Partitioning the Bags of a Tree Decomposition into Cliques

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Abstract

We consider a variant of treewidth that we call *clique-partitioned treewidth* in which each bag is partitioned into cliques. This is motivated by the recent development of FPT-algorithms based on similar parameters for various problems. With this paper, we take a first step towards computing clique-partitioned tree decompositions.

Our focus lies on the subproblem of computing clique partitions, i.e., for each bag of a given tree decomposition, we compute an optimal partition of the induced subgraph into cliques. The goal here is to minimize the product of the clique sizes (plus 1). We show that this problem is NP-hard. We also describe four heuristic approaches as well as an exact branch-and-bound algorithm. Our evaluation shows that the branch-and-bound solver is sufficiently efficient to serve as a good baseline. Moreover, our heuristics yield solutions close to the optimum. As a bonus, our algorithms allow us to compute first upper bounds for the clique-partitioned treewidth of real-world networks. A comparison to traditional treewidth indicates that clique-partitioned treewidth is a promising parameter for graphs with high clustering.

2012 ACM Subject Classification Mathematics of computing → Graph algorithms; Theory of computation → Graph algorithms analysis

Keywords and phrases treewidth, weighted treewidth, algorithm engineering, cliques, clustering, complex networks

Digital Object Identifier 10.4230/LIPIcs.SEA.2023.3

Related Version *Full Version*: https://arxiv.org/abs/2302.08870

Supplementary Material *Software (Source Code)*: https://github.com/marcwil/cptw_code
archived at swh:1:dir:d611a7236b805d6eb409147b28b514f9132f96c1
Software (Source Code: Archive, Docker Image): https://doi.org/10.5281/zenodo.7816985

1 Introduction

The treewidth is a measure for how treelike a graph is in terms of its separators. It is defined via a tree decomposition, a collection of vertex separators called *bags* that are arranged in a tree structure. The size of the largest bag determines the width of the decomposition and the treewidth of a graph is the minimum width over all tree decompositions.

The concept of treewidth has its origins in graph theory with some deep structural insights [22, 24]. Additionally, there are algorithmic implications. Intuitively speaking, the separators of a tree decomposition split the graph into pieces that can be solved independently except for minor dependencies at the separators. This is often formalized using a dynamic program over the tree decomposition, yielding an FPT-algorithm (fixed-parameter tractable) with the treewidth as parameter [9]. As this is a versatile framework that can be applied to many problems, it comes to no surprise that there has been quite a bit of effort to develop algorithms for computing low-width tree decompositions (see, e.g., [15, 16]).

A major obstruction for low treewidth are large cliques, which inevitably lead to large separators. This is particularly true for so-called complex networks, i.e., graphs with strong community structure and heterogeneous degree distribution, which appear in various domains such as communication networks, social networks, or webgraphs. One could, however, hope for two aspects that together mitigate this negative effect of large cliques. First, though some separators need to be large, these separators are structurally simple, e.g., they form a clique or can be covered with few cliques. Second, separators that are large but structurally simple still let us solve the separated pieces individually with low dependence between them. The first hope is supported by the fact that the treewidth is asymptotically equal to the clique number in hyperbolic random graphs [5]; a popular model for complex networks [21]. This indicates that cliques are indeed the main obstruction for low treewidth in these kinds of networks. The second hope is supported by the results of de Berg et al. [14], who introduced the concept $\mathcal{P}$-flattened tree decompositions. There, the graph is partitioned into cliques and the width of the tree decomposition is measured in terms of the (weighted) number of cliques in a bag. Thus, the width does measure the complexity of separators rather than their size. Based on this definition, the authors then show that these structurally simple separators help to solve various graph problems efficiently.

To the best of our knowledge, these extended concepts have not yet been studied from a practical perspective. With this paper, we want to initiate this line of research by addressing two questions. First, can such clique-partitioned tree decompositions lead to substantially smaller width values than classical tree decompositions? Second, how can such tree decompositions be computed? For the second question, we design and evaluate different algorithmic strategies for computing a novel yet closely related variant of tree decompositions. Our experiments yield some interesting algorithmic insights and provide a good starting point for further development. On networks that do exhibit clique structures, the constructed tree decompositions indeed have sufficiently low width to answer the first question affirmatively. We believe that there is plenty of room for improvement in our approaches, which may yield even better insights into the applicability of the new parameter. In the following, we discuss related work before stating our contribution more precisely.

1.1 Related Work

There are multiple lines of research that investigate variants of treewidth where additional structural properties are taken into account. As mentioned above, De Berg et al. [14] propose a variant of tree decompositions where the initial graph is partitioned into cliques (or unions of constantly many connected cliques) that are contracted into weighted vertices. The weight of a clique of size s is $\log(s + 1)$ and the weight of a bag of the tree decomposition is the sum of its weights. Using this technique, they give subexponential algorithms for a range of problems on geometric intersection graphs, including Independent Set, Steiner Tree and Feedback Vertex Set. For some of these problems, the algorithms are also representation agnostic, while for most others, the geometric representation is required. They also prove that the running time of the algorithms is tight under the exponential-time-hypothesis (ETH). Kisfaludi-Bak [20] applied the same algorithmic framework to intersection graphs of constantly sized objects in the hyperbolic plane.

A similar parameter called *tree clique width* has been proposed by Aronis [2]. Here, the idea is to consider tree decompositions where each bag is annotated with an edge clique cover (ecc) and where the size of the cover determines the width of a bag. The paper shows several hardness results and adapts common treewidth algorithms to the newly proposed parameter.

Another approach to capture graph structures that lead to high treewidth despite being structurally simple has been proposed by Dallard, Milanič, and Štorgel. They define the *independence number* of a tree decomposition as the size of the largest independent set of any of its bags and the *tree-independence number* of a graph as the minimum independence number of any tree decomposition [13]. This parameter connects to the more theoretical study of (tw, ω)-bounded graphs, i.e., graph classes in which the treewidth depends only on the clique number [11, 12]. This line of research is mostly concerned with the classification and characterization of the considered graph classes both in terms of graph theory and algorithmic exploitability. However, apart from a factor 8 approximation with running time $2^{O(k^2)} \cdot n^{O(k)}$ due to Dallard, Fomin, Golovach, Korhonen, and Milanič [10], we are not aware of any work that tries to actually build algorithms for this or similar parameters.

1.2 Contribution

In this paper, we propose *clique-partitioned* treewidth as a parameter that captures structurally simple separators in graphs. It can be seen as a close adaptation of $\mathcal{P}$-flattened treewidth [14], where we *first* compute a tree decomposition and *then* determine clique partitions of the subgraphs induced by the bags. Thus, instead of using a global clique partition of the whole graph, we consider clique partitions that are local to a single bag.

The remainder of this paper is structured as follows. In Section 2, we formalize our definition for clique-partitioned treewidth and prove several statements comparing it with $\mathcal{P}$-flattened treewidth. In Section 3, we present multiple approaches to compute low-weight clique partitions for the bags of a tree decomposition. They include various heuristic methods, as well as an exact branch-and-bound algorithm for which we propose several adjustments with the potential to improve its running time in practice. Afterwards, in Section 4 we combine an implementation of our approaches with existing methods for computing tree decompositions and study the upper bounds on the clique-partitioned treewidth of real-world networks. Furthermore, we evaluate the performance of the exact and heuristic clique partition solvers proposed in Section 3. Due to space limitations, some proofs are in Appendix B.

