A heuristic for listing almost-clique minimal separators of a graph

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Abstract

Bodlaender and Koster (Discrete Mathematics 2006) introduced the notion of almost-clique separators in the context of computing the treewidth $\text{tw}(G)$ of a given graph $G$. A separator $S \subseteq V(G)$ of $G$ is an almost-clique separator if $S \setminus \{v\}$ is a clique of $G$ for some $v \in S$. $S$ is a minimal separator if $S$ has at least two full components, where a full component of $S$ is a connected component $C$ of $G \setminus S$ such that $N_G(C) = S$. They observed that if $S$ is an almost-clique minimal separator of $G$ then $\text{tw}(G \cup K(S)) = \text{tw}(G)$, where $K(S)$ is the complete graph on a vertex set $S$: in words, filling an almost-clique minimal separator into a clique does not increase the treewidth. Based on this observation, they proposed a preprocessing method for treewidth computation, a fundamental step of which is to find a preferably maximal set of pairwise non-crossing almost-clique minimal separators of a graph.

In this paper, we present a heuristic for this step, which is based on the following empirical observation. For a graph $G$ and a minimal triangulation $H$ of $G$, let $\mathcal{A}(H, G)$ denote the set of all almost-clique minimal separators of $G$ that are minimal separators of $H$. Note that since the minimal separators of $H$ are pairwise non-crossing, so are those in $\mathcal{A}(H, G)$. We observe from experiments that $\mathcal{A}(H, G)$ is remarkably close to maximal, especially when the minimal triangulation $H$ is computed by an algorithm aiming for small treewidth. For example, consider the 200 graph instances from the exact treewidth track of PACE 2017 algorithm implementation challenge. For each instance $G$, we compute a minimal triangulation $H$ of $G$ using a variant of the MMD algorithm due to Berry et al., extract $\mathcal{A} = \mathcal{A}(H, G)$, and then expand $\mathcal{A}$ into a maximal set $\mathcal{A}'$ of pairwise non-crossing almost-clique minimal separators of $G$. Then, we have $|\mathcal{A}'| = |\mathcal{A}|$ for 79 instances, $|\mathcal{A}'| \leq 1.1 \cdot |\mathcal{A}|$ for 194 instance, and $|\mathcal{A}'| \leq 1.24 \cdot |\mathcal{A}|$ for all the 200 instances.

This observation leads to an efficient implementation of the preprocessing method proposed by Bodlaender and Koster. Experiments on instances from PACE 2017 and other sources show that this implementation is extremely fast and effective for graphs of practical interest.
1 Introduction

Treewidth is a graph parameter which plays an essential role in the graph minor theory \cite{18,19,20} and is an indispensable tool in designing graph algorithms (see, for example, a survey \cite{7}). See Section 2 for the definition of treewidth and tree-decompositions. Deciding the treewidth of a given graph is NP-complete \cite{2}, but admits a fixed-parameter linear time algorithm \cite{6}.

Practical algorithms for treewidth have also been actively studied \cite{3,10,6,23,22,11}, with recent rapid progresses stimulated by PACE 2016 and 2017 algorithm implementation challenges.

The goal of our present work is to re-evaluate a classical approach to preprocessing for treewidth computation due to Bodlaender and Koster \cite{8}, namely that of almost-clique separator decomposition, in the modern setting. This approach was shown to be effective for relatively small graphs by experiments in their original work but, somewhat surprisingly, no work is found in the literature that attempts to evaluate the approach on larger graph instances that are becoming practically tractable for treewidth computation.

Let us first review their approach. Let tw(G) denote the treewidth of a graph G. A separator S ⊆ V(G) of G is a minimal separator of G if, for at least two connected components C of G[V(G) \ {S}], the neighborhood of C is S. Suppose that G has a clique minimal separator S, a minimal separator that is also a clique. Then, tw(G) is the maximum of tw(G[C \ N_G(C)]) where C ranges over all connected components of G \ S. Thus, a clique minimal separator can be used to reduce the task of computing treewidth to the tasks on separated parts. Given G, all clique minimal separators of G can be listed by an algorithm due to Tarjan \cite{24} in $O(nm)$ time, where $n$ and $m$ are the numbers of vertices and edges of G respectively. Indeed, his algorithm constructs a clique-separator decomposition of G, which is a tree-decomposition T of G satisfying the following conditions:

1. the intersection of every pair of adjacent bags in T is a clique minimal separator of G, and
2. for every bag X of T, G[X] does not contain a clique separator.

Let T be a clique-separator decomposition of G. Following Tarjan, we call G[X] for each bag X of T an atom of the decomposition. Repeatedly applying the reduction described above, we see that tw(G) equals the maximum of tw(A), where A ranges over all atoms of T.

