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Exact (exponential) algorithms for treewidth and minimum fill-in

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Abstract

We show that for a graph G on n vertices its treewidth and minimum fill-in can be computed roughly in 1.9601^n time. Our result is based on a combinatorial proof that the number of minimal separators in a graph is $\mathcal{O}(n \cdot 1.7087^n)$ and that the number of potential maximal cliques is $\mathcal{O}(n^4 \cdot 1.9601^n)$.

1 Introduction

The last few years have seen an emerging interest in fast exponential algorithms for NP-hard problems. There are several explanations to this interest. Today almost everyone does expect that there is no polynomial time algorithm solving an NP-hard problem. Trying different ways of avoiding intractability several approaches were proposed such as: approximation algorithms, randomized algorithms, heuristic methods etc. Each of these approaches has weak points like necessity of exact solutions, difficulty of approximation, limited power of the method itself and many others. All these obstacles encourage us to try a direct (and perhaps desperate) way of coping with NP-hardness: Design of exponential algorithms that are significantly faster than exhaustive search. With the increased speed of modern computers, fast algorithms, even though they have exponential running times in the worst case, may actually lead to practical algorithms for certain NP-hard problems, at least for moderate instance sizes. Nice examples of fast exponential algorithms are Eppstein's graph coloring algorithm with time complexity $\mathcal{O}^*(2.4150^n)$ [14] and an $\mathcal{O}^*(1.4802^n)$ time algorithm for 3-SAT [12]. (In this paper we use a modified big-Oh notation that suppresses all other (polynomially bounded) terms. For functions f and g we write $f(n) = \mathcal{O}^*(g(n))$ if $f(n) = \mathcal{O}(g(n)poly(|n|))$, where $poly(|n|)$ is a polynomial. This modification may be justified by the exponential growth of $f(n)$.) Many natural questions in the field of exact algorithms can not be answered by the classical complexity theory, for example why some NP-hard problems can be solved significantly faster than others? For a good overview of the field see the recent survey written by Gerhard Woeginger [24].

Treewidth is one of the most basic parameters in algorithms and it plays an important role in structural graph theory. It serves as one of the main tools in Robertson & Seymour's Graph Minors project [23]. It is well known that many intractable problems can be solved in polynomial (and very often in linear time) when the input is restricted to graphs of bounded treewidth. In recent years [11] it was shown that the results on graphs of bounded treewidth (branchwidth) are not

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only of theoretical interest but can successfully be applied to find optimal solutions or lower bounds for diverse optimization problems. (See also [5] for a comprehensive survey.) Treewidth also plays a crucial role in Downey & Fellows parameterized complexity theory [13]. An efficient solution to treewidth is the base for many applications in artificial intelligence, databases and logical-circuit design. See [1] for further references.

The minimum fill-in problem has important applications in sparse matrix computations and computational biology.

Previous results. Treewidth and minimum fill-in are known to be NP-hard even when the input is restricted to complements of bipartite graphs (so called cobipartite graphs) [2, 25]. Despite of the importance of treewidth almost nothing is known on how to cope with its intractability. It is known that it can be approximated with a factor $\log OPT$ [1, 9] and it is an old open question if the treewidth can be approximated with a constant factor. Treewidth is known to be fixed parameter tractable, moreover, for a fixed k , the treewidth of size k can be computed in linear time (with a huge hidden constant) [4]. There is a number of algorithms that for a given graph G and integer k , either reports that the treewidth of G is at least k , or produces a tree decomposition of width at most $c_1 \cdot k$ in time $O(c_2^k n^{O(1)})$, where c_1, c_2 are some constants (see e.g. [1]). Fixed parameter algorithms are known for fill-in problem as well [10, 19].

There is no previous work on exact algorithms for treewidth or fill-in and almost nothing was known about it. Both problems can be solved in $\mathcal{O}^*(2^n)$ either by using the algorithm of Arnborg et al. [2] or by reformulating them as problems of finding a special vertex ordering and using the technique proposed by Held & Karp [18] for the travelling salesman problem.

