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Abstract

In the game of Kayles, two players select alternatingly a vertex from a given graph G, but may never choose a vertex that is adjacent or equal to an already chosen vertex. The last player that can select a vertex wins the game. In this paper, we give an exact algorithm to determine which player has a winning strategy in this game. To analyze the running time of the algorithm, we introduce the notion of a K-set: a nonempty set of vertices $W \subseteq V$ is a K-set in a graph $G = (V, E)$, if $G[W]$ is connected and there exists an independent set X such that $W = V - N[X]$. The running time of the algorithm is bounded by a polynomial factor times the number of K-sets in G. We prove that the number of K-sets in a graph with n vertices and m edges is bounded by $O(1.6052^n)$. A computer generated case analysis improves this bound to $O(1.6031^n)$ K-sets, and thus we have an upper bound of $O(1.6031^n)$ on the running time of the algorithm for Kayles. We also show that the number of K-sets in a tree is bounded by $n \cdot 3^{n/3}$ and thus KAYLES can be solved on trees in $O(1.4423^n)$ time. We show that apart from a polynomial factor, the number of K-sets in a tree is sharp.

Keywords: Graph algorithms; exact algorithms; combinatorial games; analysis of algorithms; moderately exponential time algorithms; Kayles; independent sets

1 Introduction

When a problem is computationally hard, then there still are many situations in which the need can arise to solve it exactly. This motivates the field of exact algorithms, where exact, exponential time algorithms whose running time is as small as possible are sought. Many such exact algorithms have been designed and analyzed for problems that are NP-complete or $\#P$-complete, see [8]. Of course, also problems that are complete for a 'harder'

*The work of the second author was supported by the ANR project AGAPE. An earlier version [4] of this paper appeared in the proceedings of the 37th International Workshop on Graph-Theoretic Concepts in Computer Science, WG 2011. That version has one case missing in the proof of the upper bound for general graphs. The current paper has a corrected proof, and gives in addition an improved computer generated bound.

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complexity class, e.g., PSPACE-complete often ask for exact solutions. Many PSPACE-complete problems arrive from the question which player has a winning strategy for a given position in a combinatorial game. Exact algorithms are of great relevance here, e.g., a program could use a heuristic to find a move, but once a position is simple enough, it switches to an exact algorithm to give optimal play in the endgame.

In this paper, we study exact algorithms for one such PSPACE-complete problem, namely the problem to determine which player has a winning strategy in an given instance of the game Kayles. Kayles is a two-player game that is played on a graph $G = (V, E)$. Alternatingly, the players choose a vertex from the graph, but players are not allowed to choose a vertex that already has been chosen or is adjacent to a vertex that already has been chosen. Thus, the player build together an independent set in G. The last player that chooses a vertex (i.e., turns the independent set into a maximal independent set) wins the game. Alternatively, one can describe the game as follows: the chosen vertex and its neighbors are removed and a player wins when his move empties the graph. The problem to determine the winning player for a given instance of the game is also called Kayles. This problem was shown to be PSPACE-complete by Schaefer [13]. In an earlier paper [3], we showed that by exploiting Sprague-Grundy theory, Kayles can be solved in polynomial time on several special graph classes, in particular graphs with a bounded asteroidal number (which includes well known classes of graphs like interval graphs, cocomparability graphs and cographs). Fleischer and Trippen [6] showed that Kayles can be solved in polynomial time on stars of bounded degree, and also analyzed this special case experimentally. For general trees, the complexity of Kayles is a long standing open problem. Variants of the game on paths were studied and shown to be linear time solvable by Guignard and Sopena [9]. For more background, the reader can consult [1, 2, 5].

It is not hard to find an algorithm that solves Kayles in $O^*(2^n)$ time, by tabulating for each induced subgraph of G which player has a winning strategy from that position. In this paper, we improve upon this trivial algorithm, and give an algorithm that uses $O(1.6031^n)$ time. The algorithm uses ideas from [3], exploiting results from Sprague-Grundy theory (also known as the theory of *nimbers*). To analyze the running time of the algorithm, we introduce the notion of K-set: a set of nonempty vertices $W \subseteq V$ is a K-set in a graph $G = (V, E)$, if $G[W]$ is connected and there exists an independent set X such that $W = V - N[X]$. In this paper, we give two upper bounds on the number of K-sets of a graph. For the first one, an upper bound of $O(1.6052^n)$, we give a proof based on a nontrivial case analysis. We then obtained a much more extensive With help of a computer generated case analysis, we obtained an improved bound of $O(1.6031^n)$ for the number of K-sets in a graph. We also show that if G is a tree, then G has at most $n \cdot 3^{n/3}$ K-sets, and thus, Kayles can be solved in $O^*(3^{n/3}) = O(1.4423^n)$ time on trees (and forests). [1] We also give lower bounds for the number of K-sets. In particular, our bound of $3^{n/3}$ K-sets for trees is sharp except for polynomial terms.

This paper is organized as follows. In Section 2, some preliminary notions and results

[1] We use the so called O^* notation: $f(n) = O^*(g(n))$ if $f(n) = O(g(n)p(n))$ for some polynomial $p(n)$. See also [8].

from graph theory and Sprague-Grundy theory are given. In Section 3, we give an algorithm for determining the winning player for Kayles played on a given graph G, and show that the running time is bounded by a polynomial in the number of vertices n times the number of K-sets in G. In Section 4, we present the proof that the number of K-sets in a graph is bounded by $O(1.6052^n)$. We explain how the computer generated bound of $O(1.6031^n)$ is obtained in Section 5. In Section 6, we give an upper bound on the number of K-sets in a tree; these match up to a constant multiplicative term. Section 7 discusses lower bounds for the number of K-sets in graphs; our bounds for trees are sharp up to a polynomial factor. Some final remarks are made in Section 8.