A separator S of G is safe for treewidth \cite{8}, or simply safe for short, if tw(G[K(S)]) = tw(G), where K(S) denotes the complete graph on vertex set S. If we find a minimal separator S that is safe in G then, we may treat S as if S is a clique minimal separator and apply the reduction described above. A separator S of G is an almost-clique separator of G if there is a vertex $v \in S$ such that $S \setminus \{v\}$ is a clique of $G$. One of the sufficient conditions for S being safe, due to Bodlaender and Koster, is that S is an almost-clique minimal separator. Based on this observation, they proposed a preprocessing approach to treewidth computation, which we formulate as follows.

**Input:** Graph G

**Output:** tw(G)

1. repeat
2. A ⇔ a set of pairwise non-crossing almost-clique minimal separators of G
3. Update G by filling each $S \in A$ into a clique
4. until G becomes unchanged
5. Construct a clique separator decomposition T of G
6. Compute the treewidth of each atom in T
7. return the maximum of tw(A) over all atoms A of T

**Algorithm 1:** Computing treewidth with almost-clique separator based preprocessing

We call the clique-separator decomposition T of the filled graph, constructed at line 5 of the algorithm, an almost-clique separator decomposition of the original graph. To compute a set of pairwise non-crossing almost-clique separators of G at line 2, Bodlaender and Koster suggest applying Tarjan’s algorithm \cite{8} to list clique separators of $G \setminus \{v\}$ for every $v \in V(G)$. We formulate their suggestion as Algorithm 2 which we call the standard algorithm for listing almost-clique minimal separators.

Although the running time of the standard algorithm is polynomial, the complexity of $O(n^2m)$ is too high to be practically applicable to large graphs. This might be the reason why the authors of modern implementations...
of treewidth algorithms \cite{BodlaenderK08} have not adopted the preprocessing method based on almost-clique separators as proposed by Bodlaender and Koster. We need a practically faster alternative to the standard algorithm in order to exploit the potential of the approach.

We present a heuristic algorithm for this task, which is based on the following empirical observation. For a graph $G$ and a minimal triangulation $H$ of $G$, let $S(H)$ denote the set of minimal separators of $H$ and $\mathcal{A}(H, G)$ the set of almost-clique minimal separators of $G$ belonging to $S(H)$. Note that, since the separators in $S(H)$ are pairwise non-crossing, so are those in $\mathcal{A}(H, G)$. We observe from experiments that $\mathcal{A}(H, G)$ is remarkably close to maximal, especially when the minimal triangulation $H$ is computed by an algorithm aiming for small treewidth.

For example, consider the 200 graph instances from the exact treewidth track of PACE 2017 algorithm implementation challenge \cite{BerryFR17}. For each instance $G$, we compute a minimal triangulation $H$ of $G$ using a variant, which we call MMAF, of the MMD algorithm due to Berry et al. \cite{BerryFR17}, extract $\mathcal{A} = \mathcal{A}(H, G)$, and then expand $\mathcal{A}$ into a maximal set $\mathcal{A}'$ of pairwise non-crossing almost-clique minimal separators of $G$. For this expansion, we use the list of all almost-clique minimal separators of $G$, constructed in advance, and apply a straightforward greedy algorithm. Then, we have $\mathcal{A}' = \mathcal{A}$ for 79 instances, $|\mathcal{A}'| \leq 1.1 \cdot |\mathcal{A}|$ for 194 instances, and $|\mathcal{A}'| \leq 1.24 \cdot |\mathcal{A}|$ for all the 200 instances. See Section \ref{sec:exp} for more details and the results when minimal triangulation algorithms other than MMAF are used.

This observation suggests that, at line 2 of Algorithm \ref{alg1}, we let $\mathcal{A} = \mathcal{A}(H, G)$ where $H$ is a minimal triangulation of $G$ computed by the MMAF algorithm. Although $\mathcal{A}$ thus computed is not necessarily maximal, it is expected to be close to maximal, as the above observation shows. Moreover, except for the last round of the iteration, the non-maximality may not be a serious drawback since some of the missed non-crossing almost-clique minimal separators may be discovered in subsequent rounds. We experimentally compare this implementation of Algorithm \ref{alg1} with the standard implementation where Algorithm \ref{alg2} is used to compute $\mathcal{A}$.

When applied to the 200 graph instances from the exact treewidth track of PACE 2017, our implementation is by orders of magnitudes faster than the standard one. Let $\rho_1(G)$ denote the ratio $t_{\text{ours}}(G)/t_{\text{standard}}(G)$, where $t_{\text{ours}}(G)$ and $t_{\text{standard}}(G)$ denote the time spent on $G$ by our implementation and the standard implementation respectively. See Section \ref{sec:exp} for the experimental environment. Then, $\rho_1(G) \leq 0.005$ for 156 out of the 200 instances, $\rho_1(G) \leq 0.05$ for 193 instances, and $\rho_1(G) \leq 0.12$ for all the instances.