Our results. In this paper we break the $\mathcal{O}^*(2^n)$ barrier by obtaining the first exact algorithm for treewidth of running time $\mathcal{O}^*(c^n)$ for $c < 2$. Our algorithm can be adapted not only for treewidth but for a number of other minimal triangulation problems like minimum fill-in. Our main result is the $\mathcal{O}^*(1.9601^n)$ algorithm computing the treewidth and minimum fill-in of a graph on n vertices. The algorithm can be regarded as dynamic programming across partial solutions and is based on results of Bouchitté & Todinca [7, 8]. The running time analysis of the algorithm is difficult and is based on a careful counting of potential maximal cliques, i.e. vertex subsets in a graph that can be maximal cliques in some minimal triangulation of this graph. More precisely, we start by modifying the algorithm due to Bouchitté & Todinca [7] to compute the treewidth and minimum fill-in of a graph G with the given set Π_G of all potential maximal cliques of G in time $\mathcal{O}^*(|\Pi_G|)$. Then we obtain a number of structural results which provide us with the proof that $|\Pi_G| = \mathcal{O}^*(1.9601^n)$ and with an algorithm computing all potential maximal cliques in time $\mathcal{O}^*(1.9601^n)$. Our analysis is based on combinatorial bounds for the number of minimal separators as well as for the number of potential maximal cliques in a graph on n vertices. Determining such bounds is an attractive combinatorial problem on its own.

For the class of AT-free graphs, for which both problems remain NP-complete, we were able to prove that the number of minimal separators and potential maximal cliques, and thus the running time of our algorithm, is $\Theta^*(2^{n/2})$ (see the full version of the paper [16]).

2 Basic definitions

We denote by $G = (V, E)$ a finite, undirected and simple graph with $|V| = n$ vertices and $|E| = m$ edges. For any non-empty subset $W \subseteq V$, the subgraph of G induced by W is denoted by $G[W]$. For $S \subseteq V$ we often use $G \setminus S$ to denote $G[V \setminus S]$. The

neighborhood of a vertex v is $N(v) = \{u \in V : \{u, v\} \in E\}$ and for a vertex set $S \subseteq V$ we put $N(S) = \bigcup_{v \in S} N(v) \setminus S$. A *clique* C of a graph G is a subset of V such that all the vertices of C are pairwise adjacent. By $\omega(G)$ we denote the maximum clique-size of a graph G .

The notion of treewidth is due to Robertson & Seymour [22]. A *tree decomposition* of a graph $G = (V, E)$, denoted by $TD(G)$, is a pair (X, T) in which $T = (V_T, E_T)$ is a tree and $X = \{X_i | i \in V_T\}$ is a family of subsets of V such that: (i) $\bigcup_{i \in V_T} X_i = V$; (ii) for each edge $e = \{u, v\} \in E$ there exists an $i \in V_T$ such that both u and v belong to X_i ; and (iii) for all $v \in V$, the set of nodes $\{i \in V_T | v \in X_i\}$ forms a connected subtree of T .

The maximum of $|X_i| - 1$, $i \in V_T$, is called the *width* of the tree decomposition. The *treewidth* of a graph G ($\text{tw}(G)$) is the minimum width over all tree decompositions of G .

A graph H is *chordal* (or *triangulated*) if every cycle of length at least four has a chord, i.e. an edge between two non-consecutive vertices of the cycle. A *triangulation* of a graph $G = (V, E)$ is a chordal graph $H = (V, E')$ such that $E \subseteq E'$. H is a *minimal triangulation* if for any intermediate set E'' with $E \subseteq E'' \subset E'$, the graph $F = (V, E'')$ is not chordal.

The following result is very useful for our algorithms.

Theorem 1 (Folklore). *For any graph G , $\text{tw}(G) \leq k$ if and only if there is a triangulation H of G such that $\omega(H) \leq k + 1$.*

Thus the treewidth of G can be defined as the minimum over all triangulations H of G , of $\omega(H) - 1$.

The *minimum fill-in* of a graph $G = (V, E)$, denoted by $\text{mfi}(G)$, is the smallest value of $|E_H - E|$, where the minimum is taken over all triangulations $H = (V, E_H)$ of G .

In other words, computing the treewidth of G means finding a triangulation with the smallest maximum clique-size, while computing the minimum fill-in means finding a triangulation with the smallest number of edges. In both cases we can restrict our work to minimal triangulations.