2 Preliminaries

Graph terminology Throughout this paper all graphs $G = (V, E)$ are undirected and simple. Let $S \subseteq V$. Then $N[S] = \cup_{s \in S} N[s]$ is the *closed neighborhood* of S, $N(S) = N[S] \setminus S$ is the *open neighborhood* of S, and $G[S]$ denotes the *subgraph of G induced by S*.

A nonempty set of vertices $W \subseteq V$ of a graph $G = (V, E)$ is called a *K-set* (*Kayles set*) of G, if it fulfills each of the following criteria:

- $G[W]$ is connected
- there exists an independent set $X \subseteq V$ such that $W = V - N[X]$

Sprague-Grundy theory Next, we review some notions and results from Sprague-Grundy theory, and give some preliminary results on how this theory can be used for Kayles. For a good introduction to Sprague-Grundy theory, the reader is referred to [1, 5].

A *nimber* is an integer belonging to $\mathbf{N} = \{0, 1, 2, \ldots\}$. For a finite set of nimbers $S \subseteq \mathbf{N}$, define the minimum excluded nimber of S as $mex(S) = \min\{i \in \mathbf{N} \mid i \notin S\}$.

To each position in a two player game that is finite, deterministic, full-information, impartial, and with 'last player wins rule', one can associate a nimber in the following way. If no move is possible in the position (and hence the player that must move loses the game), the position gets nimber 0. Otherwise the nimber is the minimum excluded nimber of the set of nimbers of positions that can be reached in one move.

Theorem 1 *[1, 5] There is a winning strategy for player 1 from a position, if and only if the nimber of that position is at least 1.*

Denote the nimber of a position p by $nb(p)$. Given two (finite, deterministic, impartial, ...) games $\mathcal{G}_1$, $\mathcal{G}_2$, the *sum* of $\mathcal{G}_1$ and $\mathcal{G}_2$, denoted $\mathcal{G}_1 + \mathcal{G}_2$ is the game where a move consists of choosing $\mathcal{G}_1$ or $\mathcal{G}_2$ and then making a move in that game. A player that cannot make a move in $\mathcal{G}_1$ nor in $\mathcal{G}_2$ looses the game $\mathcal{G}_1 + \mathcal{G}_2$. With (p_1, p_2) we denote the position in $\mathcal{G}_1 + \mathcal{G}_2$, where the position in $\mathcal{G}_i$ is p_i $(i = 1, 2)$.

The binary XOR operation is denoted by $\oplus$, i.e., for nimbers i_1, i_2, $i_1 \oplus i_2 = \sum\{2^j \mid (\lfloor i_1/2^j \rfloor$ is odd) $\Leftrightarrow$ ($\lfloor i_2/2^j \rfloor$ is even)$\}$.

Theorem 2 *[1, 5] Let p_1 be a position in $\mathcal{G}_1$, p_2 a position in $\mathcal{G}_2$. The nimber of position (p_1, p_2) in $\mathcal{G}_1 + \mathcal{G}_2$ equals $nb((p_1, p_2)) = nb(p_1) \oplus nb(p_2)$.*

As Kayles is an impartial, deterministic, finite, full-information, two-player game with the rule that the last player that moves wins the game, we can apply Sprague-Grundy theory to Kayles, and we can associate with every graph G the nimber of the start position of the game Kayles, played on G. We denote this nimber $nb(G)$, and call it the nimber of G.

An important observation is the following: when $G = G_1 \cup G_2$ for disjoint graphs G_1 and G_2, then the game Kayles, played on G is the sum of the game Kayles, played on G_1, and the game Kayles, played on G_2. Hence, by Theorem 2, we have the following result.

Lemma 3 $nb(G_1 \cup G_2) = nb(G_1) \oplus nb(G_2)$.

Note that G_1 and G_2 might be disconnected graphs.

Our second observation shows how to express the nimber of a graph G in the nimbers of some subgraphs of G. Consider Kayles, played on $G = (V, E)$, and suppose that a vertex $v \in V$ is played. Then, the nimber of the resulting position is the same as the nimber of $G - N[v]$, as the effect of playing on v is the same as the effect of removing v and its neighbors from the graph. As the nimber of a position is the minimum nimber that is not in the set of nimbers of positions that can be reached in one move, we have:

Lemma 4 *(i) If $G = (V, E)$ is the empty graph, then $nb(G) = 0$.*
(ii) If $G = (V, E)$ is not the empty graph, then $nb(G) = mex(nb(\{G - N[v] \mid v \in V\})$.

3 An Exact Algorithm for Kayles

In this section we present our exact exponential time algorithm solving Kayles. The algorithm starts with a call to the procedure `compute_nimber` shown in Figure 1, with input $G = (V, E)$. If it returns a nimber that is at least one, then Player 1 has a winning strategy on G; if it otherwise returns nimber zero, then Player 2 has a winning strategy. Correctness of the procedure directly follows from the discussion in Section 2.

Note that the procedure `compute_nimber`$(G[W])$ is only called for K-sets, and thus $G[W]$ is always connected, with one possible exception: if G is not connected, then the first call to the procedure is for $G[V]$ with V not a K-set. As the overhead per recursive call is polynomial, the running time is a polynomial factor times the number of K-sets in G. The procedure computes the nimber $nb(W)$ of $G[W]$ for all K-sets W of G and stores the value in a table using Memoisation, i.e., computed values are stored in a table, and by look-up no value $nb(W)$ is computed more than once. It follows that the running time of the algorithm is $O^*(|\mathcal{K}(G)|)$ where $\mathcal{K}(G)$ is the set of K-sets of G.