For the quality of decompositions, first consider the following measure. Let $\text{MA}_{\text{ours}}(G)$ and $\text{MA}_{\text{standard}}(G)$ denote the maximum numbers of vertices in an atom of the decomposition of $G$ produced by our implementation and by the standard implementation, respectively, and let $\rho_2(G) = \text{MA}_{\text{ours}}(G)/\text{MA}_{\text{standard}}(G)$. Then, $\text{MA}_{\text{ours}}(G) = \text{MA}_{\text{standard}}(G)$ on 153 instances, $\rho_2(G) \leq 1.1$ for 195 instances, and $\rho_2(G) \leq 1.5$ for all the 200 instances.

We also consider the time for treewidth computation after the preprocessing, where we use our implementation of the treewidth algorithm due to Tamaki \cite{Tamaki10}. Let $t'_{\text{ours}}(G)$ and $t'_{\text{standard}}(G)$ denote the time to compute the treewidth of $G$, given the almost-clique separator decomposition of $G$ produced by our implementation and the standard implementation respectively, and let $\rho_3(G) = t'_{\text{ours}}(G)/t'_{\text{standard}}(G)$. Then $\rho_3(G) \leq 1.1$ for 168 instances, $\rho_3(G) \leq 1.2$ for 184 instances, and $\rho_3(G) \leq 1.5$ for all the 200 instances.

To summarize, in both measures, the performance of our implementation is almost equal to that of the

\begin{verbatim}
Input: Graph $G$
Output: A maximal set of pairwise non-crossing almost-clique minimal separators of $G$
1: \textbf{A} \leftarrow \emptyset
2: \textbf{for} each $v \in V(G)$ \textbf{do}
3: \quad Use Targan’s algorithm to compute the set $S_v$ of all clique separators of $G \setminus \{v\}$
4: \quad \textbf{for} each $S \in S_v$ \textbf{do}
5: \quad \quad \textbf{if} $S \cup \{v\}$ is a minimal separator of $G$ not crossing any separator in $\mathcal{A}$ \textbf{then}
6: \quad \quad \quad add $S \cup \{v\}$ to $\mathcal{A}$
7: \quad \textbf{end if}
8: \textbf{end for}
9: \textbf{end for}
10: \textbf{return} $\mathcal{A}$
\end{verbatim}

\textbf{Algorithm 2:} Standard algorithm for listing almost-clique minimal separators

standard implementation for most of the instances and is not seriously inferior for any of the instances. See Section 3 for more details and experiments on other benchmark instances.

The Java source code of the implementations of the algorithms used in our experiments is available at a Github repository https://github.com/twalgor/tw

2 Concepts and algorithms

2.1 Graph notation In this paper, all graphs are undirected and simple, that is, without self-loops or parallel edges. Let $G$ be a graph. We denote by $V(G)$ the vertex set of $G$ and by $E(G)$ the edge set of $G$. As $G$ is simple and undirected, each member of $E(G)$ is a two-member subset of $V(G)$. The subgraph of $G$ induced by $U \subseteq V(G)$ is denoted by $G[U]$. We sometimes use an abbreviation $G \setminus U$ to stand for $G[V(G) \setminus U]$, where $U \subseteq V(G)$. A graph $G$ is complete if $E(V)$ contains all two-member subsets of $V(G)$. We denote by $K(U)$ the complete graph on vertex set $U$. For a graph $G$ and an edge set $F \subseteq E(K(V(G)))$, we denote by $G \cup F$ the graph $G'$ with $V(G') = V(G)$ and $E(G') = E(G) \cup F$.

A vertex set $S \subseteq V(G)$ is a clique of $G$ if $G[S]$ is a complete graph. A clique $S$ of $G$ is maximal if no proper superset of $S$ is a clique of $G$. In this paper, it is often needed to add edges to $G$ so that some given vertex set $U \subseteq V(G)$ becomes a clique. We say that we fill $U$ into a clique in $G$ in this situation; the resulting graph is $G \cup K(U)$. For each $v \in V(G)$, $N_G(v)$ denotes the set of neighbors of $v$ in $G$: $N_G(v) = \{u \in V(G) \mid \{u, v\} \in E(G)\}$. For $U \subseteq V(G)$, the neighborhood of $U$ in $G$, denoted by $N_G(U)$, is the set of vertices adjacent to some vertex in $U$ but not belonging to $U$ itself: $N_G(U) = (\bigcup_{v \in U} N_G(v)) \setminus U$.

We say that vertex set $C \subseteq V(G)$ is connected in $G$ if, for every $u, v \in C$, there is a path in $G[C]$ between $u$ and $v$. It is a connected component or simply a component of $G$ if it is connected and is inclusion-maximal subject to this condition. A vertex set $S \subseteq V(G)$ is a separator of $G$ if $G \setminus S$ has more than one component. For brevity, we will sometimes refer to those components as the components of $S$ in $G$ when our intention is clear (that we are not talking of components of $G[S]$). A component $C$ of $S$ in $G$ is full if $N_G(C) = S$. A separator $S$ of $G$ separates two vertices $a$ and $b$ if $a$ and $b$ belong to distinct components of $S$ in $G$. We also say that $S$ is an $a$-$b$ separator in this situation. $S$ is a minimal $a$-$b$ separator if it is an $a$-$b$ separator and is inclusion-minimal subject to this condition. $S$ is a minimal separator if it is a minimal $a$-$b$ separator for some pair of vertices $a$ and $b$. It is straightforward to see that $S$ is a minimal separator if and only if $S$ has at least two full components in $G$. Let $R$ and $S$ be separators of $G$. We say that $R$ crosses $S$ if $R$ separates some pair of vertices in $S$. When $R$ and $S$ are minimal separators, $R$ crosses $S$ if and only if $S$ crosses $R$.