Minimal separators and potential maximal cliques. Minimal separators and potential maximal cliques are the most important tools used in our proofs. Let a and b be two non adjacent vertices of a graph $G = (V, E)$. A set of vertices $S \subseteq V$ is an *a, b -separator* if a and b are in different connected components of the graph $G[V \setminus S]$. S is a *minimal a, b -separator* if no proper subset of S is an a, b -separator. We say that S is a *minimal separator* of G if there are two vertices a and b such that S is a minimal a, b -separator. Notice that a minimal separator can be strictly included in another one. We denote by Δ_G the set of all minimal separators of G . A set of vertices Ω of a graph G is called a *potential maximal clique* if there is a minimal triangulation H of G such that Ω is a maximal clique of H . We denote by Π_G the set of all potential maximal cliques of G .

The following result will be used to list all minimal separators.

Theorem 2 ([3]). *There is an algorithm listing all minimal separators of an input graph G in $\mathcal{O}(n^3 |\Delta_G|)$ time.*

For a set $K \subseteq V$, a connected component C of $G \setminus K$ is a *full component associated to K* if $N(C) = K$.

The following structural characterization of potential maximal cliques is extremely useful for our purposes.

Theorem 3 ([7]). *Let $K \subseteq V$ be a set of vertices and let $\mathcal{C}(K) = \{C_1, \dots, C_p\}$ be the set of the connected components of $G \setminus K$. Let $\mathcal{S}(K) = \{S_1, S_2, \dots, S_p\}$ where*

$S_i(K)$ is the set of vertices of K adjacent to at least one vertex of $C_i(K)$. Then K is a potential maximal clique if and only if :

1. $G \setminus K$ has no full components associated to K , and
2. the graph on the vertex set K obtained from $G[K]$ by turning each $S_i \in \mathcal{S}(K)$ into a clique, is a complete graph.

Moreover, if K is a potential maximal clique, then $\mathcal{S}(K)$ is the set of the minimal separators of G contained in K .

By Theorem 3, for every potential maximal clique Ω of G , the sets $S_i(\Omega)$ are exactly the minimal separators of G contained in K . Let us point out that for each minimal separator S_i , $\Omega \setminus S_i$ is contained in a same component of $G \setminus S_i$.

The following result is an easy consequence of Theorem 3.

Theorem 4 ([7]). *There is an algorithm that, given a graph $G = (V, E)$ and a set of vertices $K \subseteq V$, verifies if K is a potential maximal clique of G . The time complexity of the algorithm is $\mathcal{O}(nm)$.*

3 Computing treewidth and minimum fill-in

We describe the algorithm of [7] that, given a graph, all its minimal separators and all its potential maximal cliques, computes the treewidth and the minimum fill-in of the graph. New observation here is that this algorithm can be implemented to run in $\mathcal{O}^*(|\Pi_G|)$ time.

For a minimal separator S and a component $C \in \mathcal{C}(S)$ of $G \setminus S$, we say that (S, C) is a *block* associated to S . We sometimes use the notation (S, C) to denote the set of vertices $S \cup C$ of the block. It is easy to notice that if $X \subseteq V$ corresponds the set of vertices of a block, then this block (S, C) is unique: indeed $S = N(V \setminus X)$ and $C = X \setminus S$.

A block (S, C) is called *full* if C is a full component associated to S . The graph $R(S, C) = G_S[S \cup C]$ obtained from $G[S \cup C]$ by completing S into a clique is called the *realization* of the block B .

Theorem 5 ([20]). *Let G be a non-complete graph. Then*

$$\begin{aligned} \text{tw}(G) &= \min_{S \in \Delta_G} \max_{C \in \mathcal{C}(S)} \text{tw}(R(S, C)) \\ \text{mfi}(G) &= \min_{S \in \Delta_G} \left(\text{fill}(S) + \sum_{C \in \mathcal{C}(S)} \text{mfi}(R(S, C)) \right) \end{aligned}$$

where $\text{fill}(S)$ is the number of non-edges of $G[S]$.

In the equations of Theorem 5 we may take the minimum only over the inclusion-minimal separators of G . Then all the blocks in the equations are full.