2 Clique-partitioned treewidth

We first introduce some basic notation and give the definition for traditional tree decompositions. We write $[n] = \{1, \ldots, n\}$ for the first n natural numbers. Throughout the paper, we assume graphs $G = (V, E)$ to be simple and undirected and write $V(G)$ and $E(G)$ for the sets of vertices and edges, respectively. For a subset $X \subseteq V$ we write $G[X]$ for the subgraph of G induced by X.

A *tree decomposition* of G is a pair (T, B), for a tree T and a function B mapping vertices of T to subsets of V called *bags* such that T and B have the following three properties: (1) every vertex of G is contained in some bag, (2) for every edge, there is a bag containing both endpoints, and (3) for any vertex v of G, the set of bags containing v forms a connected subtree of T. The *width* of a tree decomposition is the size of the largest bag minus 1. The *treewidth* $\mathrm{tw}(G)$ is the smallest width obtainable by any tree decomposition of G.

We define a *clique-partitioned* tree decomposition of G as a tree decomposition where for every $t \in V(T)$ we have a partition $\mathcal{P}_t$ of the subgraph induced by the corresponding bag (i.e., the graph $G[B(t)]$) into cliques. Following de Berg et al. [14], we define the *weight* of a clique C as $\log(|C| + 1)$ and the weight of a bag $B(t)$ as the sum of weights of the cliques in its partition $\mathcal{P}_t$. Throughout this paper we assume 2 to be the default base of logarithms.

The weight of a clique-partitioned tree decomposition is the maximum weight of any of its bags and the *clique-partitioned treewidth* (short: cp-treewidth) of G, denoted by $\mathrm{cptw}(G)$, is the minimum weight of any clique-partitioned tree decomposition.

As mentioned before, the clique-partitioned treewidth is closely related to the parameter defined by de Berg et al. [14]. For a clique partition $\mathcal{P}$ of the whole graph G, we say that a *$\mathcal{P}$-flattened tree decomposition* is a clique-partitioned tree decomposition of G where the partition into cliques within a bag is induced by the global partition $\mathcal{P}$. As before, the weight of a $\mathcal{P}$-flattened tree decomposition is the maximum total weight of the cliques in any of its bags. In reference to the authors [14], we call the minimum weight over all $\mathcal{P}$ the BBKMZ-treewidth.

We note that our parameter can also be seen as an adaptation of *tree clique width* [2], where instead of considering the size of an *edge clique cover* of each bag, we consider the logarithmically weighted sum of clique sizes of a clique partition. That is, we are using the weight function of the $\mathcal{P}$-flattened treewidth to define a parameter which considers individual clique partitions, similar to tree clique width.

In the following, we compare the clique-partitioned treewidth to the more closely related BBKMZ-treewidth. First, as a global partition $\mathcal{P}$ can also be used locally in each bag of a clique-partitioned tree decomposition, we obtain that the clique-partitioned treewidth of a graph is at most its BBKMZ-treewidth. Additionally, the clique-partitioned treewidth can also be substantially smaller than the BBKMZ-treewidth, as shown in the following lemma.

▶ **Lemma 1.** *There is an infinite family of graphs $\mathcal{G}$ such that a graph $G \in \mathcal{G}$ with n vertices, has clique-partitioned treewidth in $\mathcal{O}(\log\log n)$ and BBKMZ-treewidth in $\Omega(\log n)$.*

Proof. The family $\mathcal{G}$ contains for every $h \in \mathbb{N}$ one graph G_h. The Graph G_h is a complete binary tree of height h, where additionally for every leaf ℓ we connect all h vertices that lie on a path between the root r and ℓ into a clique. Note that we have $h \in \Theta(\log n)$.

Let $\mathcal{P}_h$ be a clique partition of G_h. Then, via a simple induction over h, it is easy to see that in G_h there is a path between the root r and some leaf ℓ of G_h such that every vertex on the path belongs to a different partition class. These vertices form a clique in G_h that has to be prosent in some bag of any $\mathcal{P}_h$-flattened tree decomposition of G_h. This bag thus contains all h partition classes on the path and has weight $h \cdot \log(1+1) \in \Omega(\log n)$.

At the same time we can construct a clique-partitioned tree decomposition (T, σ), that has one bag for every path between the root r and each leaf ℓ. Then, T forms a path. As every bag consists of a single clique on h vertices, there is a clique partition of this tree decomposition with weighted width $\log(h+1) \in O(\log\log n)$. ◀

Finally, we show the algorithmic usefulness of clique-partitioned treewidth in the following lemma, which is an extension of the one proposed by de Berg et al. [14].

▶ **Lemma 2.** *Let G be a graph with a clique-partitioned tree decomposition (T, σ) of weight τ. Then a largest independent set of G can be found in $O(2^\tau \cdot \mathrm{poly}(n))$ time.*

By the above argumentation, it follows that the clique-partitioned treewidth introduced in this paper is upper bounded by the version of de Berg et al. and can be exponentially lower. Additionally, it retains some power in solving NP-hard problems in FPT-time.

3 The weighted clique partition problem

We split the task of computing a clique-partitioned tree decomposition in two phases. First, we compute a tree decomposition, minimizing the traditional tree width. Secondly, fixing the structure and bags of this decomposition, we compute a clique partition for every bag. We note that we already lose optimality by this separation, i.e., the result may be suboptimal even if we get optimal solutions in each of the two phases. However, we expect that small bags should also allow for low-weight clique partitions.

In the first phase, we use established algorithms for the computation of tree decompositions. Consequently, we focus on the second step in this section. To this end, we define the WEIGHTED CLIQUE PARTITION problem, short CLIQUE PARTITION. For a given graph G and an integer w, decide if there is a partition of $V(G)$ into cliques $P_1, \dots, P_k$ such that $\prod_{i \in [k]}(|P_i| + 1) \leq w$. Note that this function differs from the one in the definition of clique-partitioned treewidth, but is equivalent, as $\sum_{i \in [k]} \log(|P_i| + 1) = \log(\prod_{1 \leq i \leq k}(|P_i| + 1))$ and the logarithm is monotonic.

In the following, we prove some technical lemmas that are useful throughout the section, before showing that WEIGHTED CLIQUE PARTITION is NP-complete (Section 3.1). Afterwards, we give different heuristic approaches (Section 3.2) and an optimal branch-and-bound algorithm in (Section 3.3). We start with following lemma, which intuitively states that the weight of a partition is smaller the more imbalanced the individual weights are, i.e., moving a vertex from a smaller to a larger clique reduces the total weight.

▶ **Lemma 3.** *Let $a, b, c, d \in \mathbb{N}_0$ such that $a + b = c + d$ and $a \geq b$, $c \geq d$, $d > b$. Then $(a + 1)(b + 1) < (c + 1)(d + 1)$.*

With the above lemma (i.e., repeated applications thereof) we can compare the weight of two partitions.