2.2 Tree-decompositions A tree-decomposition of a graph $G$ is a pair $(T, \mathcal{X})$ where $T$ is a tree and $\mathcal{X}$ is a family $\{X_i\}_{i \in V(T)}$ of vertex sets of $G$, indexed by the nodes of $T$, such that the following three conditions are satisfied. We call each $X_i$ the bag at node $i$.

1. $\bigcup_{i \in V(T)} X_i = V(G)$.

2. For each edge $\{u, v\} \in E(G)$, there is some $i \in V(T)$ such that $u, v \in X_i$.

3. For each $v \in V(G)$, the set of nodes $I_v = \{i \in V(T) \mid v \in X_i\} \subseteq V(T)$ is connected in $T$.

The width of this tree-decomposition is $\max_{i \in V(T)} |X_i| - 1$. The treewidth of $G$, denoted by $tw(G)$ is the smallest $k$ such that there is a tree-decomposition of $G$ of width $k$. A tree-decomposition of $G$ is optimal if its width equals $tw(G)$.

The following facts are easy to verify.

**Proposition 2.1.** Let $G$ be a graph and $K$ a clique of $G$. Then, every tree-decomposition of $G$ contains a bag that is a superset of $K$.

**Corollary 2.1.** For every graph $G$, $tw(G) \geq \omega(G) - 1$ holds, where $\omega(G)$ is the clique number of $G$.

Let $G$ be a graph and $(T, \mathcal{X})$ a tree-decomposition of $G$. For a pair $i, j$ of adjacent nodes in $T$, let $T(i, j)$ denote the maximal subtree of $T$ containing $i$ but not $j$. Furthermore, we define $V_T(i, j) = \bigcup_{i \in V(T(i,j))} X_i \setminus X_i$: this is the union of the bags in $T(i, j)$ with vertices in $X_i$ removed.
Proposition 2.2. Let $(T, X)$ be a tree-decomposition of $G$. For each edge $\{i, j\}$ of $T$, let $S_{ij}$ denote $X_i \cap X_j$. Then, $S_{ij}$ equals $V_T(i, j) \cap V_T(j, i)$ and is an $a$-$b$ separator for every pair of vertices $a \in V_T(i, j) \setminus V_T(j, i)$ and $b \in V_T(j, i) \setminus V_T(i, j)$.

We say that each edge $\{i, j\}$ of this tree-decomposition induces separator $S_{ij}$. We say that tree-decomposition $(T, X)$ induces separator $S$ if some edge of $T$ induces $S$.

2.3 Chordal graphs and triangulations Tree-decompositions of graphs are closely related to triangulations of graphs, defined as follows. Let $G$ be a graph and $C$ a cycle in $G$. An edge $\{u, v\}$ of $G$ is a chord of $C$ if $u, v \in V(C)$ but $\{u, v\} \notin E(C)$. A graph $G$ is chordal if every cycle $C$ of $G$ with $|V(C)| > 3$ has a chord. A vertex $v$ in $G$ is a simplicial vertex of $G$ if $N_G(v)$ is a clique. A total ordering $v_1, v_2, \ldots, v_n$ of $V(G)$ is a perfect elimination order of $G$ if $v_i$ is a simplicial vertex of $G[\{v_i, v_{i+1}, \ldots, v_n\}]$ for $1 \leq i \leq n$. The following characterization of chordal graphs due to [12] is fundamental.

Proposition 2.3. A graph $G$ is chordal if and only if it has a perfect elimination order.

A graph $H$ is a triangulation of a graph $G$ if it is chordal, $V(H) = V(G)$, and $E(H) \subseteq E(G)$: it is a minimal triangulation of $G$ if, furthermore, its edge set is inclusion-minimal subject to this condition. For a graph $G$ and a tree-decomposition $T = (T, \{X_i\})$ of $G$, let $fill(G, T)$ denote the graph $G \cup \bigcup_{i \in V(T)} K(X_i)$ obtained by filling every bag of $T$ into a clique.

The following facts are known. (See [13] for example).

Proposition 2.4. If $G$ is chordal, then there is a tree-decomposition $T$ of $G$ in which every bag is a maximal clique of $G$. For every such $T$, the set of separators induced by edges of $T$ is the set of all minimal separators of $G$.

