On the number of minimal separators in graphs

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Abstract
We consider the largest number of minimal separators a graph on \( n \) vertices can have.

- We give a new proof that this number is in \( \mathcal{O} \left( \left( \frac{1 + \sqrt{5}}{2} \right)^n \cdot n \right) \).

- We prove that this number is in \( \omega(1.4457^n) \), improving on the previous best lower bound of \( \Omega(3^{n/3}) \subseteq \omega(1.4422^n) \).

This gives also an improved lower bound on the number of potential maximal cliques in a graph. We would like to emphasize that our proofs are short, simple, and elementary.

KEYWORDS
combinatorial bounds, enumeration algorithms, extremal combinatorics

1 INTRODUCTION

For a graph \( G = (V, E) \), and two vertices \( a, b \in V \), a vertex subset \( S \subseteq V \setminus \{a, b\} \) is an \((a,b)\)-separator if \( a \) and \( b \) are in different connected components of \( G - S \), the graph obtained from \( G \) by removing the vertices in \( S \). An \((a,b)\)-separator is minimal if it does not contain another \((a,b)\)-separator as a subset. A vertex subset \( S \subset V \) is a minimal separator in \( G \) if it is a minimal \((a,b)\)-separator for some pair of distinct vertices \( a, b \in V \).

By \( \text{sep}(G) \), we denote the number of minimal separators in the graph \( G \). By \( \text{sep}(n) \), we denote the maximum number of minimal separators, taken over all graphs on \( n \) vertices.

Potential maximal cliques are closely related to minimal separators, especially in the context of chordal graphs. A graph is chordal if every induced cycle has length 3. A triangulation of a graph \( G \) is a chordal supergraph of \( G \) obtained by adding edges. A graph \( H \) is a minimal triangulation of \( G \) if it is a triangulation of \( G \) and \( G \) has no other triangulation that is a subgraph of \( H \). A vertex set is a potential maximal clique in \( G \) if it is a maximal clique in at least one minimal triangulation of \( G \).
By \(\text{pmc}(G)\), we denote the number of potential maximal cliques in the graph \(G\). By \(\text{pmc}(n)\), we denote the maximum number of potential maximal cliques, taken over all graphs on \(n\) vertices.

Minimal separators and potential maximal cliques have been studied extensively [1–3,10,12,16,17, 20–22]. Upper bounds on \(\text{sep}(n)\) are used to upper bound the running time of algorithms for enumerating all minimal separators [1,17,21]. Bounds on both \(\text{sep}(n)\) and \(\text{pmc}(n)\) are used in analyses of algorithmic running times for computing the treewidth and minimum fill-in of a graph [3,10,12], and for computing a maximum induced subgraph isomorphic to a graph from a family of bounded treewidth graphs [11].

1.1 | Our results

Fomin et al. [10] proved that \(\text{pmc}(n) \in O(1.7087^n)\). Fomin and Villanger [12] improved the upper bound and showed that \(\text{pmc}(n) \in O(\rho^n \cdot n)\), where \(\rho = \frac{1 + \sqrt{5}}{2} = 1.6180 \ldots\). We prove the same upper bound with simpler arguments.

As for lower bounds, it is known [10] that \(\text{sep}(n) \in \Omega(3^{n/3})\); see Fig. 1. We improve on this lower bound by giving an infinite family of graphs with \(\omega(1.4457^n)\) minimal separators. This answers an open question raised numerous times (see, e.g. [9,10]), for example by Fomin and Kratsch [9, p. 100], who state

It is an open question, whether the number of minimal separators in every \(n\)-vertex graph is \(O^\ast(3^{n/3})\).

Here, the \(O^\ast\)-notation is similar to the \(O\)-notation, but hides polynomial factors.

As a corollary, we have that there is an infinite family of graphs, all with \(\omega(1.4457^n)\) potential maximal cliques. This answers another open question on lower bounds for the number of potential maximal cliques in graphs. For example, Fomin et al. [11] state

There are graphs with roughly \(3^{n/3} \approx 1.442^n\) potential maximal cliques [10]. Let us remind ourselves that by the classical result of Moon and Moser [19] (see also Miller and Muller [18]), the number of maximal cliques in a graph on \(n\) vertices is at most \(3^{n/3}\). Can it be that the right upper bound on the number of potential maximal cliques is also of order \(3^{n/3}\)? Can we enumerate potential maximal cliques within this time? By Theorem 3.9, this would yield a dramatic improvement for numerous exact algorithms.