In Section 4, we give a combinatorial proof that the number of K-sets in a graph with n vertices is bounded by $O(1.6052^n)$. With a computer generated analysis, this bound can be brought back to $O(1.6031^n)$, as discussed in Section 5. In Section 6, we show that the

```
Procedure compute_nimber(G[W]).
  if nb(W) already computed then
    return nb(W)
  else
    M := ∅;
    for all v ∈ W do
      let Z_1, Z_2, ..., Z_r (r ≥ 1) be the components of G − N[w];
      nim := 0;
      for i ← 1 to r do
        nim := nim ⊕ compute_nimber(G[Z_i]);
        M := M ∪ {nim}
      answer := mex(M);
    nb(W) := answer;
    return answer
```

Figure 1: Procedure `compute_nimber`

number of K-sets in a tree with n vertices is bounded by $O(1.4423^n)$. If we combine these bounds with the algorithm of this section, we establish the following result. (The result for forests follows directly from the result for trees, as each K-set in a forest belongs to one connected component.)

Theorem 5 KAYLES *can be solved in time* $O(1.6031^n)$ *for graphs on* n *vertices.* KAYLES *can be solved in time* $O(1.4423^n)$ *for trees and forests on* n *nodes.*

4 An Upper Bound on the Number of K-sets

In this section, we give an explicit proof for an upper bound on the number of K-sets in a graph. Note that we give a slightly better, but computer generated bound in Section 5. As discussed in Section 3, this bound gives an upper bound on the running time of our algorithm for KAYLES on arbitrary graphs.

Theorem 6 *Let* G *be a graph with* n *vertices. Then* G *has* $O(1.6052^n)$ *K-sets.*

The proof of Theorem 6 is algorithmic: we give a branching procedure that generates all K-sets. By distinguishing different types of vertices, assigning these different weights, and considering the different branching vectors, we obtain a set of recurrences, whose solution gives us the desired bound. For information on branching algorithms and their analysis, in particular branching vectors and the corresponding recurrences we refer to [8].

We say that a K-set is *nontrivial*, if it has at least three vertices; otherwise we call it trivial. As each trivial set either consists of a single vertex or the two endpoints of an edge, the number of trivial K-sets is at most $n+m$, where m is the number of edges of the graph.

During our branching process, we decide at some points to put some vertices in an independent set X and forbid for some vertices to put them in the independent set. When placing a vertex in X, we say we *select* the vertex. The vertices in G are of four types:

- **White** or free vertices. Originally all vertices in G are white. We have not made any decision yet for a white vertex. All white vertices have weight one.
- **Red** vertices. Red vertices may not be placed in the independent set X: i.e., we already decided this during the branching. It still is possible that a red vertex becomes deleted later, however. Red vertices have a weight $\alpha = 0.5685$.
- **Green** vertices. A green vertex is 'safe': it never will be removed. I.e., we cannot place the green vertex nor any of its neighbors in the independent set X. Green vertices have weight zero.
- **Removed vertices**: these are either placed in the independent set or are a neighbor of a vertex in the independent set. All removed vertices have weight zero. Removed vertices are considered not existing, i.e., when discussing the neighbors of a vertex, these neighbors will be white, red, or green.

The *measure* of an instance G is the total weight of all vertices, and the difference in the measure from an instance to one of a subproblem often called *gain* is used to analyse the branching algorithm via branching vectors. Our branching process may be overcounting the number of K-sets (in particular, in some cases, we will not detect that a generated set is not connected), but the obtained bound nevertheless is valid as an upper bound.

The semantics of the colors implies that we can always perform the following actions:

- **Rule 1**: If a red vertex v has no white neighbors, we can color it green. This is valid, as we can no longer place a neighbor of v in X.
- **Rule 2**: If a green vertex v has a white neighbor w, we can color w red. This is valid, as placing w in X would remove v, which we are not allowed by the green color of v.

Rules 1 and 2 will always decrease the measure. They ensure that each red vertex will have a white neighbor, and that white vertices have no green neighbors.

The following action also can always be performed; the removed vertices can no longer be part of a nontrivial K-set.

- **Rule 3**: If $W \subseteq V$ is a set of white vertices that are not incident to nondeleted vertices not in W, and $|W| \leq 2$, then remove all vertices of W.

Before starting the main recursive branching, we first fix one vertex $v_0 \in V$, of which we will assume that it is an element of the K-set. In terms of colors, this means that we color v_0 green and all neighbors of v_0 red. Clearly, the total number of K-sets will be at most n times the bound on the number of K-sets that contain a specific vertex.

We obtain a fourth rule.

- **Rule 4**: If G has more than one connected component, then remove all vertices from components that do not contain v_0.

As a consequence, we have that when no rule can be applied and there is at least one white vertex, then there exists a white vertex that is adjacent to a red vertex.

We consider two main types of branching. The first type of branching is a *vertex branch*. Let $v \in V$ be a white vertex. We consider two cases: v is placed in X (called select v), and v is not placed in X. In the former case, we remove and decrease the measure by the total weight of all white and red vertices in the closed neighborhood of v. In the latter case, we color v red and have a measure decrease of $1 - \alpha$. In some cases, we gain more by applications of Rules 1, 2, and 3.

In the second type of branching, we consider a number of cases, of which one must apply. Again, in some cases, we can gain more by applications of Rules 1, 2, and 3.

In the sequel we present all branching rules in a preference order. Hence when Case i branching is applied to an instance all earlier cases do not apply.