Because of this fact, minimal triangulation algorithms can be regarded as algorithms for tree-decomposition. Indeed, due to the following additional fact and Corollary 2.1, $tw(G)$ equals the smallest $k$ such that there is a minimal triangulation with the clique number $k + 1$.

Proposition 2.5. For every graph $G$ and every tree-decomposition $T$ of $G$, $fill(G, T)$ is a triangulation of $G$.

The following facts are already used in the introduction to reason about minimal separators of a graph $G$ obtained from a minimal triangulation of $G$.

Proposition 2.6. If $G$ is chordal, then no pair of minimal separators $S_1$ and $S_2$ of $G$ cross each other.

Proposition 2.7. If $H$ is a minimal triangulation of $G$, then every minimal separator of $H$ is a minimal separator of $G$.

Corollary 2.2. If $H$ is a minimal triangulation of $G$, then the set of all minimal separators of $H$ is a maximal set of mutually non-crossing minimal separators of $G$.

2.4 Minors Let $G$ be a graph and $e = \{u, v\}$ an edge of $G$. The contraction of $e$ in $G$ is an operation to turn $G$ into a graph $G'$ in which $u$ and $v$ are replaced by a vertex $w$ with $N_{G'}(w) = N_G(\{u, v\})$. This vertex $w$ may be chosen to be $u$, $v$, or any vertex not in $G$. A graph $H$ is a minor of $G$ if it is obtained by a sequence of zero or more edge contractions, vertex deletions, and edge deletions. Let $T$ be a tree-decomposition of $G$. If we apply any of these three operations to $G$ and obtain $G'$, $T$ is straightforwardly converted into a tree-decomposition $T'$ of $G'$ (by replacing $u$ and/or $v$ in each bag with $w$ in case of contracting $\{u, v\}$ into $w$) with width not larger than that of $T$. Therefore, we have the following:

Proposition 2.8. If $H$ is a minor of $G$ then $tw(H) \leq tw(G)$.

A minor is a clique minor if it is a complete graph. Let $R$ be a vertex set of $G$. A minor $M$ of $G$ is rooted on $R$ if $V(M) = R$ and each contraction in the sequence that leads from $G$ to $M$ is always on an edge between some $u \in V(M)$ and some $v \notin V(M)$, with $u$ chosen to be the vertex into which this edge is contracted.
2.5 Clique separator decompositions A separator $S$ of $G$ is a clique separator if it is a clique of $G$. The following well-known fact follows immediately from Proposition 2.1.

**Proposition 2.9.** Let $S$ be a clique separator of $G$. Then $\text{tw}(G)$ is the larger of $|S| - 1$ and the maximum of $\text{tw}(G[C \cup N_G(C)])$ over all components $C$ of $S$.

**Corollary 2.3.** Let $S$ be a clique minimal separator of $G$. Then $\text{tw}(G)$ is the maximum of $\text{tw}(G[C \cup N_G(C)])$ over all components $C$ of $S$.

A tree-decomposition $\mathcal{T}$ of $G$ is a clique-separator decomposition of $G$ [24] if it satisfies the following conditions:

1. the intersection of every pair of adjacent bags in $\mathcal{T}$ is a minimal clique separator of $G$, and
2. for every bag $X$ of $\mathcal{T}$, $G[X]$ does not contain a clique separator.

Tarjan [24] gives an $O(nm)$ time algorithm for constructing a clique separator decomposition of a graph with $n$ vertices and $m$ edges. Following Tarjan, we call the subgraph of $G$ induced by a bag of a clique separator decomposition an atom of the decomposition.

By repeated applications of Corollary 2.3, we have:

**Proposition 2.10.** Let $\mathcal{T}$ be a clique separator decomposition of $G$. Then $\text{tw}(G)$ is the maximum of $\text{tw}(A)$ where $A$ ranges over all the atoms of $\mathcal{T}$.

2.6 Safe separators Bodlaender and Koster [8] introduced the notion of safe separators for treewidth. Let $S$ be a separator of a graph $G$. We say that $S$ is safe for treewidth, or simply safe, if $\text{tw}(G) = \text{tw}(G \cup K(S))$. As every tree-decomposition of $G \cup K(S)$ must have a bag containing $S$, $\text{tw}(G)$ is the larger of $|S| - 1$ and $\max\{\text{tw}(G[C \cup S] \cup K(S))\}$, where $C$ ranges over all the components of $S$.

Let us say that a separator $S$ of $G$ is minor-safe if for every component $C$ of $S$ in $G$, there is a clique-minor of $G \setminus C$ rooted on $N_G(C)$.

**Theorem 2.1.** [Bodlaender and Koster [8]] If $S$ is a minor-safe separator of $G$ then $S$ is safe.

A vertex set $S \subseteq V(G)$ is an almost-clique of $G$ if $S \setminus q$ is a clique of $G$ for some $q \in S$. We call a separator $S$ of $G$ an almost-clique minimal separator if it is an almost-clique and a minimal separator at the same time. The following observation is also due to Bodlaender and Koster [8]. It is originally stated for inclusion-minimal almost-clique separators, but it is clear that it holds more generally with almost-clique minimal separators.