We now express the treewidth and the minimum fill-in of realizations of full blocks from realizations of smaller full blocks. Let Ω be a potential maximal clique of G . We say that a block (S', C') is *associated to* Ω if C' is a component of $G \setminus \Omega$ and $S' = N(C')$.

Theorem 6 ([7]). *Let (S, C) be a full block of G . Then*

$$\begin{aligned} \text{tw}(R(S, C)) &= \min_{S \subset \Omega \subseteq (S, C)} \max(|\Omega| - 1, \text{tw}(R(S_i, C_i))) \\ \text{mfi}(R(S, C)) &= \min_{S \subset \Omega \subseteq (S, C)} \left(\text{fill}(\Omega) - \text{fill}(S) + \sum \text{mfi}(R(S_i, C_i)) \right) \end{aligned}$$

where the minimum is taken over all potential maximal cliques Ω such that $S \subset \Omega \subseteq (S, C)$ and (S_i, C_i) are the blocks associated to Ω in G such that $S_i \cup C_i \subset S \cup C$.

Theorem 7. *There is an algorithm that, given a graph G together with the list of its minimal separators Δ_G and the list of its potential maximal cliques Π_G , computes the treewidth and the minimum fill-in of G in $\mathcal{O}^*(|\Pi_G|)$ time. Moreover, the algorithm constructs optimal triangulations for the treewidth and the minimum fill-in.*

Proof's sketch. We provide here only some ideas, for a complete proof see [16]. W.l.o.g. we can assume that G is connected graph (otherwise we can run the algorithm for each connected component of G). First the algorithm computes all the full blocks and sorts them by their size. If there is no block, then G is a complete graph and in this case the solution is trivial. For each inclusion minimal full block (S, C) (i.e. block containing no other full blocks), we assign $\text{tw}(R(S, C)) = |S \cup C| - 1$ and $\text{mfi}(R(S, C)) = \text{fill}(S \cup C)$. Then, for each full block (S, C) in the increasing order, the treewidth and the minimum fill-in of the realization $R(S, C)$ is computed by making use of Theorem 6. Finally, $\text{tw}(G)$ and $\text{mfi}(G)$ are obtained by Theorem 5.

The time complexity is given by the computation of the treewidth and minimum fill-in parameters for the realizations of all the full blocks, which works as follows:

```

for each full block  $(S, C)$ 
  for each potential maximal clique  $\Omega$  such that  $S \subset \Omega \subseteq S \cup C$ 
    apply a polynomial time treatment to each block  $(S_i, C_i)$ 
    associated to  $\Omega$  s.t.  $S_i \cup C_i \subset S \cup C$ .

```

When S , C and Ω are fixed, the number of blocks associated to Ω is at most n . Indeed, each of these blocks corresponds to a component of $G \setminus \Omega$. These blocks can be computed in polynomial time. Let us show that the number of triples (S, C, Ω) with $S \subset \Omega \subseteq S \cup C$ is bounded by $n|\Pi_G|$. By Theorem 3, for a fixed potential maximal clique Ω there are at most n minimal separators $S \subset \Omega$. (The number of components in $G \setminus \Omega$, and hence the number of sets $S_i(\Omega)$ is at most n .) Also by Theorem 3, for each minimal separator $S \subset \Omega$, there is a unique component C of $G \setminus S$ such that $\Omega \subseteq S \cup C$.

It remains to turn this argument into an implementation such that the two nested loops have at most $n|\Pi_G|$ iterations. During a preprocessing step, for each potential maximal clique Ω we compute all minimal separators contained in Ω (by Theorem 3, they are the neighborhoods of the components of $G \setminus \Omega$). For each $S \subset \Omega$, we compute the unique component C of $G \setminus S$ containing $\Omega \setminus S$. For each block (S, C) we keep a pointer to Ω . Using appropriate data structures these preprocessing costs $\mathcal{O}(nm)$ for each potential maximal clique. In this way, each block (S, C) will keep the list of all the potential maximal cliques Ω s.t. $S \subset \Omega \subseteq S \cup C$. The number of iterations of the two loops is then the number of “good” triples (S, C, Ω) , i.e. at most $n|\Pi_G|$. \square

After Theorem 7, the only missing ingredient of our algorithms is listing of all the minimal separators and the potential maximal cliques of a graph in time $\mathcal{O}^*(c^n)$ for some $c < 2$. In the next two sections we discuss this issue.