1.2 | Preliminaries

We use standard graph notation from [4]. For an edge \(u v\) in a graph \(G\), we denote by \(G/uv\) the graph obtained from \(G\) by contracting the edge \(uv\), i.e. making \(u\) adjacent to \(N_G(\{u, v\})\) and removing \(v\).
2 | UPPER BOUND ON THE NUMBER OF MINIMAL SEPARATORS

Measure and Conquer is a technique developed for the analysis of exponential time algorithms [7]. Its main idea is to assign a cleverly chosen (sometimes, by solving mathematical programs [5,13,15]) potential function to the instance—a so-called measure—to track several features of an instance in solving it. While developed in the realm of exponential-time algorithms, it has also been used to upper bound the number of extremal vertex sets in graphs (see, e.g., [6,8]).

Our new proof upper bounding \( \text{sep}(n) \) uses a measure that takes into account the number of vertices of the graph and the difference in size between the separated components of the graph. This simple trick allows us to avoid several complications from [12], including the use of the firefighter lemma (Lemma 3.1 in [12]), fixing the size of the separators, the discussion of “full components,” and distinguishing between separators of size at most \( n/3 \) and at least \( n/3 \).

The upper bound will follow as a corollary of the next lemma, which is more general than needed, but can also used as a replacement of the firefighter lemma in recent upper bound proofs on the number of potential maximal cliques [11,12].

**Lemma 1.** Let \( 1 \leq \alpha \leq 2 \). In any graph \( G = (V, E) \) and for any vertex \( a \in V \), the number of connected vertex sets \( A \subseteq V \) with \( a \in A \) and \( |A| \leq \frac{n - |N_G(A)|}{\alpha} \) is in \( O(\beta^n) \), where \( \beta \) is the positive real root of \( x^{-1} + x^{-\alpha} = 1 \) and \( n \) is the number of vertices of \( G \).

**Proof 2.** Let \( G = (V, E) \) be any graph on \( n \) vertices and \( a \in V \). For \( d \leq n \), an \([a,d]\)-set is a set \( A \subseteq V \) such that

- \( a \in A \),
- \( G[A] \) is connected, and
- \( |A| \leq n - |N_G[A]| - d \).

Let \( \text{sep}_a(G, d) \) denote the number of \([a,d]\)-sets in \( G \). To upper bound \( \text{sep}_a(G, d) \), we will use the measure

\[
\mu(G, d) = n - d \cdot (\alpha - 1).
\]

Observe that \( \mu(G, d) \leq n \) for every \( d \) with \( 0 \leq d \leq n \). The theorem will follow from the claim that \( \text{sep}_a(G, 0) \leq \beta^{\mu(G,0)} \). We will prove the more general claim that \( \text{sep}_a(G, d) \leq \beta^{\mu(G,d)} \) for each \( d \) with \( 0 \leq d \leq n \).

If \( \mu(G, d) \leq 0 \), then \( d \geq \frac{n}{\alpha - 1} \geq n \) and \( \text{sep}_a(G, d) = 0 \) since there is no \( A \subseteq V \) with \( |A| \leq n - |N_G[A]| - d \leq -|N_G[A]| \leq 0 \) and \( a \in A \). If \( d_G(a) = 0 \), then there is at most one \([a,d]\)-set, which is \([a]\). Therefore, assume \( \mu(G, d) > 0 \), the vertex \( a \) has at least one neighbor, and assume the claim holds for smaller measures. Consider a vertex \( u \in N_G(a) \). For each \([a,d]\)-set \( A \), either \( u \in A \) or \( u \in N_G(A) \). Therefore, we can upper bound the \([a,d]\)-sets \( A \) counted in \( \text{sep}_a(G, d) \) with \( u \in N_G(A) \) by \( \beta^{\mu(G-[u],d)} = \beta^{\mu(G,d)-1} \), and those with \( u \in A \) by \( \beta^{\mu(G/Au,d+1)} = \beta^{\mu(G,d)-\alpha} \). It remains to observe that \( \beta^{\mu(G,d)-1} + \beta^{\mu(G,d)-\alpha} = \beta^{\mu(G,d)} \).

We can use the bound in Lemma 1 with \( \alpha = 2 \) for each vertex \( v \in V \) to upper bound \( \text{sep}(n) \) since for every minimal separator \( S \) of a graph \( G = (V, E) \), which is a minimal \((a,b)\)-separator for some pair of vertices \((a,b)\), either the connected component \( A \) of \( G - S \) containing \( a \) or the connected component \( B \) of \( G - S \) containing \( b \) has size at most \((|V| - |S|)/2 \). Moreover, minimality of the separator ensures that each vertex from \( S \) is adjacent to a vertex from \( A \) and a vertex from \( B \).
Corollary 1. $\text{sep}(n) \in O(\rho^n \cdot n)$, where $\rho = \frac{1 + \sqrt{5}}{2} = 1.6180...$ is the golden ratio.