**Proposition 2.11.** If $S$ is an almost-clique minimal separator of a graph $G$, then $S$ is minor-safe.

**Proof.** Let $v \in S$ such that $S \setminus \{v\}$ is a clique. Let $C$ be an arbitrary component of $S$ in $G$. Since $S$ is a minimal separator, $S$ has a full component $C'$ distinct from $C$. Contracting $C'$ into $v$, we have a clique-minor of $G \setminus C$ rooted on $S$. Deleting vertices in $S \setminus N_G(C)$, we have a clique-minor of $G \setminus C$ rooted on $N_G(C)$.

Combining Propositions 2.10, 2.11 and Theorem 2.1, we see that Algorithm 1 for treewidth computation given in the introduction is correct.

2.7 Computing minimal triangulations Several algorithms are known for computing a minimal triangulation of a given graph [16, 21, 4, 5], see a survey [13] for more. In our experiments, we use MCS-M (Maximum Cardinality Search for Minimal triangulation) [4] and MMD (Minimal Minimum Degree) [5]. The principal different of these algorithms, from our perspective, is that MMD is a good heuristic for upperbounding treewidth while MCS-M is not intended for treewidth computation at all.

We also use a variant, we call MMAF (Minimal Minimum Average Fill), of MMD. To describe this variant, we need to review MMD. MMD is based on MD [15] (see also [9]), which is one of the several heuristics for triangulation based on elimination orders. In these heuristics, given graph $G$, a total ordering $v_1, v_2, \ldots, v_n$ of $V(G)$ is constructed together with a triangulation $H$ of $G$ such that this ordering is a perfect elimination order of $H$. This is done as follows. Let $H_0 = G$. At step $i$, $1 \leq i \leq n$, we choose the next vertex $v_i$ in the ordering and
let $H_i = (H_{i-1} \setminus \{v_i\}) \cup K(N_{H_{i-1}}(v_i))$. In words, we fill the neighborhood of the chosen vertex $v_i$ in $H_{i-1}$, remove $v_i$, and let the resulting graph be $H_i$. Letting $H$ be the union of $H_i$, $1 \leq i \leq n$, we see that the vertex ordering constructed is a perfect elimination order of $H$. Note also that all the maximal cliques of $H$ can be found among $N_{H_{i-1}}(v_i)$, $1 \leq i \leq n$.

In MD, $v_i$ is chosen from the vertices of the minimum degree in $H_{i-1}$. In another heuristic MF (minimum fill), $v_i$ is chosen from the vertices of minimum fill in $H_{i-1}$, where the fill of $v$ in $H_{i-1}$ is the number of missing edges of $H_{i-1}$ in the neighborhood of $v$. It is observed [9] that MF often outperforms MD as a treewidth heuristic. In [17], it is observed that MAF (Minimum Average Fill) heuristic often performs even better, where $v_i$ is chosen from vertices $v$ such that the fill of $v$ divided by the degree of $v$ is the smallest.

These methods based on elimination orders do not produce a minimal triangulation in general. Berry et al. [5] gives a scheme of turning those methods into a minimal triangulation algorithm, which we sketch as follows. Let $H$ be the triangulation of $G$ computed, say, by MD. For each separator $S$ of $G$ that is filled into a clique in $H$, we compute minimal separators of $G$ contained in $S$. Rather than filling $S$ into a clique, we fill those minimal separators. The resulting graph $G'$ is a subgraph of $H$ and, in general, is not a triangulation of $G$. Since we have filled only minimal separators of $G$ in $G'$, a minimal triangulation of $G'$ is a minimal triangulation of $G$. So we apply MD to $G'$ and repeat until we get a triangulation of $G$, which is necessarily minimal.

MMD is the result of applying the above scheme to MD. Our variant MMAF is the result of applying the scheme to MAF. In Section 3, we will see how these two minimal triangulation methods together with MCS-M perform in our context of generating almost-clique minimal separators.

3 Experiments

3.1 Computational environments The computing environment for our experiments is as follows. CPU: Intel Core i7-8700, 3.20GHz; RAM: 32GB; Operating system: Windows 10, 64bit; Programming language: Java 1.8; JVM: jre1.8.0_201. The maximum heap size is set to 28GB. The implementation is single-threaded, except that multiple threads may be invoked for garbage collection by JVM. The time is measured by System.nanoTime() method and is rounded up to the nearest millisecond.

3.2 Graph instances We use two sets of instances. One is from PACE 2017 exact treewidth track [11] and consists of 200 instances. We call them PACE2017 instances. The other is from the DIMACS challenge on graph-coloring [14] and consists of 73 instances. We call them DIMACS instances. Figure 1 shows the PACE2017 instances for which $|A|$ is 161. The maximum of $|A|$ among the 200 instances is 716, achieved by ex150, $|V(G)| = 839$, $|A_{\text{max}}(G)| = 102$, and $|A_{\text{all}}(G)|$ is 148; for ex150, $|V(G)| = 839$, $|A_{\text{max}}(G)| = 102$, and $|A_{\text{all}}(G)|$ is 161. The maximum of $|A_{\text{max}}(G)|$ is 716, achieved by
Figure 1: PACE2017 graph instances

Figure 2: DIMACS graph instances
instance ex109 with 1212 vertices, for which $|A_{\text{all}}(G)|$ is 1588.