4 Upper bounding the number of minimal separators

In this section we show that any graph with n vertices has $\mathcal{O}(n \cdot 1.7087^n)$ minimal separators. For the main algorithm of this paper the upper bound $\mathcal{O}^*(1.9601^n)$ would be sufficient. However, bounding the number of minimal separators in a graph is a nice combinatorial problem and we prefer to give here the best upper bound we were able to find.

Let S be a separator in a graph $G = (V, E)$. For $x \in V \setminus S$, we denote by $C_x(S)$ the component of $G \setminus S$ containing x . The following lemma is an exercise in [17].

Lemma 8 (Folklore). *A set S of vertices of G is a minimal a, b -separator if and only if a and b are in different full components associated to S . In particular, S is a minimal separator if and only if there are at least two distinct full components associated to S .*

Theorem 9. *For any graph G , $|\Delta_G| = \mathcal{O}(n \cdot 1.7087^n)$.*

Let us note, that by Theorem 2, Theorem 9 yields immediately that all minimal separators of a graph can be listed in time $\mathcal{O}(n^4 \cdot 1.7087^n)$.

Proof. For a constant α , $0 < \alpha < 1$, we distinguish two types of minimal separators: *small* separators, of size at most αn , and *big* separators, of size more than αn . We denote the cardinalities of these sets by `#small sep` and `#big sep`. Notice that $|\Delta_G| = \text{\code\#small sep} + \text{\code\#big sep}$.

Counting big separators. Let S be a minimal separator. By Lemma 8, there are at least two full components associated to S . Hence at least one of these full components has at most $n(1 - \alpha)/2$ vertices. For every $S \in \Delta_G$ we choose one of these full components, and call it the *small* component of S , denoted by $s(S)$.

By the definition of a full component, $S = N(s(S))$. In particular, for distinct minimal separators S and T , we have that $s(S) \neq s(T)$. Therefore the number `#big sep` of big minimal separators is at most the number of small components and we conclude that `#big sep` does not exceed the number of subsets of V of cardinality at most $n(1 - \alpha)/2$, i.e.

$$\text{\code\#big sep} \leq \sum_{i=1}^{\lceil n(1-\alpha)/2 \rceil} \binom{n}{i} \quad (1)$$

Counting small separators. To count small separators we use a different technique. Let S be a minimal separator, let x be a vertex of a full component $C_x(S)$ associated to S with minimum number of vertices and let $X \subset V$ be a vertex subset. We say that (x, X) is a *bad pair* associated to S if $C_x(S) \subseteq X \subseteq V \setminus S$.

Note that the connected component of $G[X]$ containing x is $C_x(S)$, by the fact that $C_x(S) \subseteq X$ and $X \cap S = \emptyset$. Let S and T be two distinct minimal separators. Consider two bad pairs (x, X) and (y, Y) , associated to S and T respectively. We prove that $(x, X) \neq (y, Y)$. Suppose that $x = y$ and $X = Y$. By the observation above, we have $C_x(S) = C_y(T)$. Since $C_x(S)$ is a full component associated to S in G , we have that $S = N(C_x(S))$ and $T = N(C_y(T))$. Thus $S = T$ which is a contradiction.

By Lemma 8, there are at least two full components associated to every small separator S . For a full component $C_x(S)$ associated to S with the minimum number of vertices, $|V \setminus (S \cup C_x(S))| \geq n \cdot (1 - \alpha)/2$. For any $Z \subseteq V \setminus (S \cup C_x(S))$, the pair $(x, Z \cup C_x(S))$ is a bad pair associated to S . Therefore there are at least $2^{n \cdot (1-\alpha)/2}$ distinct bad pairs associated to S . Hence the total number of bad pairs is at least `#small sep` $\cdot 2^{n \cdot (1-\alpha)/2}$. On the other hand, the number of bad pairs is at most $n \cdot 2^n$. We conclude that

$$\text{\code\#small sep} \leq n 2^{n \cdot (1+\alpha)/2} \quad (2)$$

For $\alpha = 0.5456$, by making use of Stirling's formula (1) and (2) yield that `#small sep` + `#big sep` = $\mathcal{O}(n \cdot 1.7087^n)$. \square \square

5 Final step: Counting potential maximal cliques

We prove in this section the main technical result of this paper, namely that a graph with n vertices has at most $\mathcal{O}^*\left(\binom{n}{2n/5}\right)$ potential maximal cliques, that is $\mathcal{O}^*(1.9601^n)$, enumerable with the same time complexity.