▶ **Lemma 4.** *Let $\langle s_1, \dots, s_k \rangle$ and $\langle r_1, \dots, r_\ell \rangle$ be different non-increasing sequences of natural numbers such that $2 \leq k \leq \ell$, $\sum_{i \in [k]} s_i = \sum_{i \in [\ell]} r_i$, and $s_i \geq r_i$ for all $i \in [k - 1]$. Then $\prod_{i \in [k]}(s_i + 1) < \prod_{i \in [\ell]}(r_i + 1)$.*

Proof. This follows from repeatedly applying Lemma 3 to go from $R = \langle r_1, \dots, r_\ell \rangle$ to $S = \langle s_1, \dots, s_k \rangle$ while reducing the product in each step. To make this precise let i be the first index where $s_i > r_i$. We adjust R by adding 1 to r_i and subtracting 1 from r_ℓ. Note that this maintains the sum. We apply Lemma 3 with $a = r_i + 1$, $b = r_\ell - 1$, $c = r_i$, and $d = r_\ell$. Then, we have $(a + 1)(b + 1) < (c + 1)(d + 1)$, i.e., the product of the adjusted sequence is smaller than that of the original sequence R. Moreover, after a finite number of steps, we reach S and thus the product for S is smaller than the product for R. ◀

3.1 Hardness

To prove that WEIGHTED CLIQUE PARTITION is NP-complete, we perform a reduction in two steps. We start with the NP-hard problem 3-COLORING. It asks for a given graph whether each vertex can be colored with one of three colors such that no two neighbors have the same color. As an intermediate problem in the reduction, we introduce WEIGHTED INDEPENDENT SET PARTITION. It is defined equivalently to WEIGHTED CLIQUE PARTITION, but instead of partitioning the graph into cliques, we partition it into independent sets, i.e., sets of pairwise non-adjacent vertices. Note that independent sets are cliques in the complement graph and vice versa. Thus, WEIGHTED INDEPENDENT SET PARTITION and WEIGHTED CLIQUE PARTITION are computationally equivalent. Thus, to obtain the following theorem, it remains to reduce 3-COLORING to WEIGHTED INDEPENDENT SET PARTITION.

▶ **Theorem 5.** *WEIGHTED CLIQUE PARTITION is NP-complete.*

Proof. Membership in NP is easy to see as polynomial time verification of a solution is straightforward. For hardness, we reduce from 3-COLORING to WEIGHTED INDEPENDENT SET PARTITION. Thus, we now assume that we are given a graph G and need to transform it into a graph G' and integer w such that G can be colored with three colors if and only if G' has a partition into independent sets of weight at most w. We construct G' as follows. For every vertex v of G, we add two new vertices v_1 and v_2 that form a triangle together with v, but have no other edges. We denote $n = |V(G)|$ and set $w = (n+1)^3$. Note that any independent set in G' contains at most n vertices, because every appended triangle admits only one independent vertex.

Assume that G admits a proper three-coloring. This coloring directly translates to a three-coloring of G' as follows. Every vertex v of G keeps its color in G'. moreover, v_1 and v_2 each get one of the two other colors. Thus, the coloring classes in G' have size exactly n each and form an independent set partition with weight $(n+1)^3$.

If otherwise G does not admit a proper three-coloring, then neither does G' and there is no partition of G' into at most three independent sets. Any partition of $V(G')$ into more than three independent sets has a weight larger than $(n+1)^3$ by Lemma 4, as no independent set in G' can have more than n vertices. Consequently, G is three-colorable if and only if there is a partition of $V(G')$ into independent sets with weight at most $(n+1)^3$. ◀

3.2 Heuristic approaches

We now explain different approaches to solving the optimization variant of WEIGHTED CLIQUE PARTITION both optimally and heuristically.

Throughout this section we make use of the fact that enumerating all maximal cliques of a graph is not only output polynomial [19], but also highly feasible in practice as shown by Eppstein, Löffler, and Strash [17]. We use an implementation of their algorithm from the `igraph`[1] library.

Maximal clique heuristic. Recall from Lemma 3 that the weight function favors imbalanced clique sizes over more balanced ones. It therefore makes sense to try to find few large cliques that cover all vertices. A basic greedy heuristic that tries to achieve this works as follows. First, we enumerate all maximal cliques $\mathcal{C}$ of the graph. Then we iteratively add one clique to the partition by greedily selecting the clique with the largest number of remaining uncovered vertices. We call this the *maximal clique heuristic.*

In order to efficiently implement this heuristic, we use a priority queue to fetch the largest clique and keep track of the cliques $\mathcal{C}_v \subseteq \mathcal{C}$ that a vertex v is part of. This way, after choosing the remaining vertices of a clique $C \in \mathcal{C}$ as a partition, we have to update the sizes of $\mathcal{O}(\sum_{v\in C} |\mathcal{C}_v|)$ cliques. The total number of such updates throughout the whole algorithm is at most the sum of clique sizes in $\mathcal{C}$. Thus, using a Fibonacci Heap, a total running time of $\mathcal{O}(|V| \log |\mathcal{C}| + \sum_{C\in\mathcal{C}} |C|)$ can be achieved. In our implementation we use a binary heap due to it being faster in practice. This costs an additional factor of $\log |\mathcal{C}|$ for the second term.

Repeated maximal clique heuristic. Note that the MC heuristic does not recompute the maximal cliques of the remaining graph after selecting a clique. As deleting the vertices of one clique can have the effect that a non-maximal clique becomes maximal, the MC heuristic might miss a clique we would want to select. The *repeated maximal clique heuristic* recomputes the set of maximal cliques after each decision, i.e., it selects a maximum clique of the remaining graph in each step.

[1] `https://igraph.org/`

Set Cover heuristics. Observe that for the Weighted Clique Partition problem, we have to choose a set of cliques of minimum weight that cover all vertices. Thus, we essentially have to solve a weighted Set Cover problem. As there are reasonably efficient solvers for Set Cover (or the equivalent Hitting Set problem), it seems like a promising approach to use those. However, this has the disadvantage, that we would need to list all cliques and not only the maximal cliques. Nonetheless, it seems like a good heuristic to just consider maximal cliques and find a minimum set cover (unweighted or weighted).

The heuristic consists of two steps. First, we compute a minimum set cover, using the maximum cliques as sets and the vertices as elements. We consider two variants for this steps; weighted (a set of size k has weight $\log(k+1)$) and unweighted (each set has weight 1). Afterwards, in the second step, we convert the cover into a partition by assigning the overlap between selected cliques to only one clique. We call the resulting two approaches the *(maximal clique) set cover* and *(maximal clique) weighted set cover* heuristics.

For the first step, i.e., solving Set Cover, we use a state of the art branch-and-bound solver [6] for the unweighted case. Additionally, for the weighted case, we use the straightforward formulation of set cover as an ILP and solve it with Gurobi [18]. To the best of our knowledge, ILP solvers are currently the state-of-the-art for weighted set cover.

For the second step, we have to compute clique partitions from the resulting set covers by assigning each vertex that is covered by multiple cliques to a single one of these cliques. The goal is to minimize the weight of the resulting cliques, i.e., by Lemma 3, we want to distribute them as unevenly as possible. We employ a simple greedy heuristic, assigning each vertex to the largest clique it is part of and braking ties arbitrarily in case of ambiguity.

At a first glance it seems possible that doing both steps optimally (solving set cover and resolving the overlaps) could yield an overall optimal solution. However, this is not the case, as briefly discussed in Appendix A.