For the base case of the proof of Lemma 1, we need that $\alpha \leq 2$. This limitation can be avoided at the expense of a factor $O(n^2)$ in the upper bound, as proved in the following lemma, which also uses a somewhat more intuitive measure.

Lemma 2. Let $\alpha \geq 1$. In any graph $G = (V, E)$ and for any vertex $a \in V$, the number of connected vertex sets $A \subseteq V$ with $a \in A$ and $|A| \leq \frac{n - |N_G(A)|}{\alpha}$ is in $O(\beta^n \cdot n^2)$, where $\beta$ is the positive real root of $x^2 - 1 + x^{-\alpha} = 1$ and $n$ is the number of vertices of $G$.

Proof 5. Let $G = (V, E)$ be any graph on $n$ vertices with $a \in V$. For any $0 \leq b, s \leq n$ with $b \leq \frac{n - s}{\alpha}$, an $[a, b, s]$-set is a set $A \subseteq V$ such that
- $a \in A$,
- $G[A]$ is connected,
- $|A| = b$, and
- $|N_G(A)| = s$.

Let $\text{sep}_a(G, b, s)$ denote the number of $[a, b, s]$-sets in $G$. To upper bound this value, we will use the measure

$$
\mu(G, b, s) = \alpha \cdot b + s.
$$

Note that there are $O(n^2)$ combinations of values for $b$ and $s$ such that $b \leq \frac{n - s}{\alpha}$, and for each of them we have that $\mu(G, b, s) \leq \frac{n - s}{\alpha} + s \leq n$. The theorem will therefore follow from the claim that $\text{sep}_a(G, b, s) \leq \beta^{\mu(G,b,s)}$ for $0 \leq b, s \leq |V|$.

If $b = 0$, then $\text{sep}_a(G, b, s) = 0$ since there is no $A \subseteq V$ with $|A| = 0$ and $a \in A$. If $s = 0$, then $\text{sep}_a(G, b, s) = 1$ if the connected component of $G$ containing $a$ has $b$ vertices and $\text{sep}_a(G, b, s) = 0$ otherwise. Now, assume $b, s \geq 1$. If $d_G(a) = 0$, then there is no $[a, b, s]$-set since $s \geq 1$. Therefore, assume $a$ has at least one neighbor, and assume the claim holds for smaller measures. Consider a vertex $u \in N_G(a)$. For every $[a, b, s]$-set $A$, either $u \in A$ or $u \in N_G(A)$. Therefore, we can upper bound the $[a, b, s]$-sets $A$ counted in $\text{sep}_a(G, b, s)$ with $u \in N_G(A)$ by $\beta^{\mu(G \setminus \{u\}, b, s - 1)} = \beta^{\mu(G, b, s - 1)}$, and those with $u \in A$ by $\beta^{\mu(G / \{a, u, b - 1, s\})} = \beta^{\mu(G, b, s) - \alpha}$. It remains to observe that $\beta^{\mu(G, b, s) - 1} + \beta^{\mu(G, b, s) - \alpha} = \beta^{\mu(G, b, s)}$. \[\blacksquare\]

We note that the inductive proofs of Lemma 1, Corollary 1, and Lemma 2 can easily be turned into recursive algorithms enumerating these objects at the expense of a multiplicative polynomial factor.

3 | LOWER BOUND ON THE MAXIMUM NUMBER OF MINIMAL SEPARATORS

In the melon graph in Fig. 1, each horizontal layer implies a choice between three vertices. Each such choice also “costs” three vertices. The new construction improves the bound by adding vertical choices on top of the horizontal choices. This is achieved by “sacrificing” horizontal choices and adding 18 vertices for 126 horizontal layers. For most minimal separators, two horizontal choices are sacrificed, and their order matters, giving $126 \cdot 125$ possibilities, at the cost of 24 vertices (18 new vertices and six from the horizontal choices). Since $126 \cdot 125 > 3^{24/3}$, this gives more choices than the melon graph on the same number of vertices.
**Theorem 1.** $\text{sep}(n) \in o(1.4457^n)$.

*Proof.* We prove the theorem by exhibiting a family of graphs $\{G_1, G_2, \ldots\}$ and lower bounding their number of minimal separators.