Roughly speaking, the idea is to show that each potential maximal clique of a graph can be identified by a set of vertices of size at most $2n/5$. The algorithm for generating all the potential maximal cliques of a graph lists all the sets of vertices of size at most $2n/5$ and then, by applying a polynomial time procedure for each set, generates all the potential maximal cliques of the input graph.

Lemma 10. *Let Ω be a potential maximal clique of G , S be a minimal separator contained in Ω and C be the component of $G \setminus S$ intersecting Ω . Then one of the following holds:*

1. $\Omega = N(C \setminus \Omega)$;
2. there is $a \in \Omega \setminus S$ such that $\Omega = N[a]$;
3. there is $a \in S$ such that $\Omega = S \cup (N(a) \cap C)$.

Proof. Since C is a component of $G \setminus S$ and S is contained in Ω , we have that $N(C \setminus \Omega) \subseteq \Omega$. If every vertex of Ω is adjacent to a vertex of $C \setminus \Omega$, then $\Omega = N(C \setminus \Omega)$.

Suppose that there is a vertex $a \in \Omega$ having no neighbors in $C \setminus \Omega$. We consider first the case $a \in \Omega \setminus S$. We claim that in this case $\Omega = N[a]$. Because $a \in \Omega \setminus S \subseteq C$ we conclude that $N[a] \subseteq \Omega$. Thus to prove the claim we need to show that $\Omega \subseteq N[a]$. For sake of contradiction, suppose that there is $b \in \Omega$ which is not adjacent to a . By Theorem 3, every two non adjacent vertices of a potential maximal clique are contained in some minimal separator $S_i(\Omega)$. Thus both a and b should have neighbors in a component $C_i(\Omega)$ of $G \setminus \Omega$. Since $a \in \Omega \setminus S \subseteq C$, we have that $C_i(\Omega) \subseteq C \setminus \Omega$. But this contradicts our assumption that a has no neighbors in $C \setminus \Omega$.

The case $a \in S$ is similar. Suppose that $\Omega \setminus S \neq N(a) \cap C$, i.e. there is $b \in \Omega \setminus S$ non adjacent to a . Then again, a and b are contained in some minimal separator and thus should have neighbors in a component $C_i(\Omega) \subseteq C$ of $G \setminus \Omega$ which is a contradiction. □ □

Let Ω be a potential maximal clique of G . The triple (S, a, b) is called a *separator representation* of Ω if S is a minimal separator of G , $a \in S$, $b \in V \setminus S$ and $\Omega = S \cup (N(a) \cap C_b(S))$, where $C_b(S)$ is the component of $G \setminus S$ containing b . Let us note that for a given triple (S, a, b) , one can check in polynomial time whether (S, a, b) is the separator representation of a (unique) potential maximal clique Ω .

The number of all possible separator representations of a graph is bounded by $n^2 |\Delta_G|$. Unfortunately, in the case when a potential maximal clique Ω has no separator representation, we cannot say that Ω is small (i.e. of size at most βn for some $\beta < 0.5$) or is the neighborhood of a small set. In the next subsection we introduce another type of representation, the *neighborhood representation*, that allows us to show that all the potential maximal cliques can be represented by small sets of vertices.

Counting nice potential maximal cliques. Let Ω be a potential maximal clique of a graph G and let $S \subset \Omega$ be a minimal separator of G . We say that S is an *active separator* for Ω if Ω is not a clique in the graph $G_{S(\Omega) \setminus \{S\}}$, obtained from G by completing all the minimal separators contained in Ω , except S . If S is active, a pair of vertices $x, y \in S$ non adjacent in $G_{S(\Omega) \setminus \{S\}}$ is called an *active pair*.