3.3 Exact branch-and-bound solver

Our branch-and-bound branches on which clique to select next. How to branch is described in Section 3.3.1 where we show that we can, in each step, select a maximal clique and that the cliques of the resulting sequence are non-increasing in size. In Section 3.3.2 and Section 3.3.3, we describe lower bounds for pruning the search space, i.e., if the best solution found so far is better than the lower bound in the current branch, we can prune that branch.

3.3.1 Branching

The following structural insight enables us to branch on the maximal cliques.

▶ **Lemma 6.** *Let $\mathcal{P}$ be a minimum weight clique partition of a graph G and let $C \in \mathcal{P}$ be the largest clique of $\mathcal{P}$. Then C is maximal clique in G.*

Thus, even though not all cliques of an optimal solution might be maximal, we at least know that the largest one is. We can use the decision of which maximal clique to select as the largest one as the branching decision of our algorithm. This way, we can solve the optimization variant of Weighted Clique Partition, i.e., the algorithm takes a graph G and finds a minimum weight clique partitioning.

After a clique C has been selected as the largest one, the remaining problem is to find a clique partition of $G[V \setminus C]$ that does not use any clique larger than C. This means that we can view our algorithm as a simple recursive subroutine that solves the same problem at every node of the recursion tree. As input it gets the graph G and the cliques $\langle C_1, \ldots, C_i \rangle$

that have already been selected by previous recursive calls. It then tries to compute an optimal clique partition of the remaining graph $G' := G \setminus \bigcup_{j\in[i]} C_j$. This is done by either returning a trivial solution if G' can be covered with a single clique or by branching on the decision of which maximal clique to select as the largest one for the partition of G'. Note that for this decision, only maximal cliques that are at most as large as any of the previously selected cliques $\langle C_1, \ldots, C_i\rangle$ need to be considered. The result of the subroutine call is then the cheapest solution found in any of the branches.

In order to quickly obtain a good upper bound, we explore branches corresponding to larger cliques first. This way, the first leaf of the search tree constructs the same solution as the repeated maximal clique heuristic.

3.3.2 Size lower bound

We call the lower bound given by the following lemma the *size lower bound.*

▶ **Lemma 7.** *Let G be a graph with n vertices and $\mathcal{P}$ be a clique partition of G consisting of cliques of size at most s. Then $\mathcal{P}$ has weight at least $(s+1)^{\lfloor n/s\rfloor} \cdot ((n \mod s)+1)$.*

Proof. The stated minimum weight is achieved by a partitioning $\mathcal{P}'$ that uses as many cliques of size s as possible and one clique with all remaining vertices. Any other partitioning $\mathcal{P}$ using only cliques of size at most s is at least as expensive, as it can be transformed into $\mathcal{P}'$ by Lemma 4. ◀

Note that the size lower bound can trivially be evaluated in constant time. Even though it is rather basic, we expect this lower bound to be effective at pruning branches in which very small cliques are selected early on.

3.3.3 Valuable sequence lower bound

Note that the size lower bound optimistically assumes that there are $\lfloor n/s\rfloor$ non-overlapping cliques of size s. This yields a bad lower bound if, e.g., there is only one clique of size s while all other cliques are much smaller. In the following, we describe an improved bound based on this observation. We note that we have to be careful when considering what clique sizes are available for the following reason. Assume the branching has already picked a clique of size s, i.e., subsequent selected cliques have to have size at most s. Then it seems natural to derive a lower bound by summing over the sizes of all maximal cliques of size at most s. However, we have to account for the fact that selecting (and deleting) one clique can shrink a maximal clique that was larger than s to become a clique of size s. Thus, there might me more cliques of size s available than initially thought. In order to formalize this, we first introduce a different problem that considers only sizes of the cliques without making any assumptions on the overlap between the cliques.

In the Valuable Sequence problem, we are given a multiset A of natural numbers and a natural number n. The task is to construct a sequence of total value n and minimum weight. Such a sequence $S = \langle s_1, s_2, \ldots, s_k\rangle$ consists of elements $s_i \in A$ such that each number is repeated at most as often as it appears in A. In the following, we define value and weight of a sequence and give additional restrictions to what constitutes a valid sequence. To this end, let $S_i = \langle s_1, \ldots, s_i\rangle$ for $i \le k$ denote a prefix of S. We define a value $\mathrm{val}(s_i)$ for each s_i in the sequence as follows. The first element s_1 has value $\mathrm{val}(s_1) = s_1$. For subsequent elements s_{i+1}, we have $\mathrm{val}(s_{i+1}) = \min\{s_{i+1}, \mathrm{val}(s_i), n - \mathrm{val}(S_i)\}$, where $\mathrm{val}(S_i) = \sum_{j\in[i]} \mathrm{val}(s_j)$ is the total value of the prefix S_i.[2] If $\text{val}(s_i) = s_i$, we say that the element contributes *fully* to the sequence. Otherwise, it contributes *partially.* The *weight* of S is $\prod_{i\in[k]}(\text{val}(s_i) + 1)$. For the subsequence S_i, we call the next element s_{i+1} *eligible* if $s_{i+1} - \text{val}(S_i) \leq \text{val}(s_i)$; s_1 is always eligible. The sequence S is *valid* if each element is eligible.

To make the connection back to Weighted Clique Partition, interpret the numbers in A as the clique sizes. The total value n corresponds to the number of vertices that have to be covered. The value $\text{val}(s_i)$ corresponds to the number of vertices from the maximal clique of size s_i in G that have not been covered by previous cliques, i.e., the number of vertices that are newly covered in step i. Note that in step $i + 1$, at least $s_i - \text{val}(S_i)$ new vertices are covered as only $\text{val}(S_i)$ have been covered previously. Thus, the eligibility requirement ensures that the number of vertices covered in step $i + 1$ is not larger than the number of vertices covered in step i (recall, that we can assume the chosen cliques to form a non-increasing sequence). Moreover, for the definition of $\text{val}(s_{i+1})$, note that the minimum with $\text{val}(s_i)$ ensures that the sequence of values is non-increasing and the minimum with $n - \text{val}(S_i)$ ensures that the total value is n.

The following two lemmas formalize this connection between Valuable Sequence and Weighted Clique Partition. Afterwards, we discuss how Valuable Sequence can be solved optimally.

▶ **Lemma 8.** *Let $\mathcal{P}$ be a minimum weight clique partition of a graph G and let $\mathcal{C}$ be the set of maximal cliques in G. Then, any mapping $f : \mathcal{P} \to \mathcal{C}$ with $P \subseteq f(P)$ for each $P \in \mathcal{P}$ is injective and there exists at least one such mapping.*

Proof. There are mappings from $\mathcal{P}$ to $\mathcal{C}$, because each clique $P \in \mathcal{P}$ is either a maximal clique or a subset of a larger maximal clique. Assume that a mapping $f : \mathcal{P} \mapsto \mathcal{C}$ is not injective. Then, there are two partition classes P and P' that are mapped to the same clique $C \in \mathcal{C}$. Thus, these partition classes could be merged, contradicting the optimality of $\mathcal{P}$. ◀

▶ **Lemma 9.** *Let G be a graph with maximal cliques $\mathcal{C} = \{C_1, \dots, C_k\}$ and let (A, n) with $A = \{|C_1|, \dots, |C_k|\}$ and $n = |V(G)|$ be an instance of Valuable Sequence. The weight of a minimum solution of (A, n) is a lower bound for the weight of every clique partition of G.*

Proof. We now show that for a minimum clique partition $\mathcal{P}$ of G, we find a solution S of (A, n) whose weight is at most the weight of $\mathcal{P}$.

