all k_i, thus proving the theorem. □

4.2 Bridged Melon Graphs

A *bridged melon graph* is constructed similarly to a melon graph. The difference lies in the *bridges*, which are edges between pairs of nodes v_{i_1,j_1}, v_{i_2,j_2} for $i_1 \neq i_2$. Figure 9 shows an example of a bridged melon graph.

The aim of this section is to provide support for the following conjecture:

Conjecture. *For a melon graph* M*, when adding bridges between any number of pairs* $(v_{i_1,j_1}, v_{i_2,j_2})$*, the number of minimal* (a, b)*-separators either decreases or stays constant.*

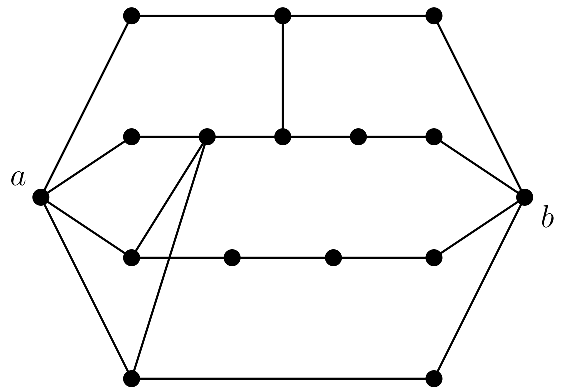

Figure 9: Bridged melon graph with $\ell = 4$, $k_1 = 3, k_2 = 5, k_3 = 4, k_4 = 2$, and bridges $(v_{1,2}, v_{2,3})$, $(v_{2,2}, v_{3,1})$ and $(v_{2,2}, v_{4,1})$.

4.2.1 One Bridge

Theorem 4.3. *A bridged melon graph* $M' = (V', E')$*, obtained by adding exactly one bridge to the melon graph* $M = (V, E)$*, satisfies* $\text{sep}(M') \leq \text{sep}(M)$*.*

Proof. Assume without loss of generality that the bridge connects $v_{1,x}$ and $v_{2,y}$ for some $x \in [k_1]$ and $y \in [k_2]$. Note that this adds the paths $(a, v_{1,1}, ..., v_{1,x-1}, v_{1,x}, v_{2,y}, ..., v_{2,k_2}, b)$ and $(a, v_{2,1}, ..., v_{2,y-1}, v_{2,y}, v_{1,x}, ..., v_{1,k_1})$ to E'. To create a minimal separator in M', we need to block these new paths in addition to all paths between a and b in M. Note that for all layers except the first two, it is still the case that exactly one node from each layer will be in any minimal separator.

Let S be a minimal (a, b)-separator in M'. We want to show that every minimal separator will have exactly one node in the first and second layer. If this is the case, it must be that $\text{sep}(M') \leq \text{sep}(M)$, since $\text{sep}(M)$ is given in (1) to be the number of ways to chose one node from each layer. This means the minimal separators of M' make up a subset of the minimal separators of M, thus confirming the inequality.

First note that there is no separator with no nodes in layer $l \in \{1, 2\}$. If this were the case, the path $(a, v_{l,1}, ..., v_{l,k_l})$ would still be traversable in $M' \backslash S$.

Assume, for sake of contradiction, that there are at least two different nodes $v_{1,j_1}, v_{1,j_2} \in \{v_{1,j} : \forall j\} \cap S$. It is obvious that either $j_1 \leq x \leq j_2$ or $j_2 \leq x \leq j_1$, since if not, one of the two nodes could be removed from the separators and it would still block exactly

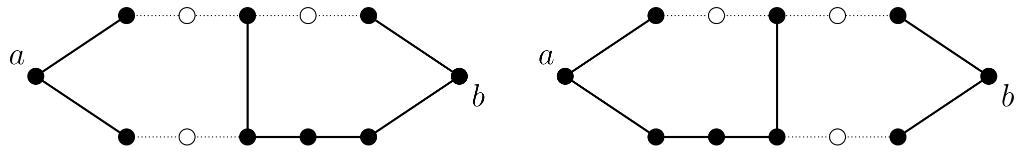

Figure 10: A bridged melon graph with bridge $(v_{1,x}, v_{2,y})$. Two different separators including v_{1,j_1}, v_{1,j_2} for $j_1 \leq x \leq j_2$ and some v_{2,j_3}. In the leftmost graph, $j_3 \leq y$. Neither separator is minimal.

the same paths. Assume without loss of generality $j_1 \leq x \leq j_2$. Let v_{2,j_3} be some node in S. Figure 10 shows how the separator might look. If $j_3 \leq y$ then the separator is not minimal since v_{1,j_2} can be removed from it. If $j_3 > y$ then v_{1,j_1} can be removed. Thus, we have that any minimal separator in M' will have exactly one node in each layer, which proves the theorem. □

For other amounts of bridges, a similar reasoning may apply. However, note that it is not the case that any separator will have exactly one node in each layer for any bridged melon graph. Figure 11 gives an example of this. This particular bridged melon graph will still have less (a, b)-separators than the corresponding melon graph $M_{6,2}$. Comparing the two, we see that the bridged one has 10 unique (a, b)-separators, whereas $M_{6,2}$ has 36. Thus, despite the large amount of nodes included in some separators, this particular example is consistent with the conjecture.

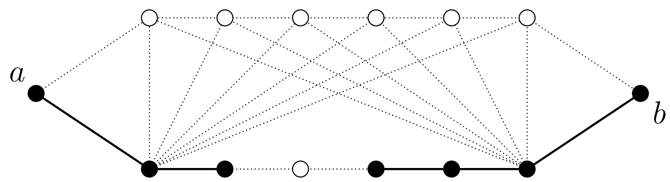

Figure 11: Bridged melon graph with two layers. A minimal (a, b)-separator of size 7 is shown.

5 Conclusion

The main result of this paper is that the best known lower bound of ξ_n is once again $\Omega(3^{\frac{n}{3}})$. Consequently, the existence of a graph with more than $\Omega(3^{\frac{n}{3}})$ minimal separators, that is, whether $\xi_n \notin \Theta(3^{\frac{n}{3}})$, is once again an open problem.

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