Case 1: There is a white vertex with at least three white neighbors If v has three white neighbors, we can perform a vertex branch on v. The branching vector in this case will be $(4, 1 - \alpha)$, i.e., in one case, we decrease the measure by at least four, and in the other case, we decrease the measure by $1 - \alpha$.

Case 2: There is a white vertex with two white neighbors and at least one red neighbor If v has two white neighbors and at least one red neighbor, then a vertex branch on v gives a branching vector of $(3 + \alpha, 1 - \alpha)$.

Suppose Cases 1 and 2 cannot be applied anymore. Then all white vertices have at most two white neighbors. Moreover, there cannot be a cycle of white vertices, as such a cycle would either be removed by Rule 4 or contains a vertex to which Case 2 applies. Similar for white vertices forming paths. Only the endpoints of such a path can be adjacent to a red vertex, and at least one endpoint is adjacent to a red vertex.

Case 3: The subgraph induced by white vertices contains a path of length at least two, with both endpoints incident to at least one red vertex Suppose now we have a path of white vertices $v_1, \ldots, v_r$, $r \geq 2$, with v_1 and v_r incident to a red vertex. As Case 2 no longer applies, we can assume that $v_2, \ldots, v_{r-1}$ have no nondeleted neighbors outside the path.

Let R be the set of red vertices that are adjacent to v_1 and/or v_r.

Case 3.1: $r = 2$ We must either select v_1, or select v_2, or select neither v_1 nor v_2. In the latter case, both v_1 and v_2 can be colored green, so the measure decreases by two in this case. Hence, we have a branching vector $(2 + \alpha, 2 + \alpha, 2)$.

Case 3.2: $r = 3$ **and** $|R| \geq 2$ We consider all cases of placing vertices from $\{v_1, v_2, v_3\}$ in X:

- Select v_1 and v_3: we decrease the measure by $3 + 2 \cdot \alpha$.
- Select v_1: we decrease the measure by $3 + \alpha$.
- Select v_2: we decrease the measure by 3.
- Select v_3: we decrease the measure by $3 + \alpha$.
- Choose none: we decrease the measure by 3. (All three vertices can be colored green.)

So, in this case, we obtain a branching vector $(3 + 2 \cdot \alpha, 3 + \alpha, 3, 3 + \alpha, 3)$.

Case 3.3: $r = 3$ **and** $|R| = 1$ The vertices v_1 and v_3 have a common red neighbor. Now, we can perform a vertex branch on v_1. If we select v_1, then v_3 becomes an isolated vertex, and thus we have a branching vector of $(3 + \alpha, 1 - \alpha)$.

Case 3.4: $r = 4$ **and** $|R| \geq 2$ Like in Case 3.2, we consider all cases of placing vertices from $\{v_1, v_2, v_3, v_4\}$ in X, and obtain a somewhat tedious case analysis. In each case, each vertex in $\{v_1, v_2, v_3, v_4\}$ either is removed or is green. If v_1 or v_4 is placed in X, we gain an additional α for the removal of the red neighbor of this vertex. In case we select both v_1 and v_4, we gain $2 \cdot \alpha$; here we use that $|R| \geq 2$. This gives a branching vector of $(4 + \alpha, 4 + 2 \cdot \alpha, 4 + \alpha, 4 + \alpha, 4, 4, 4 + \alpha, 4)$, corresponding to selecting $\{v_1, v_3\}$, $\{v_1, v_4\}$, $\{v_2, v_4\}$, $\{v_1\}$, $\{v_2\}$, $\{v_3\}$, $\{v_4\}$ or no vertex from this path for inclusion in X.

Case 3.5: $r = 4$ **and** $|R| = 1$ We do a vertex branch on v_1: if we select v_1, then Rule 3 will remove v_3 and v_4. So the branching vector is $(4 + \alpha, 1 - \alpha)$.

Case 3.6: $r \geq 5$ We branch as follows:

- v_1 is placed in X: we decrease the measure by $2 + \alpha$.
- v_2 is placed in X: we decrease the measure by 3.
- v_3 is placed in X and v_1 is not placed in X. v_1 can be colored green, and thus we decrease the measure by 4.
- v_4 is placed in X and v_1 and v_2 are not placed in X. v_1 and v_2 can be colored green, and thus we decrease the measure by 5.
- None of v_1, v_2, v_3, v_4 is placed in X. v_1, v_2, v_3 become green, and v_4 becomes red: a measure decrease of $4 - \alpha$.

Thus, the branching vector is $(2 + \alpha, 3, 4, 5, 4 - \alpha)$.

Case 4: v_1 is a white vertex with no white but at least two red neighbors We do a vertex branch on v_1. If we do not select v_1, it can be colored green, by Rule 1. So we obtain a branching vector $(1 + 2 \cdot \alpha, 1)$.

Case 5: v_1 is a white vertex with exactly one neighbor, which is red Let w be the red neighbor of v_1.

Case 5.1: w has a white neighbor $x \neq v_1$ If a white neighbor of w has at least two red neighbors, then we can deal with it as in Case 4, and obtain a branching vector of $(1 + 2 \cdot \alpha, 1)$. So suppose all white neighbors of w have degree one, and thus w is their unique neighbor. We now have the following branch:

- w is a vertex in the K-set. In this case, w and all white neighbors of w are colored green. So, the measure decreases by at least $2 + \alpha$.
- w is not a vertex in the K-set. In this case, we must place *all* white neighbors of w in the independent set X. Again, the measure decreases by at least $2 + \alpha$.

So, we obtain a $(2 + \alpha, 2 + \alpha)$ branching vector.