Let $P_1, \dots, P_{k'}$ be the cliques of $\mathcal{P}$ sorted by size in decreasing order. We can think of $\mathcal{P}$ as constructed iteratively in that order, so that each P_i is a maximal clique in $G[V \setminus (\bigcup_{j\in[i-1]} P_j)]$.

We construct S iteratively until $\text{val}(S) = n$. For each element s_i in the sequence, we prove by induction that $\text{val}(s_i) \geq |P_i|$ except for the last element. This then lets us use Lemma 4 to obtain that the weight of S is at most the weight of $\mathcal{P}$. For $i = 1$, we simply choose $s_1 = |P_1| \in A$. Since the first element always contributes fully, we have $\text{val}(s_1) = |P_1|$.

Assuming we constructed the sequence until i, we continue with step $i + 1$ as follows. If P_{i+1} is one of the initial maximal cliques in $\mathcal{C}$, then we can simply choose $s_{i+1} = |P_{i+1}| \in A$. Note that s_{i+1} is eligible, as $s_{i+1} = |P_{i+1}| \leq |P_i| \leq \text{val}(s_i)$, which in particular implies $s_{i+1} - \text{val}(S_i) \leq \text{val}(s_i)$. In this case, s_{i+1} contributes fully, i.e., $\text{val}(s_{i+1}) = |P_{i+1}|$, which implies the claim.

Otherwise, if P_{i+1} is not in $\mathcal{C}$, it is at least a subset of some clique $C \in \mathcal{C}$ such that $P_{i+1} = C \setminus \bigcup_{j\in[i]} P_j$. We choose $s_{i+1} = |C|$. The eligibility of s_{i+1} follows from the facts that the cliques in $\mathcal{P}$ are ordered non-increasingly, i.e. $|P_i| \geq |P_{i+1}|$, and that $\text{val}(s_j) \geq |P_j|$ holds by induction for all $j < i + 1$:

[2] Note that $\text{val}(s_{i+1})$ only depends on values of previous elements in S, i.e., the definition is not cyclic.

$$\mathrm{val}(s_i) \geq |P_i| \geq |P_{i+1}| = \left|C \setminus \bigcup_{j\in[i]} P_j\right| \geq |C| - \sum_{j\in[i]} |P_j| \geq s_{i+1} - \sum_{j\in[i]} \mathrm{val}(s_j) = s_{i+1} - \mathrm{val}(S_i).$$

Note that s_{i+1} contributes partially, i.e., $\mathrm{val}(s_{i+1}) = \mathrm{val}(s_i)$ unless this is the last item in S. As we just argued, we have $\mathrm{val}(s_i) \geq |P_{i+1}|$ and thus $\mathrm{val}(s_{i+1}) \geq |P_{i+1}|$, proving the claim.

To conclude, observe that our construction of S implicitly defines a mapping from $\mathcal{P}$ to $\mathcal{C}$ as in Lemma 8. As such a mapping is injective, no number in A is chosen twice. Moreover as we have $\mathrm{val}(s_i) \geq |P_i|$ for $i < k$, but both sum to n, the weight of $\mathcal{P}$ is at least the weight of S by Lemma 4. ◀

Valuable Sequence can be solved optimally with a simple greedy algorithm. We call the resulting lower bound the *valuable sequence* bound.

▶ **Theorem 10.** *An instance (A, n) of* Valuable Sequence *can be solved in $O(|A| + n)$ time.*

3.3.4 Sufficient weight reduction

To speed-up the computation of clique partitions for all bags of a tree decomposition, we additionally apply the following reduction rule. In the *sufficient weight* reduction, we immediately accept the first solution that is lighter or equally light as the largest weight of any of the already considered bags.

4 Evaluation

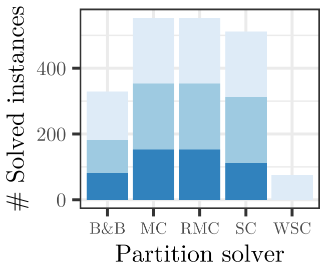
With our evaluation, we aim to answer the following questions.

1. How do the different algorithms compare in regards to run time and quality?
2. How do the algorithms scale?
3. What is the impact of the lower bounds and the reduction rules on the performance of the exact branch-and-bound solver?
4. How do different network properties influence the performance of the algorithms?
5. How do the resulting upper bounds on the clique-partitioned treewidth compare to traditional treewidth?

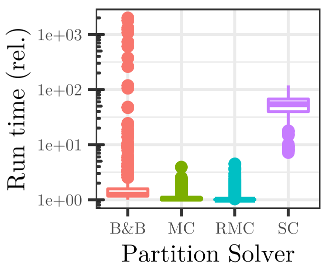
Experimental setup. Our implementation is written in Python. The source code along with all evaluation scripts and results is available on our public GitHub repository[3]. The experiments were run with Python 3.10.1 on a Gigabyte R282-Z93 (rev. 100) server (2250MHz) with 1024GB DDR4 (3200MHz) memory.

For each input graph, we perform the following two steps. First, we compute a tree decomposition using the heuristics implemented in the HTD library [1]. Specifically, we use the min-fill-in heuristic, which is known to provide a good tradeoff between run time and solution quality [23]. Secondly, we solve the Weighted Clique Partition problem for each bag of the tree decomposition using all algorithms proposed in Section 3.

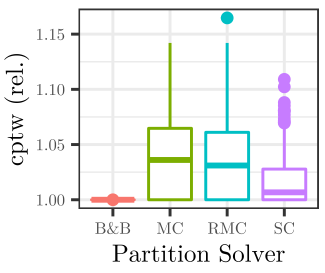
[3] `https://github.com/marcwil/cptw_code`



(a) Number of solved instances with 500 (bright) 5 k (medium) and 50 k (dark) vertices.



(b) Distribution of run time relative to fastest solver within time limit on a given graph.



(c) Distribution of obtained width relative to best found solution on a given graph.

Figure 1 Comparison of run time and solution quality of the different exact (red), greedy (green, blue) and set cover based (violet) solvers for the WEIGHTED CLIQUE PARTITION problem on GIRGs.

We use a time limit of five minutes for the heuristic computation of low-weight tree decompositions with the HTD library. For the WEIGHTED CLIQUE PARTITION algorithms, we set a time limit of three minutes per bag and five minutes in total.

To discern the different solvers from Sections 3.2 and 3.3, in our plots, we use the following abbreviations: branch and bound solver (B&B), maximal clique set cover heuristic (SC), maximal clique weighted set cover heuristic (WSC), maximal clique heuristic (MC), and repeated maximal clique heuristic (RMC).

Input instances. For the input, we use a large collection of real-world networks as well as generated networks. For the latter, we use geometric inhomogeneous random graphs (GIRGs) [8], which resemble real-world networks in regards to important properties and have been shown to be well suited for the evaluation of algorithms [3]. GIRGs can be generated efficiently [4] and allow to vary the power-law exponent (ple) of the degree distribution controlling its heterogeneity, as well as a parameter α controlling the locality by either strengthening the influence of the geometry (high values of α) or increasing the probability for random edges not based on the geometry (low values of α). We mainly use the following two datasets, where each graph has been reduced to its largest connected component.