Theorem 11 ([8]). *Let Ω be a potential maximal clique of G and $S \subset \Omega$ a minimal separator, active for Ω . Let (S, C) be the block associated to S containing Ω and let $x, y \in \Omega$ be an active pair. Then $\Omega \setminus S$ is a minimal x, y -separator in $G[C \cup \{x, y\}]$.*

We say that a potential maximal clique Ω is *nice* if at least one of the minimal separators contained in Ω is active for Ω . In this subsection we shall prove that a graph with n vertices has $\mathcal{O}^*\left(\binom{n}{2n/5}\right)$ nice potential maximal cliques.

Lemma 12. *Let Ω be a nice potential maximal clique, S be a minimal separator, active for Ω , $x, y \in S$ be an active pair, and C be the component of $G \setminus S$ containing $\Omega \setminus S$. There is a partition (D_x, D_y) of $C \setminus \Omega$ such that $N(D_x \cup \{x\}) \cap C = N(D_y \cup \{y\}) \cap C = \Omega \setminus S$.*

Proof. By Theorem 11, $\Omega \setminus S$ is a minimal x, y -separator in $G[C \cup \{x, y\}]$. Let C_x be the full component associated to $\Omega \setminus S$ in $G[C \cup \{x, y\}]$, containing x , $D_x = C_x \setminus \{x\}$, and $D_y = C \setminus D_x$. Notice that the full component associated to $\Omega \setminus S$ in $G[C \cup \{x, y\}]$ and containing y , is in $D_y \cup \{y\}$. Therefore D_x and D_y satisfy the above condition. \square \square

Let us note that if one of the two sets of the partition in Lemma 12, say D_x , is empty, then for any $z \in C$, the triple (S, x, z) is a separator representation of Ω . Let C' be a component of $G \setminus \Omega$ such that $N(C') = S$ and let $c \in C'$. If D_x is not empty, we have that the triple $(X = C' \cup D_x, x, c)$ is sufficient for computing Ω . Indeed, C' is the component of $G[X]$ containing c , $D_x = X \setminus C'$, C is the component of $G - N(C')$ containing D_x , and finally $\Omega = S \cup (\Omega \setminus S) = N(C') \cup (N(D_x \cup \{x\}) \cap C)$.

The triple $(C' \cup D_x, x, c)$ can be used to represent Ω .

More formally: For a potential maximal clique Ω of G , we say that a triple (X, x, c) , where $X \subseteq V$, $c \in X$, and $x \notin X$ is a *neighborhood representation* of Ω if the following hold:

1. $D_x = X \setminus C'$ is not empty, where C' is the component of $G[X]$ containing c ;
2. $\Omega = N(C') \cup (N(D_x \cup \{x\}) \cap C)$, where C is the component of $G - N(C')$ containing D_x .

Let us remark that for a given triple (X, x, c) , we can check in polynomial time whether (X, x, c) is a neighborhood representation of a (unique) potential maximal clique Ω .

We state now the main tool for counting the nice potential maximal cliques.

Lemma 13. *Let Ω be a nice potential maximal clique of G . Then one of the following holds:*

1. $|\Omega| \leq 2n/5$;
2. There is a vertex a such that $\Omega = N[a]$;
3. Ω has a separator representation;
4. There is a set of vertices X such that $\Omega = N(X)$ and $|X| \leq 2n/5$;
5. Ω has a neighborhood representation (X, x, c) such that $|X| \leq 2n/5$.

Proof. Let S be a minimal separator active for Ω , $x, y \in S$ be an active pair, and C be the component of $G \setminus S$ containing $\Omega \setminus S$. By Lemma 12, there is a partition (D_x, D_y) of $C \setminus \Omega$ such that $N(D_x \cup \{x\}) \cap C = N(D_y \cup \{y\}) \cap C = \Omega \setminus S$. If one of the sets D_x, D_y , say D_x , is empty, then for any $z \in C$, the triple (S, x, z) is a separator representation of Ω . Suppose that none of the first three lemma's conditions hold. Then D_x and D_y are nonempty. Let C' be a component of $G \setminus \Omega$

such that $N(C') = S$ and $c \in C'$. Since D_x and D_y are not empty, we have that $(C' \cup D_x, x, c)$ and $(C' \cup D_y, y, c)$ are neighborhood representations of Ω .