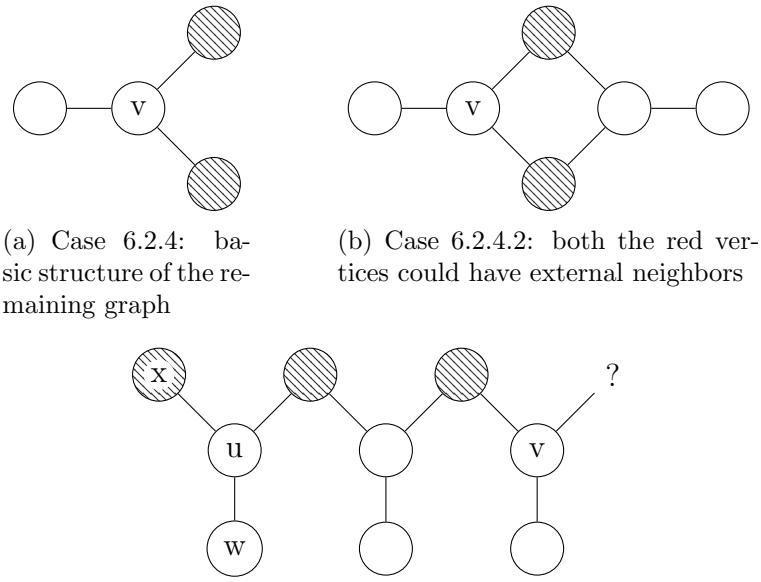
Case 5.2: v_1 is the unique white neighbor of w In this case, we do a vertex branch on v_1. If we do not place v_1 in the independent set, then both v_1 and w can be colored green. So, the branching vector is $(1 + \alpha, 1 + \alpha)$.

If Cases 1 to 3 cannot be applied, then there is no white vertex with two or more white neighbors. If Cases 4 and 5 can also not be applied then there is no white vertex without white neighbors. Thus we may assume that each white vertex has exactly one white neighbor.

Case 6: The subgraph induced by white vertices contains a path of length at least two, with exactly one endpoint incident to a red vertex Suppose $v_1, \ldots, v_r$ is a path of white vertices, and suppose $r \geq 2$ is maximal. Assume without loss of generality that v_1 has a red neighbor, say w.

Case 6.1: $r \geq 3$ We do a vertex branch on v_{r-2}. If we select v_{r-2} then we gain at least $3 + \alpha$: if $r \geq 4$, then v_{r-2} has two white neighbors, and if $r = 3$, then v_{r-2} has the white neighbor v_{r-1} and the red neighbor w. Moreover, v_r becomes an isolated vertex after v_{r-2} is placed in the independent set, and thus is removed by Rule 3. If we do not select v_{r-2}, we gain $1 - \alpha$, and thus we have a branching vector of $(3 + \alpha, 1 - \alpha)$.

Case 6.2: $r = 2$ There is a number of possibilities:



(a) Case 6.2.4: basic structure of the remaining graph

(b) Case 6.2.4.2: both the red vertices could have external neighbors

(c) Case 6.2.4.3: the cycle could be longer, but v could also be adjacent to x

Figure 2: Overview of the possibilities of Case 6.2.4. Red vertices are hatched.

Case 6.2.1: w is the unique red neighbor of v_1 and has at least one other white neighbor that we will call x We can now perform a vertex branch on x. If we place x in the independent set, then w and x are removed, but also v_1 and v_2 as Rule 3 can be applied: they form a connected component of at most two white vertices. So, the measure is decreased by at least $3 + \alpha$. If we do not select x, we color x red to obtain a measure decrease of $1 - \alpha$. So, this case gives a $(3 + \alpha, 1 - \alpha)$ branching vector.

Case 6.2.2: w is the unique red neighbor of v_1 and has no other white neighbor We either select v_1, or we select v_2, or we select neither v_1 nor v_2. If we select v_2, then w can be colored green, as its only white neighbor v_1 is removed. If we select neither v_1 nor v_2, then w, v_1 and v_2 can be colored green, so we decrease the measure $2 + \alpha$ in this case. So we obtain a branching vector of $(2 + \alpha, 2 + \alpha, 2 + \alpha)$.

Case 6.2.3: v_1 has ≥ 3 red neighbors We can do a vertex branch on v_1. If we select v, the measure is reduced by $2 + 3\alpha$. So this case gives a $(2 + 3\alpha, 1 - \alpha)$ branching.

Case 6.2.4: Each white vertex has exactly one white neighbor; each path of two white vertices consists of one white vertex without red neighbors and one white vertex with exactly two red neighbors When none of the above cases applies, there is only one very specific structure for the white vertices. This structure is shown in Figure 2(a). We now distinguish the following three possibilities. Throughout the analysis of Case 6.2.4, we denote with v a white vertex with two red neighbors.

Case 6.2.4.1: One (or both) of the red vertices has no other white neighbors We perform a vertex branch on v. If v is selected, then the measure is reduced by $2 + 2\alpha$. If v is not selected, we can color it red. The red neighbors of v that do not have white neighbors can then be colored green by Rule 1. We obtain a measure decrease of at least 1. The branching vector for this case becomes $(2 + 2\alpha, 1)$.

If the above case does not apply, then all red vertices have at least two white neighbors. The structures thus must form cycles of alternating red and white vertices. The smallest possible cycle is of length four, when two of these structures are connected.

Case 6.2.4.2: Two of the described structures share the same pair of red neighbors This situation is depicted in Figure 2(b). In this case selecting v removes both of its red neighbors and therefore changes the two vertices on the other side into a connected component. Rule 3 will remove this connected component and therefore selecting v results in a measure decrease of $4 + 2\alpha$. If v is not placed in the independent set X then the measure decreases by $1 - \alpha$. The branching vector is therefore $(4 + 2\alpha, 1 - \alpha)$ in this case.