- A collection of 2967 real-world networks [7] that essentially consists of all networks with at most 1 M edges from Network Repository [25]; see [3] for details.
- GIRGs with $n \in \{500, 5000, 50000\}$ vertices, expected average degree 10, dimension 1, ple $\in \{2.1, 2.3, 2.5, 2.7, 2.9\}$, and $\alpha \in \{1.25, 2.5, 5, \infty\}$. For each parameter configuration, we generate ten networks with different random seeds, to smooth out random variations.

4.1 Performance comparison

Here, we evaluate the performance of our CLIQUE PARTITION approaches on the two datasets.

Generated instances. In Figure 1, we compare the run times as well as the solution quality of the different considered CLIQUE PARTITION algorithms on the dataset of generated networks. In Figure 1a, we show how many of the 600 instances were solved within the time limit by each solver. While the greedy heuristics are able to finish on almost all instances, the set cover heuristic and the branch-and-bound solver get timed on some of the larger networks with 5 k and 50 k vertices. The weighted set cover heuristic performs much worse, finishing only on few networks. We therefore exclude it from the other comparisons.

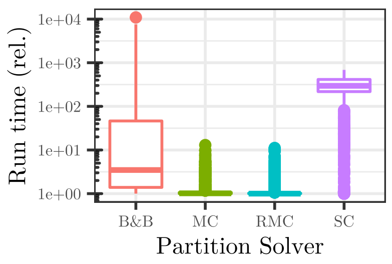


Figure 2 Distribution of run time relative to fastest solver within time limit on our set of real-world networks.

Table 1 Distribution of obtained cp-treewidth relative to optimum clique partition on our set of real-world networks.

Measure	MC	RMC	SC
Mean	1.008	1.009	1.002
Median	1	1	1
90th percentile	1.035	1.036	1.000
99th percentile	1.108	1.121	1.046
Maximum	1.254	1.192	1.113

In Figures 1b and 1c, we compare the performance for all instances that were solved within the time limit by all other algorithms. Figure 1b shows the run time of each algorithm relative to the fastest one on each instance. Figure 1c shows the obtained upper bound on the cp-treewidth relative to the optimal solution computed by the branch-and-bound solver.

Our findings are as follows. The branch-and-bound solver solves the fewest instances of the four considered algorithms, but is quick on most of the instances it is able to solve within the time limit. Both greedy heuristics (MC and RMC) are similarly fast, significantly outcompeting the other approaches. In terms of quality, all three heuristics perform well, achieving solutions within few percent of the optimum. The set cover heuristic slightly outperforms the greedy heuristics in terms of quality, but pays for this with substantially higher running time.

Real-world networks. We complement the above evaluation of our Clique Partition algorithms, by comparing their performance on the collection of real-world networks. As above, we exclude the weighted set cover heuristic. The other four approaches were able to finish on 1243 (B&B), 2619 (MC), 2622 (RMC), and 2204 (SC) of the 2967 networks within the time limit. We compare our algorithms on the 1237 networks that were solved by all four approaches. Figure 2 shows the run time of each solver relative to the fastest solver on each instance. In Table 1 we describe the distribution of the obtained upper bounds on the cp-treewidth relative to the optimal solution found by the branch-and-bound solver.

Our results are the following. In general, our observations on generated networks are replicated on the real-world networks. Even though the branch-and-bound algorithm solved fewer instances than the set cover heuristic, it is comparatively faster on the networks it is able to solve. Both approaches are, however, considerably slower than the greedy heuristics and this difference is more pronounced than on the generated networks. Regarding the solution quality, all three heuristic solvers perform even better than on the generated networks, with only a tiny fraction of instances not being solved almost optimally.

Discussion. We find that the proposed algorithms show good performance both on generated and real-world instances. Although, the branch-and-bound solver was only able to solve about half of the considered networks, its run time typically beats the set cover heuristic on the networks it can solve. In addition, it is a valuable tool for evaluating the solution quality of the other approaches. We find that especially the set cover heuristic, but also the greedy heuristics (MC and RMC) often find close to optimal clique partitions. Due to their excellent trade-off between speed and solution quality, the greedy heuristics are probably the best approach in most practical settings. In general, we do not expect that there is substantial

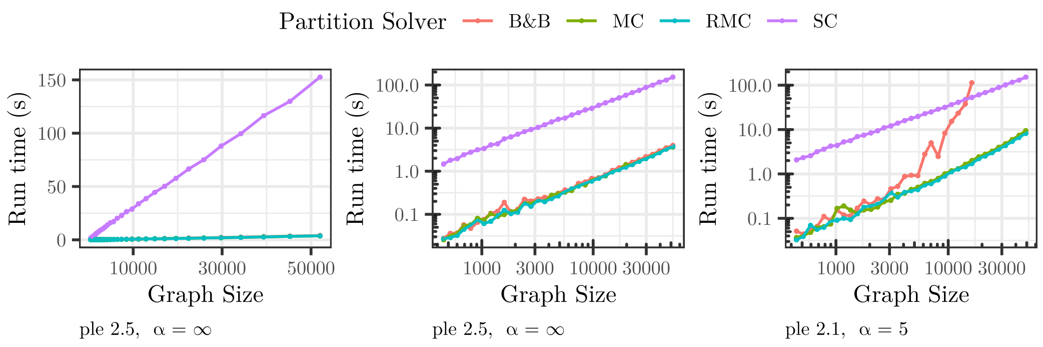


Figure 3 Scaling behavior of Clique Partition algorithms on GIRGs with different parameters.

room for improvement in the engineering of Clique Partition solvers for the computation of cp-treewidth. Instead, in order to achieve better upper bounds, we suggest future research to optimize the tree decomposition and the partition into cliques at the same time.

4.2 Run time scaling

Next, we consider the scaling behavior of our solvers. For this, we generated GIRGs of varying sizes up to around 50 k vertices for various parameters. As in Section 4.1, we did not evaluate the weighted set cover heuristic. Figure 3 shows the run times for GIRGs with two different parameter configurations. On the networks with high locality ($\alpha = \text{inf}$), all four approaches seem to have close to linear run time, despite enumerating all maximal cliques present in each bag of the tree decomposition. However, as we decrease the locality ($\alpha = 5$) the performance of the branch-and-bound solver deteriorates while the greedy heuristics and especially the set cover heuristic are only slightly affected. In the logarithmic plot, we observe clearly super-polynomial scaling behavior only for the branch-and-bound solver. Further experiments on a larger grid of parameter settings confirm the above findings.

4.3 Branch-and-bound: lower bounds and reduction rule

In the following, we evaluate the effectiveness of the lower bounds and the reduction rule in speeding up our branch-and-bound solver. For this, we use the dataset of generated networks. As the performance without lower bounds does not allow for the timely evaluation on larger instances, we consider only graphs generated with 5 k vertices. Figure 4 shows the average run time without lower bounds (none), with only the size lower bound (S) and with the valuable sequence bound in addition to the size bound (S+V) as well as with and without the sufficient weight reduction for different network parameters. We only show $\alpha \in \{5, \infty\}$, as for lower values the variant without lower bounds did not finish within the time limit.