Figure 3: The number of almost-clique minimal separators for each PACE2017 instance

Figures 4 and 5 compare $|A(G, H)|$, for each PACE2017 instance $G$, where the minimal triangulation $H$ of $G$ is computed by three methods MMD, MMAF, and MCS-M. The instances are divided into five subfigures, grouped in the increasing order of $|A_{\text{max}}(G)|$: the first three groups are in Figure 4 and the remaining two are in Figure 5. For each instance, the gray bar represents $|A_{\text{max}}(G)|$, the light-colored bars represent $|A(G, H)|$, and dark-colored bars represent $|A_{\text{max}}(G, H) \setminus A(G, H)|$, where blue is for MDD, red is for MMAF, and green is for MCS-M. We observe the following:

1. The three maximal sets $A_{\text{max}}(G, H)$, where $H$ is computed by the three methods, have cardinalities similar to each other and to the cardinality of $A_{\text{max}}(G)$ computed by the standard method.

2. MMD performs best, in terms of the gap $|A_{\text{max}}(G, H) \setminus A(G, H)|$ between the computed set of almost-clique minimal separators and the maximally expanded set; MDD is slightly inferior and MCS-M is by far inferior to the other two methods.

The second point can be confirmed by Table 1, where, for each method and each bound $\rho$ on the ratio, the number of instances satisfying $|A_{\text{max}}(G, H)|/|A(G, H)| \leq \rho$ is listed.

Table 2 compares the treewidth of the minimal triangulation computed by these three methods. For each method and each bound $\rho$ on the ratio, the number of instances with $\text{tw}(H)/\text{tw}(G) \leq \rho$, where $H$ is the minimal triangulation computed by the method, is listed. MMAF performs the best and MCS-M is considerably inferior, which is not surprising since MCS-M is not intended for small treewidth. The correlations of the performances
Figure 4: The number of almost-clique minimal separators from minimal triangulations for each PACE2017 instance: Groups 1, 2, 3
Figure 5: The number of almost-clique minimal separators from minimal triangulations for each PACE2017 instance: Groups 4, 5

Table 1: The numbers of instances with the ratio $|A_{\text{max}}(G, H)|/|A(G, H)|$ within the given bound
shown by these two tables are not surprising either. For each almost-clique minimal separator $S$ of $G$, there exists a tree-decomposition of $tw(G)$ that induces $S$ as a separator. It is natural to expect that the chances of a tree-decomposition $T$ of $G$ inducing $S$ are larger when the width of $T$ is closer to $tw(G)$.

|       | 1.0 | 1.1 | 1.2 | 1.3 | 1.4 | 2.6 | 3.9 | 8.8 |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|
| MMD   | 22  | 40  | 76  | 125 | 146 | 200 |     |     |
| MMAF  | 48  | 94  | 160 | 181 | 194 | 200 |     |     |
| MCE-M | 14  | 18  | 29  | 42  | 53  | 164 | 190 | 200 |

Table 2: The numbers of instances with the ratio $tw(H)/tw(G)$ within the given bound

3.4 Almost-clique separator decomposition In this subsection, we compare two implementations of Algorithm 1 given in the introduction for computing treewidth using an almost-clique separator decomposition: one uses the standard algorithm for listing almost-clique minimal separators and the other uses our heuristic based on minimal triangulations. For the latter implementation, we use MMAF for computing the minimal triangulation, as it is the best among the three methods compared by the experiments in the previous subsection. In the figures in this subsection, instances are plotted with circles whose areas are proportional to the number of vertices of the instances. The constant of proportionality, however, may not be consistent across figures.

3.4.1 PACE2017 instances We start with comparisons on PACE2017 instances.

We first compare the time for computing the almost-clique separator decomposition by the two implementations. Recall the notation in the introduction: $t_{ours}(G)$ and $t_{standard}(G)$ denote time spent on $G$ by our heuristic implementation and by the standard implementation, respectively. Figure 6 plots PACE2017 instances, where the $x$-coordinate is $t_{ours}(G)$ and the $y$-coordinate is $t_{standard}(G)$. We see that our heuristic implementation is by orders of magnitudes faster than the standard implementation.