Case 6.2.4.3: There is no cycle of length four Since there must be a cycle, it has length at least six. Part of the graph is drawn in Figure 2(c). Note that v may or may not be could adjacent to x. For the branching we distinguish four possibilities; note that at least one of these cases must apply:

Select u and v: the remaining white vertices are disconnected and removed by Rule 3, so the measure decreases by $6 + 3 \cdot \alpha$

Select u but do not select v: the measure decreases by $3 + \alpha$

Select v but do not select u: the measure decreases by 2

Select neither u nor w: both u and w are first colored red, but then they can be removed by Rule 1. Thus the measure decreases by 2.

The branching vector for this case amounts to $(6 + 3 \cdot \alpha, 3 + \alpha, 2, 2)$.

If no case applies, then there are no white, and hence also no red vertices left, so we found one (or zero, in case the green vertices are not connected) K-set. Our choice of $\alpha = 0.5685$ gives the best value for the base of the exponent for the given branching vectors, namely the claimed 1.6052. The tight branching vectors are $(4 + \alpha, 4 + 2 \cdot \alpha, 4 + \alpha, 4 + \alpha, 4, 4, 4 + \alpha, 4)$ (from Case 3.4) and $(3 + \alpha, 1 - \alpha)$. The latter one occurs in all of the Cases 2, 3.3, 6.1 and 6.2.1. From the above, it follows that there are $O(1.6052^n)$ nontrivial K-sets that contain v_0. As the value 1.6052 is obtained by rounding, and there are at most $n + m$ trivial K-sets, the result follows.

5 A Bound Obtained with an Automated Analysis

The case analysis that was presented in Section 4 can be extended further to reach a branching number of 1.6031. As the number of cases to consider becomes very large, we did not carry out this case analysis by hand, but instead used a computer generated proof. The code of our program that was used for this automated case analysis can be downloaded from `https://bitbucket.org/sjoerdtimmer/kayles`. We will now outline the followed procedure.

The main idea is to maintain a collection of objects, where each of these objects corresponds to a 'case' in the case analysis. The program computes branching vectors for these cases, and from these the corresponding bound on the number of K-sets. At runtime, the algorithm will 'expand' a case: a case is replaced by a larger collection of cases, that together cover the replaced case. More precise details are given below.

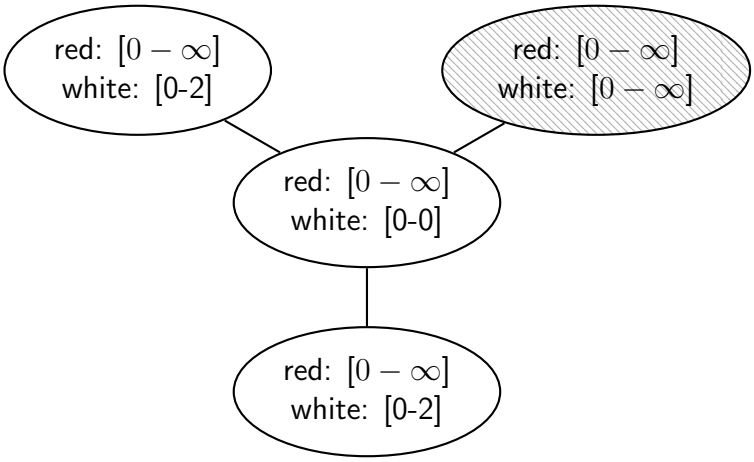


Figure 3: Example of a configuration

Modeling a case Every case can be described by a 'configuration' or 'pattern' in the input graph. A configuration is modeled with an incomplete graph. I.e. we have a colored graph that is assumed to be a subgraph of the input graph; vertices are not only labeled with a color, but also with intervals. These intervals describe how many white and how many red neighbors the vertex has outside the subgraph. The neighbors of a vertex outside of the configuration will be called its 'external' neighbors. In general a vertex starts with zero to infinite external white neighbors and zero to infinite external red neighbors, but during the branching this could change. An example configuration is drawn in Figure 3. This particular configuration corresponds to Case 2. Since Case 1 no longer applies, each white vertex has at most two white neighbors.

Modeling a proof The analysis given in Section 4 is already three levels deep, but we can go even further. We have created a mechanism to automatically explore a certain

configuration and generate a set of new configurations that covers all possibilities in which the old case could occur. The generation of these subcases will from here on be referred to as 'expansion'.

A very important aspect of the case analysis is the fact that some of these cases rely on the fact that all earlier cases do not apply. More specifically, Cases 1 and 2 are used in the analysis of the other cases, Case 4 is used in the analysis of Case 5 and Case 6.2 relies on the fact that all other cases have been removed. To use or infer these dependencies automatically is generally hard. But in this case we did not need to do so, since we could just start the automated analysis from the point where these cases are present.

Expansion strategies There are two ways to automatically expand a case: we can either look at the red neighborhood, or at the white neighborhood. When we look for instance at the white neighborhood of a vertex that can still have zero to infinity external white neighbors, we can split this into one configuration where it has exactly zero, one where it has exactly one and one configuration where it has two or more white neighbors. It is then guaranteed that the original case is covered, and we can ignore it in the analysis from that point onwards. The same argument holds however for the expansion of the red neighborhood of the vertex. This means the algorithm has to make an automated decision with respect to the vertex and the type of neighborhood to expand on. We will introduce a very efficient heuristic for this purpose later on.

Analysis After the generation of a new configuration we recalculate the branching number. When doing a branching by hand there was always a good intuition for the vertex to branch on, but now that we automate the process it is not that easy to know which vertex this is. The solution is to branch on all vertices that do not have external white neighbors (we will call these 'inner vertices' from now on). We simply test all possible selections of these inner vertices, and determine the reduction that would follow from selecting those vertices. When two or more selections result in the same coloring afterward, we only have to consider it once for the branching vector.