We find that especially for smaller power-law exponents, the lower bounds bring large speed-ups of up to multiple orders of magnitude. The additional gain of using the size lower bound is much larger than that of the much simpler valuable sequence bound. The sufficient weight reduction yields similar speed-ups for all settings. Overall, we conclude that the lower bounds are effective in speeding up the branch-and-bound solver. On a more general note, it is striking how strongly all variants of the solver are affected by lower values of α, especially also below the values shown in Figure 4. In additional experiments we found that the above observations also apply to the remainder of the dataset, even though for 50 k vertices the time limit is reached even more frequently.

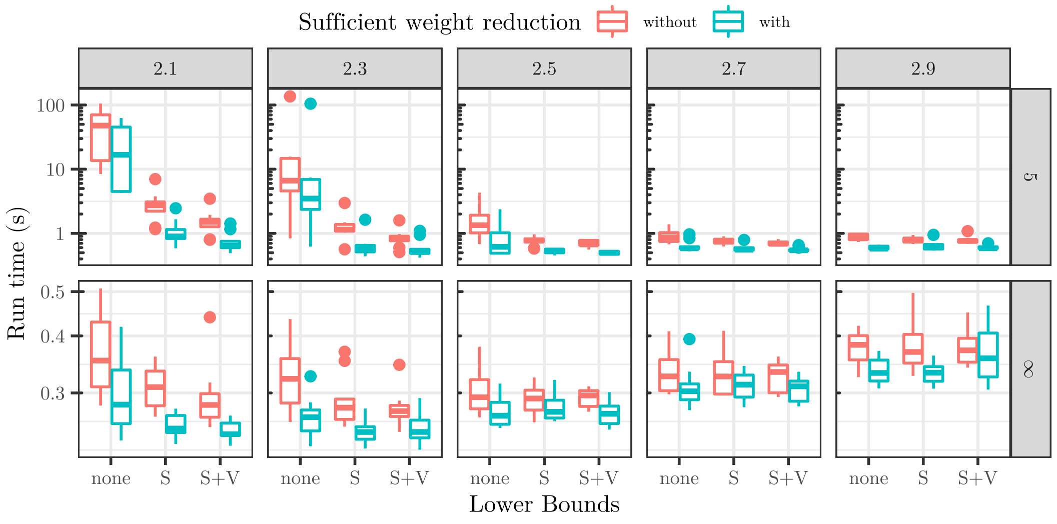


Figure 4 Run time of different variants of the branch-and-bound solver on GIRGs with 5 k vertices and different values for the power-law exponent (left to right) and α (top / bottom).

4.4 Impact of network properties

At multiple points throughout the last sections, we found that, especially for the branch-and-bound algorithm, the performance strongly depended on the parameter α controlling the locality of the generated networks.

In order to better understand this, we study the structure of cliques in the generated networks depending on their parameters. Specifically, for each network we count the number of maximal cliques in the graph, we count the number of maximal cliques in each bag of the tree decomposition and take the maximum, we count the number of cliques used per bag in the clique-partitioned tree decomposition and take the maximum, and consider the width of the clique-partitioned tree decomposition. The clique-partitioned tree decompositions are obtained using the MC and MCR heuristic. Figure 5 shows these values for GIRGs with varying power-law exponent and α.

We see that with decreasing values of α, all considered measures increase. However, while the total number of maximal cliques in the network only increases by a factor of roughly 4 to 10, the highest number of cliques intersecting some bag of the tree decomposition as well as the highest number of cliques in a lowest-weight clique partition increase by multiple orders of magnitude. Intuitively, this can be explained by cliques starting to fray if the locality is too low. This explains, why the CLIQUE PARTITION problem is harder on GIRGs with lower values of α, which slows down the branch-and-bound algorithm. We also observe, that the obtained upper bounds on the cp-treewidth are not much lower than the highest number of cliques per bag of a solution, explaining the good performance of the set cover heuristic.

4.5 Clique-partitioned treewidth compared to traditional treewidth

Here we consider the data set of real-world networks. As we have seen in Section 4.1, the maximal clique and repeated maximal clique heuristics are efficient and tend to perform well in terms of quality. Thus, we use these two heuristics to find an upper bound on the clique-partitioned treewidth.

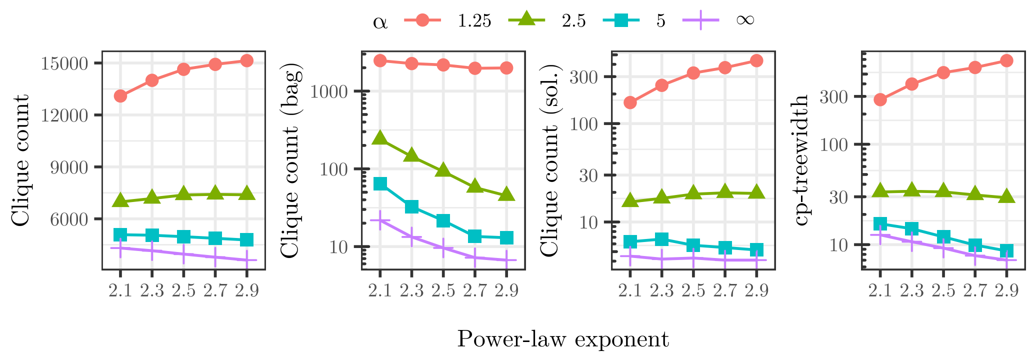
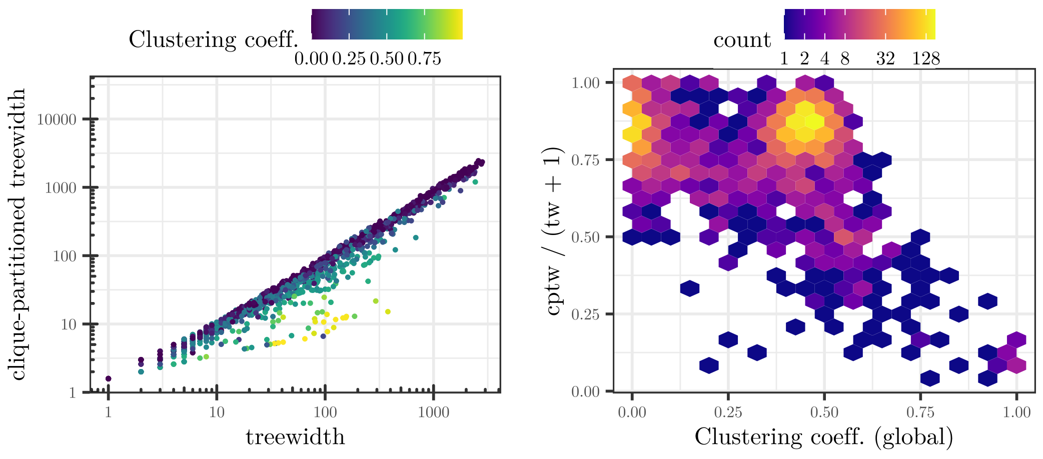


Figure 5 Total clique count (number of maximal cliques) per network, and highest clique count in any bag of a greedy tree decomposition as well in the lowest weight clique partition of any bag, and clique-partitioned treewidth (lowest upper bound) of the entire instance on GIRGs with 5 k vertices and varying parameters. Note the logarithmic y-axes on all except the first plot.