To compare the quality of the almost-clique separator decomposition produced by the two implementations, we first consider the number of vertices in the largest atom of the decomposition. Recall the notation in the introduction: $MA_{ours}(G)$ and $MA_{standard}(G)$ denote the maximum number of vertices in an atom of the decomposition of $G$ produced by our heuristic implementation and by the standard implementation, respectively. Figure 7 plots PACE2017 instances, where the $x$-coordinate is $|MA_{ours}(G)|/|V(G)|$ and the $y$-coordinate is $|MA_{standard}(G)|/|V(G)|$. We see that the performances of the two implementations in this measure are almost equal for most of the instances. Note also that, for a majority of the instances, the number of vertices in the largest atom is smaller than half of the total number of vertices: the almost-clique separator decomposition approach itself is quite effective.

We next consider the time for computing $tw(G)$ given the almost-clique separator decomposition. Recall the notation in the introduction: $t'_{ours}(G)$ and $t'_{standard}(G)$ denote the time for computing $tw(G)$ given the almost-clique separator decomposition of $G$ produced by our heuristic implementation and by the standard implementation, respectively. For this treewidth computation, we use our implementation of the treewidth algorithm due to Tamaki [22]. Figure 8 plots PACE2017 instances, where the $x$-coordinate is $t'_{ours}(G)$ and the $y$-coordinate is $t'_{standard}(G)$. We see that the performances of the two implementations in this measure are also almost equal for most of the instances.

We finally compare the total time for computing the treewidth by the two implementations. Figure 9 plots PACE2017 instances, where the $x$-coordinate is $t_{ours}(G) + t_{ours}(G)$ and the $y$-coordinate is $t_{standard}(G) + t_{standard}(G)$. We see that our heuristic implementation consistently outperforms the standard implementation in this measure.

3.4.2 DIMACS graph coloring instances We have also compared the two implementations on DIMACS instances. Of the total of 73 instances in this set, 41 instances have no almost-clique separators. We call them sterile instances and treat them separately in the following figures.

We first compare the time for computing the almost-clique separator by the two implementations. We continue to use the same notation: $t_{ours}(G)$ and $t_{standard}(G)$ denote time spent on $G$ by our heuristic implementation and by the standard implementation, respectively. We have two figures: Figure 10 for sterile instances and Figure 11 for
Figure 6: Time for computing the almost-clique separator decomposition of PACE2017 instances
Figure 7: Relative size of the largest atom in the almost-clique separator decomposition of PACE2017 instances
Figure 8: Time for computing the treewidth of PACE2017 instances given the almost-clique separator decomposition
Figure 9: Total time for computing the treewidth of PACE2017 instances
non-sterile instances. In both figures, each instance is plotted where the $x$-coordinate is $t_{\text{ours}}(G)$ and $y$-coordinate is $t_{\text{standard}}(G)$. From these figures, we see that the advantage of our heuristic implementation over the standard one is larger on non-sterile instances than on sterile instances. Our implementation, however, is at least ten times faster than the standard one even on sterile instances.

Figure 10: Time for computing the almost-clique separator decomposition of for sterile DIMACS instance

We compare the size of the largest atom in the almost-clique separator decomposition only on non-sterile instances. In Figure 12, each instance is plotted with $|\text{MA}_{\text{ours}}(G)|/|V(G)|$ as the $x$-coordinate and $|\text{MA}_{\text{standard}}(G)|/|V(G)|$ as the $y$-coordinate. We see that, similarly to the case of PACE2017 instances, the performances of the two implementations in this measure are almost equal for most of the instances.

We do not include the comparison on the time to compute treewidth given the almost-clique separator decompositions, because not all of the instances in this set are solvable in a reasonable amount of time. The comparisons of the largest atom size alone, however, show that the quality of the almost-clique separator decompositions produced by the two implementations are almost equal.

The effectiveness of the almost-clique separator based preprocessing itself is somewhat limited on DIMACS instances as more than half of them are sterile. There are, however, a non-negligible number of instances in this set where the reduction of the problem size by this approach is dramatic. In view of the small running time of our heuristic algorithm, it seems a good strategy to try this approach in general, unless there is a strong evidence that the instance at hand is sterile.
Figure 11: Time for computing the almost-clique separator decomposition of non-sterile DIMACS instances
Figure 12: Relative size of the largest atom in the almost-clique separator decomposition of DIMACS graph coloring instances
4 Conclusions

We have developed a practically efficient heuristic method of listing almost-clique minimal separators of a given graph. Because of this new method, we may now regard the preprocessing method of Bodlaender and Koster based on almost-clique separator decompositions as a standard component to be included in any practical implementations of treewidth algorithms.

As stated in Subsection 2.6, this preprocessing approach is a special case of their approach of using minor-safety as a sufficient condition for the safety of separators. The problem of deciding if a given separator is minor-safe is NP-complete. Therefore, we need a good heuristic for this task. Although some heuristic methods have been developed and successfully used in previous work [23,1], the effect of applying those heuristics is not sufficiently predictable. Although some hard instances become easily solvable due to the problem reduction by the preprocessing, there are some other instances on which the heuristics discover no safe separators after expensive combinatorial searches, contributing only to a huge overhead. It appears difficult to know in advance which would happen. To turn this more general preprocessing approach into a preprocessing component as stable as the one developed here, more research is required.

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