Each branching vector results in a lower bound on the base of the exponent. This is however still depending on the choice of α. Every branching vector can thus be seen as a constraint on x (the base of the exponent) given the value of α. We can use a Golden Ratio Search (see [11]) to efficiently determine the value of α which minimizes the base x of the exponential upper bound x^n on the number of K-sets.

Choosing the right expansion We have seen that there are always multiple options for the expansion. The question that arises is: "How do you choose the vertex to expand and the neighborhood to expand on?" In order to make progress (improve the branching vector) it is import to choose the right expansion, since choosing a disadvantageous expansion might lead to a lot more work later on, or even to a worse solution. One approach would be to expand in all possible directions and use a backtracking technique to find the optimum

sequence of expansions. This is however a lot of work and there is a good heuristic for making the choice.

To understand this heuristic, we should take a look at the four possible kinds of expansions that we could perform:

1. Expand the white neighborhood of a white vertex; this is a perfectly fine expansion, because afterwards this vertex has become an inner vertex. Any white neighbor that this inner vertex now has is removed when we select the inner vertex, thus contributing to a higher branching vector. If the new inner vertex has enough white neighbors this will result in a good branching vector. If, on the other hand, it has only a few white neighbors, then the number of branches becomes smaller which also makes the branching number better.

2. Expand the red neighborhood of a white vertex; this is also good to do, but less advantageous because you only win α for each neighbor if you select the vertex, and you do not win anything if this is not an inner vertex, so the above expansion should be preferred.

3. Expand the white neighborhood of a red vertex; we call this 'jumping over' the red vertex. If both of the above expansions cannot be applied and there is one red vertex with external white neighbors, selecting any of those white vertex disconnects the graph on this side and might even make the whole graph disconnected. This is a trick that was also applied manually in the paper to gain some measure in cases 5 and 6. This is of course mainly a good expansion if the above two expansions cannot be applied.

4. Expand the red neighborhood of a red vertex; this is a very disadvantageous expansion because you do not gain anything in the resulting configurations.

From the above reasoning we deduce a very effective heuristic for this problem:

- If there is a white vertex with external white neighbors, branch on that vertex.
- If not, but there is a white vertex with external red neighbors, branch on the red neighborhood of that vertex.
- If not, branch on the white neighborhood of a red vertex.
- repeat

Note that in our experiment the third case occurred only very rarely, and only if it was really necessary in order to make progress.

Automated result We applied our program to the case analysis given in Section 4. This helped us to identify a missing case in the original proof (given in [4]), and helped to obtain the corrected proof, given here in Section 4. In addition, the program showed that Case 3.4 of the proof given in Section 4 can be replaced by a collection of 95 new cases. This new case analysis is twelve expansions deep; the new collection of cases (all cases from Section 4 except Case 3.4 and the 95 new cases) lead to an upper bound of of $O(1.6031^n)$ on the number of K-sets in graphs.

All sources of the automated analysis can be downloaded from `https://bitbucket.org/sjoerdtimmer/kayles`. Due to space constraints, we do not give the full case analysis here; the reader can however reproduce the results from the program.

6 A Bound on the Number of K-sets in Trees

In this section, we establish an upper bound on the number of K-sets in a tree. This bound was used in Section 3 to show a bound on the running time of our algorithm, when the input graph is a tree or a forest.

Theorem 7 *Let $T(n)$ be the maximum number of K-sets in a tree on n nodes. Then $T(n) \leq n \cdot 3^{n/3}$.*

Proof. We denote as a *rooted K-set* of a rooted tree T any K-set of T containing r, where r denotes the root of T. Let $R(n)$ be the maximum number of rooted K-sets in any rooted tree on n nodes. We claim that $R(n) \leq 3^{n/3} - 1$ for all $n \geq 2$.

We are going to prove this claim by induction. To see that the claim is true for the base case $n = 2$, note that the only K-set containing r is the one containing both nodes of the tree, and that $3^{2/3} - 1 > 1.08$.

As induction hypothesis let us assume that the claim is true for all $n' < n$ and consider any rooted tree T on $n > 2$ nodes. Let r be the root of the tree and $u_1, u_2, \ldots, u_p$ be the children of v. For every $i = 1, 2, \ldots, p$, let T_i be the subtree of T rooted at u_i. Furthermore for all $i = 1, 2, \ldots, p$, we denote by n_i the number of nodes of T_i.

Let W be any K-set of T containing its root r. Then for every i, the intersection of W with T_i is either empty or a K-set of T_i containing its root u_i. Note that $n_i = 1$ implies that W also contains u_i since $r \in W$ (and thus r cannot be taken into the independent set X generating W). Using the induction hypothesis and $\sum_{i=1}^{p} n_i = n - 1$, we establish the following upper bound for the number of rooted K-sets of a rooted tree on n nodes

$$\begin{aligned} R(n) &\leq \prod_{i:n_i \geq 2} (R(n_i) + 1) \leq \prod_{i:n_i \geq 2} 3^{n_i/3} \\ &\leq \prod 3^{(n-1)/3} \leq 3^{n/3} - 1. \end{aligned}$$

This completes the proof of our claim.

To complete the proof of the theorem simply note that any K-set is counted at least once as a rooted K-set for some vertex v chosen to be the root, and thus $T(n) \leq n \cdot R(n)$. □

The above proof can be used to obtain an algorithm to enumerate all K-sets of a tree in time $O^*(3^{n/3})$. This algorithm chooses any vertex r of maximum degree and branches into two subproblems: in one r is taken into W and in the other one r is I suggest to mention the tight recurrences when summarizing the result. This way readers can at least get an impression what has to be improved to achieve a better bound. ed from W and thus all neighbors of r are discarded from S.