Let $p = 9$ and $q = 4$. Let $I = \{1, \ldots, 3\}$, $J = \{1, \ldots, \binom{p}{q}\}$, and $K = \{1, \ldots, p\}$. The graph $G_1$ is constructed as follows (see Fig. 2). Construct disjoint vertex sets $V_i = \{v_{i,j} : j \in J\}$ for each $i \in I$, and the vertex sets $U = \{u_i : i \in K\}$ and $W = \{w_i : i \in K\}$. The vertex set of $G_1$ is $\{a, b\} \cup U \cup W \cup \bigcup_{i \in I} V_i$. The edge set of $G_1$ is obtained by first adding the paths $(v_{1,j}, v_{2,j}, v_{3,j})$ for all $j \in J$ and the edges $\{au_i : i \in K\}$ and $\{w_ib : i \in K\}$. Then, add edges between $U$ and $V_1$ such that each vertex in $V_1$ has $q$ neighbors in $U$ and no two vertices from $V_1$ have the same neighbors in $U$. This is possible, since there are $\binom{p}{q}$ distinct subsets of $U$ of size $q$. Similarly, add edges between $V_3$ and $W$ such that each vertex in $V_3$ has $q$ neighbors in $W$ and no two vertices from $V_3$ have the same neighbors in $W$. The graph $G_{\ell}$, $\ell \geq 2$, is obtained from $\ell$ disjoint copies of $G_1$, merging the copies of $a$, and merging the copies of $b$.

Let us now consider the sets $S_{r,s}$ of minimal $(a, b)$-separators in $G_1$ that contain $r$ vertices from $U$ and $s$ vertices from $W$. The separators in $S_{0,0}$ contain one vertex among $\{v_{1,j}, v_{2,j}, v_{3,j}\}$ for each $j \in J$, giving $|S_{0,0}| = 3^{|J|}$. The separators in $S_{0,s}$ with $s \geq q$ contain $s$ vertices from $W$, leaving $\binom{p}{q} - \binom{p}{s}$ vertices from $V_3$ with at least one neighbor in $W$. For each such vertex $v_{3,j}$, the separators in $S_{0,s}$ that contain $S$ also contain one vertex among $\{v_{1,j}, v_{2,j}, v_{3,j}\}$. This separates $a$ from $b$, and all these separators are minimal. In total, $|S_{0,0}| = \binom{p}{3} \cdot 3^{(p-3)/q}$. Similarly, $|S_{r,0}| = \binom{p}{r} \cdot 3^{(p-r-s)/q}$. For $r, s \geq q$, separators containing $S_U \subseteq U$ and $S_W \subseteq W$ are not minimal if $S_U \subseteq S_W$ or $S_W \subseteq S_U$. Otherwise, $S_U \cup S_W$ can be extended to a minimal $(a, b)$-separator by selecting one vertex from $\{v_{1,j}, v_{2,j}, v_{3,j}\}$ for each $j \in J$ such that $v_{1,j}$ has at least one neighbor in $U \setminus S_U$ and $v_{3,j}$ has at least one neighbor in $W \setminus S_W$. In total, $|S_{r,s}| \geq \binom{p}{r} \cdot \binom{p}{s} - \binom{p}{\max(r,s)} \cdot \binom{p}{\min(r,s)} - \binom{p}{\max(r,s)} \cdot 3^{(p-r-s)/q}$. Therefore, the number of minimal separators of $G_1$ is at least

\[
x = 3^{(p)/q} + 2 \cdot \sum_{s=q}^{p} \left( \binom{p}{r} \cdot 3^{(p-r-s)/q} \right) + \sum_{s=q}^{p} \sum_{r=q}^{p} \left( \binom{p}{r} \cdot \binom{p}{s} - \binom{p}{\max(r,s)} \cdot \binom{p}{\min(r,s)} - \binom{p}{\max(r,s)} \cdot 3^{(p-r-s)/q} \right) > 2.4603 \cdot 10^{63}.
\]
Minimal \((a, b)\)-separators for \(G_\ell\) are obtained by taking the union of minimal separators for the copies of \(G_1\). Their number is therefore at least \(x^\ell = x^{\frac{n-\ell}{2}} - \frac{1}{\ell} + 2|\mathcal{K}| + 2|\mathcal{J}| \in \omega(1.4457^n)\), where \(G_\ell\) has \(n = \ell(3^\ell p + 2p) + 2\) vertices.

Based on results from [2], Bouchitté and Todinca [3] observed that the number of potential maximal cliques in a graph is at least the number of minimal separators divided by the number of vertices \(n\). Therefore, we arrive at the following corollary of Theorem 1.

**Corollary 2.** \(\text{pmc}(n) \in \omega(1.4457^n)\).

### 4 | CONCLUSION

We have given a simpler proof for the best-known asymptotic upper bound on \(\text{sep}(n)\), and we have improved the best-known lower bound from \(\Omega(3^{n/3})\) to \(\omega(1.4457^n)\), thereby reducing the gap between the current best lower and upper bound. Before our work, it seemed reasonable to believe that \(\text{sep}(n)\) could be asymptotically equal to \(3^{n/3}\), up to polynomial factors. We showed that this is not the case, and we believe there is room to further improve the lower bound.

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### ENDNOTE

1 The bound stated in [12] is \(O(1.6181^n)\), but this stronger bound can be derived from their proof.

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