By Lemma 10, $\Omega = N(C \setminus \Omega)$. Since (D_x, D_y) form a partition of $C \setminus \Omega$, it remains to prove that at least one of the sets $C \setminus \Omega = D_x \cup D_y$, $C' \cup D_x$ and $C' \cup D_y$ has at most $2n/5$ vertices. Clearly D_x, D_y and C' are pairwise disjoint. Since $|D_x| + |D_y| + |C'| \leq |V(G) \setminus \Omega| \leq 3n/5$, the conclusion follows. \square \square

It is not hard to check that, for each case of Lemma 13 there are $\mathcal{O}^*\left(\binom{n}{2n/5}\right)$ potential maximal cliques of that type. More precisely:

Lemma 14. *A graph on n vertices has at most $n^2 \sum_{i=1}^{2n/5} \binom{n}{i}$ nice potential maximal cliques, enumerable in $\mathcal{O}^*\left(\binom{n}{2n/5}\right)$ time.*

Counting all the potential maximal cliques. Not all the potential maximal cliques of a graph are necessarily nice (see [8] for an example). For counting and enumerating all the potential maximal cliques of a graph, we need the following theorem, used in [8] for showing that the number of potential maximal cliques of G is $\mathcal{O}^*(|\Delta_G|^2)$.

Theorem 15 ([8]). *Let Ω be a potential maximal clique of G , let a be a vertex of G and $G' = G \setminus \{a\}$. Then one of the following cases holds:*

1. *either Ω or $\Omega \setminus \{a\}$ is a potential maximal clique of G' .*
2. *$\Omega = S \cup \{a\}$, where S is a minimal separator of G .*
3. *Ω is nice.*

Theorem 16. *A graph G on n vertices has at most $n^3 \sum_{i=1}^{2n/5} \binom{n}{i} = \mathcal{O}(n^4 \cdot 1.9601^n)$ potential maximal cliques, enumerable in $\mathcal{O}^*(1.9601^n)$ time.*

Proof. Let x_1, x_2, \dots, x_n be the vertices of G and $G_i = G[\{x_1, \dots, x_i\}]$, $\forall i, 1 \leq i \leq n$. Theorem 15 and Lemma 14 imply that $|\Pi_{G_i}| \leq |\Pi_{G_{i-1}}| + n|\Delta_{G_i}| + n^2 \sum_{i=1}^{2n/5} \binom{n}{i}$, for all $i, 2 \leq i < n$. By Theorem 9, $|\Pi_G| \leq n^3 \sum_{i=1}^{2n/5} \binom{n}{i}$. From the same arguments it follows that Π_G can be computed and enumerated in $\mathcal{O}^*\left(\binom{n}{2n/5}\right)$ time which is approximately $\mathcal{O}^*(1.9601^n)$. \square \square

Theorems 7 and 16 imply the main result of this paper.

Theorem 17. *For a graph G on n vertices, the treewidth and the minimum fill-in of G can be computed in $\mathcal{O}^*(1.9601^n)$ time.*

6 Open problems

An interesting question is whether the upper bounds in Theorems 9 and 16 can be improved. Let us note that the lower bound we have for minimal separators and potential cliques is of order $3^{n/3} \sim 1.4422^n$.

Our algorithms for treewidth and fill-in can also be applied for solving other problems that can be expressed in terms of minimal triangulations like finding a tree decomposition of minimum cost [6] or computing treewidth of weighted graph. However, there are two 'width' parameters related to treewidth, namely bandwidth and pathwidth and one parameter called profile, related to minimum fill-in, that do not fit into this framework. Bandwidth can be computed in time $\mathcal{O}^*(10^n)$ [15] and reducing Feige's bounds is a challenging problem. Pathwidth (and profile) can be expressed as vertex ordering problems and thus solved in $\mathcal{O}^*(2^n)$ time by applying a dynamic programming approach similar to Held & Karp's approach [18] for TSP. Let us note that reaching time complexity $\mathcal{O}^*(c^n)$, for any constant $c < 2$ even for

the Hamiltonian cycle problem is a long standing problem. So it is highly unlikely that some modification of Held & Karp's approach provide us with a better exact algorithm for pathwidth or profile. It is tempting to ask if one can reach time complexity $\mathcal{O}^*(c^n)$, for any constant $c < 2$ for these problems.

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