7 Lower Bounds

In this section we present graphs on n vertices having $\Theta(3^{n/3})$ different K-sets. This implies a lower bound on the maximum number of K-sets of any graph on n vertices as well as a lower bound on the running time of any exact algorithm solving Kayles by using all K-sets of the input graph.

Theorem 8 *There are graphs on n vertices with $3^{n/3} + 2n/3$ different K-sets.*

Proof. Consider the following family of (chordal) graphs G_n for all positive integers n on the vertex set $\{1, 2, \ldots, 3n\}$. The edge set of G_n is constructed as follows:

- $\{3i \ : \ i = 1, 2, \ldots, n\}$ is a clique of G_n, and
- for all $i = 1, 2, \ldots, n$, the vertex set $\{3i - 2, 3i - 1, 3i\}$ induces a path.

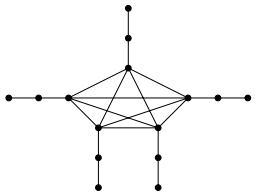


Figure 4: Example of the construction of Theorem 8, with $n = 5$

Let us count the K-sets W of G_n.
Case 1: $W \cap \{3i \ : \ i = 1, 2, \ldots, n\} = \emptyset$, which implies $|S \cap \{3i \ : \ i = 1, 2, \ldots, n\}| = 1$. Say $S \cap \{3i \ : \ i = 1, 2, \ldots, n\} = \{3i_0\}$. Hence $W \subseteq \{3i - 1, 3i - 2\}$ for some i. Thus if $i \neq i_0$ then $W = \{3i - 1, 3i - 2\}$; and if $i = i_0$ then $W = \{3i - 2\}$. thus there are $2n$ different K-sets in this case.
Case 2: $W \cap \{3i \ : \ i = 1, 2, \ldots, n\} \neq \emptyset$, which implies $S \cap \{3i \ : \ i = 1, 2, \ldots, n\} = \emptyset$. Then $W \subseteq \{3i - 2, 3i - 1, 3i\}$ may be any of the following sets $\{3i - 2, 3i - 1, 3i\}$, $\{3i\}$, $\emptyset$. Thus there are $3^n - 1$ different K-sets W in this case.
In total the graph G_n has at least $3^n + 2n$ K-sets. □

Theorem 9 *There are trees on n nodes with $3^{(n-1)/3} + 4(n-1)/3$ different K-sets.*

Proof. Consider the following family of trees T_n for all positive integers n. The node set of T_n is the set $\{0, 1, 2, \ldots, 3n+1\}$. The edgeset is constructed as follows:

- For all $i = 1, 2, \ldots, n$, the vertex set $\{3i-2, 3i-1, 3i\}$ induces a path, and
- the node 0 is adjacent to all nodes in the set $\{3i \ : \ i = 1, 2, \ldots, n\}$ and no others.

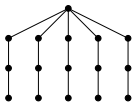


Figure 5: Example of the construction of Theorem 9, with $n = 5$

To count the K-sets W of T_n we distinguish two cases.
Case 1: $0 \notin W$. Then $S \cap \{0, 3, 6, \ldots, 3n\} \neq \emptyset$. Hence $W \subseteq \{3i, 3i-1, 3i-2\}$ for some i. Thus $W = \{3i, 3i-1, 3i-2\}$, $W = \{3i, 3i-2\}$, $W = \{3i\}$, $W = \{3i-2\}$. thus there are $4n$ different K-sets.
Case 2: $0 \in W$. Then $S \cap \{0, 3, 6, \ldots, 3n\} = \emptyset$. For every i, consider $W \cap \{3i-2, 3i-1, 3i\}$. By connectedness of $G[W]$ and $0 \in W$, we obtain that $W \cap \{3i-2, 3i-1, 3i\}$ is any of the following sets $\{3i-2, 3i-1, 3i\}$, $\{3i\}$, $\emptyset$. Thus there are $3^n - 1$ different K-sets W in this case.

Summarizing, the tree T_n has at least $3^n + 4n$ K-sets. □

8 Conclusions

In this paper, we gave an algorithm to determine which player has a winning strategy for the game Kayles. To analyse the running time, we introduced the notion of K-sets, and obtained upper and lower bounds on the maximum number of K-sets that a graph can have. We also obtained such bounds for trees; up to a polynomial factor, the bounds are sharp for trees. We obtained an upper bound with a hand-made proof, but also a somewhat better upper bound with a computer generated proof. We expect that for a even better bound, a different method of analysis should be used, e.g., it would be interesting to see if the bound can be improved using a measure and conquer analysis with a larger number of different vertex weights [7], or with the new potential method by Iwata [10].

A number of other interesting directions for further research remain. The complexity of Kayles on trees remains a long standing open problem. But one can also ask if there exists a subexponential time algorithm for Kayles on trees, e.g., with running time of the form $O(c^{\sqrt{n}})$.

Our algorithm uses exponential memory. It also is open if there exists a polynomial space algorithm with a running time of $O^*(2^n)$, and this may well be hard to obtain.

Our paper is a first example of exact algorithms for problems that are PSPACE-complete. It would be interesting to study such algorithms for other PSPACE-complete problems, e.g., for other combinatorial games, or for a problem like Quantified 3-Satisfiability [12]. An algorithm that solves Quantified (3-)Satisfiability in $O^*(2^n)$ time is not hard to find, but it seems very hard (or impossible) to find an algorithm with a running time $O^*(c^n)$ with $c < 2$ for this problem.

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