(a) Dependency between clustering coefficient and heuristic upper bounds on clique-partitioned treewidth and treewidth.

(b) Dependency between clustering coefficient and relative difference between clique-partitioned treewidth and treewidth.

Figure 6 Upper bounds for clique-partitioned treewidth on large real-world networks.

In Figure 6a we compare the obtained upper bounds for the weighted treewidth and the treewidth. Even though the parameter does not decrease much for the majority networks, there are some networks on which substantial reductions are achieved. This is particularly true for networks with high clustering coefficient, where for some instances our clique-partitioned tree decomposition has width 10 while the corresponding traditional tree decomposition has width above 100. This correspondence with the clustering coefficient fits well to the observations in Section 4.4. For the networks for which we do not yet see a big improvement, it would be interesting to see whether adjusting the computation of the initial tree decomposition can yield better bounds; see also the discussion in Section 4.1.

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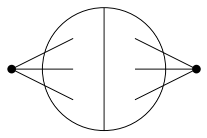
A Limits of the set cover heuristics


(a) Unweighted set cover.

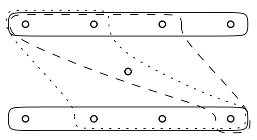

(b) Weighted set cover.

Figure 7 Counter-examples for the optimality of the set cover heuristics.

We want to briefly discuss why the set cover solutions are not always optimal clique partitions. First, we give an instance on which the unweighted set cover approach fails.

▶ **Observation 11.** *There are graphs on which the minimum size clique cover cannot give an optimal clique partition.*

Proof. Consider a clique on k vertices for even k where half of the vertices are connected to one additional vertex and the other half to another additional vertex, as illustrated in Figure 7a. Then, for $k \geq 6$ the partition into three cliques of sizes 1, 1, and k has lower weight than the partition into two cliques of size $\frac{k}{2}+1$, which corresponds to the optimal solution of the set cover instance. ◀

For the minimum weight set cover, we can use the fact that the weights of the set cover instance correspond to the size of the whole clique and do not reflect the potential overlap between multiple selected cliques.

▶ **Observation 12.** *There are graphs on which the minimum size clique cover cannot give an optimal clique partition.*

Proof. For the weighted approach, consider the instance depicted in Figure 7b. The small circles represent the vertices of a graph and the regions mark maximal cliques. The optimal clique partitioning uses cliques of sizes 6, 2, and 1 (the dotted clique plus the remainders of the two solid cliques). In the set cover instance these cliques have (partly overlapping) sizes 6, 4, and 4, which is more expensive than the set cover solution with sizes 5, 4, and 4 (using the dashed clique instead of the dotted one), which results in a solution with sizes $5, 3, 1$. ◀

The above problem could be avoided by extending the set cover instance to also include all non-maximal subsets of each clique that can be obtained by removing vertices shared with some subset of overlapping cliques. This would, however, lead to an exponential blowup of the set cover instances, which is not feasible even with state of the art solvers.

B Omitted proofs

▶ **Lemma 2.** *Let G be a graph with a clique-partitioned tree decomposition (T, σ) of weight τ. Then a largest independent set of G can be found in $O(2^\tau \cdot \operatorname{poly}(n))$ time.*

Proof. We use a standard dynamic programming approach on tree decompositions based on *introduce*, *forget*, and *join* nodes (see for example Cygan et. al [9]). For each node $t \in V(T)$, we store a number of partial solutions for the subgraph of G induced by the bags of nodes in the subtree below t.

A partial solution consists of a subset of the vertices in the current bag as well as the size of the total partial independent set for the subgraph induced by the subtree below the current bag. This makes it easy to initialize partial solutions for leaf nodes in the tree decomposition.

In an introduce node, two new partial solutions are created, one where the new vertex is in the independent set and one where it is not. In a forget node, the removed vertex is removed from each partial solution. In a join node, the partial solutions from the child-nodes are combined by taking their union.

In a traditional tree decomposition of width k, this leads to at most 2^k partial solutions per bag. In a clique-partitioned tree decomposition, this is even smaller, as there are only $k+1$ ways an independent set can intersect a clique of size k. Thus, assuming $\{\mathcal{P}_t \mid t \in V(T)\}$ denotes the clique partition of weight τ, the number of partial solutions that need to be considered per bag t are at most

$$\prod_{C\in\mathcal{P}_t}(|C|+1) = 2^{\sum_{C\in\mathcal{P}_t}\log(|C|+1)} = 2^{\tau}.$$

As the number of bags and time spent per bag is polynomial, this concludes the proof. ◀

▶ **Lemma 3.** *Let $a, b, c, d \in \mathbb{N}_0$ such that $a + b = c + d$ and $a \geq b$, $c \geq d$, $d > b$. Then $(a+1)(b+1) < (c+1)(d+1)$.*

Proof. There is an $x > 0$ such that $c = a - x$ and $d = b + x$. As $c \geq d$, x can be at most $(a - b)/2$. We derive

$$\begin{aligned}(c+1)(d+1) &= (a-x+1)(b+x+1)\\ &= ab - bx + b + ax - x^2 + x + a - x + 1\\ &= (ab + a + b + 1) + ax - bx - x^2\\ &= (a+1)(b+1) + x(a-b-x).\end{aligned}$$

We have $x(a - b - x) > 0$, as $0 < x \leq \frac{a-b}{2}$ and thus the claimed strict inequality follows. ◀

▶ **Lemma 6.** *Let $\mathcal{P}$ be a minimum weight clique partition of a graph G and let $C \in \mathcal{P}$ be the largest clique of $\mathcal{P}$. Then C is maximal clique in G.*

Proof. Assume that C is a non-maximal clique. That is, there is a vertex $v \in V(G) \setminus C$ with $C \subseteq N(v)$. Let $C' \in \mathcal{P}$ be the clique containing v. We construct a clique partition $\mathcal{P}'$ by removing v from C' and adding it to C. As C was the largest clique in $\mathcal{P}$, via Lemma 3 we have $(|C| + 2)(|C'|) < (|C| + 1)(|C'| + 1)$, contradicting the optimality of $\mathcal{P}$. ◀

▶ **Theorem 10.** *An instance (A, n) of* Valuable Sequence *can be solved in $O(|A| + n)$ time.*

Proof. We construct a solution $S = s_1, \ldots, s_i$ by iteratively choosing an eligible and not yet chosen number $a \in A$ with maximum value, until the value of the sum reaches n.

We note that this greedy strategy maximizes how many numbers in A are eligible, as the corresponding upper bound $\mathrm{val}(S) + \mathrm{val}(s_i)$ decreases as slowly as possible. The optimality of the produced sequence $S = s_1, \ldots, s_i$ follows, again, via Lemma 4 as for $j \in [i]$, the value $\mathrm{val}(s_j)$ is at least as large as the value of any other number that can be chosen in round j.

Regarding the running time, the greedy strategy can be implemented by sorting the numbers in A (in $O(|A| + n)$ time) and keeping track of the largest unchosen number that is eligible and contributes fully, as well as the smallest unchosen number that can contribute partially (which is larger than the ones that can contribute fully). Both of these values can be updated in constant time each time a number has been chosen. ◀