

# On finding directed trees with many leaves

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## Abstract

The ROOTED MAXIMUM LEAF OUTBRANCHING problem consists in finding a spanning directed tree rooted at some prescribed vertex of a digraph with the maximum number of leaves. Its parameterized version asks if there exists such a tree with at least  $k$  leaves. We use the notion of  $s - t$  numbering studied in [18], [5], [19] to exhibit combinatorial bounds on the existence of spanning directed trees with many leaves. These combinatorial bounds allow us to produce a constant factor approximation algorithm for finding directed trees with many leaves, whereas the best known approximation algorithm has a  $\sqrt{OPT}$ -factor [10]. We also show that ROOTED MAXIMUM LEAF OUTBRANCHING admits a quadratic kernel, improving over the cubic kernel given by Fernau et al [12].

## 1 Introduction

An *outbranching* of a digraph  $D$  is a spanning directed tree in  $D$ . We consider the following problem:

### ROOTED MAXIMUM LEAF OUTBRANCHING:

**Input:** A digraph  $D$ , an integer  $k$ , a vertex  $r$  of  $D$ .

**Output:** TRUE if there is an outbranching of  $D$  rooted at  $r$  with at least  $k$  leaves, otherwise FALSE.

This problem is equivalent to finding a Connected Dominating Set of size at most  $|V(D)| - k$ , connected meaning in this setting that every vertex is reachable by a directed path from  $r$ . Indeed, the set of internal nodes in an outbranching correspond to a connected dominating set.

Finding undirected trees with many leaves has many applications in the area of communication networks, see [7] or [23] for instance. An extensive literature is devoted to the paradigm of using a small connected dominating set as a backbone for a communication network.

ROOTED MAXIMUM LEAF OUTBRANCHING is NP-complete, even restricted to acyclic digraphs [2], and MaxSNP-hard, even on undirected graphs [15].

Two natural ways to tackle such a problem are, on the one hand, polynomial-time approximation algorithms, and on the other hand, parameterized complexity. Let us give a brief introduction on the parameterized approach.

An efficient way of dealing with NP-hard problems is to identify a parameter which contains its computational hardness. For instance, instead of asking for a minimum vertex cover in a graph - a classical NP-hard optimization question - one can ask for an algorithm which would decide, in  $O(f(k).n^d)$  time for some fixed  $d$ , if a graph of size  $n$  has a vertex cover of size at most  $k$ . If such an algorithm exists, the problem is called *fixed-parameter tractable*, or FPT for short. An extensive literature is devoted to FPT, the reader is invited to read [9], [13] and [20].

Kernelization is a natural way of proving that a problem is FPT. Formally, a *kernelization algorithm* receives as input an instance  $(I, k)$  of the parameterized problem, and outputs, in polynomial time in the size of the instance, another instance  $(I', k')$  such that:  $k' \leq k$ , the size of  $I'$  only depends of  $k$ , and the instances  $(I, k)$  and  $(I', k')$  are both true or both false.

The reduced instance  $(I', k')$  is called a *kernel*. The existence of a kernelization algorithm clearly implies the FPT character of the problem since one can kernelize the instance, and then solve the reduced instance  $G', k'$  using brute force, hence giving an  $O(f(k) + n^d)$  algorithm. A classical result asserts that being FPT is indeed equivalent to having kernelization. The drawback of this result is that the size of the reduced instance  $G'$  is not necessarily small with respect to  $k$ . A much more constrained condition is to be able to reduce to an instance of polynomial size in terms of  $k$ . Consequently, in the zoology of parameterized problems, the first distinction is done between three classes: W[1]-hard, FPT, polykernel.

A kernelization algorithm can be used as a preprocessing step to reduce the size of the instance before applying some other parameterized algorithm. Being able to ensure that this kernel has actually polynomial size in  $k$  enhances the overall speed of the process. See [16] for a recent review on kernelization.

An extensive literature is devoted to finding trees with many leaves in undirected and directed graphs. The undirected version of this problem, MAXIMUM LEAF SPANNING TREE, has been extensively studied. There is a factor 2 approximation algorithm for the MAXIMUM LEAF SPANNING TREE problem [21], and a  $3.75k$  kernel [11]. An  $O^*(1, 94^n)$  exact algorithm was designed in [14]. Other graph theoretical results on the existence of trees with many leaves can be found in [8] and [22].

The best approximation algorithm known for MAXIMUM LEAF OUTBRANCHING is a factor  $\sqrt{OPT}$  algorithm [10]. From the Parameterized Complexity viewpoint, Alon et al showed that MAXIMUM LEAF OUTBRANCHING restricted to a wide class of digraphs containing all strongly connected digraphs is FPT [1], and Bonsma and Dorn extended this result to all digraphs and gave a faster parameterized algorithm [4]. Very recently, Kneis, Langer and Rossmanith [17] obtained an  $O^*(4^k)$  algorithm for MAXIMUM LEAF OUTBRANCHING, which is

also an improvement for the undirected case over the numerous FPT algorithms designed for MAXIMUM LEAF SPANNING TREE. Fernau et al [12] proved that ROOTED MAXIMUM LEAF OUTBRANCHING has a polynomial kernel, exhibiting a cubic kernel. They also showed that the unrooted version of this problem admits no polynomial kernel, unless polynomial hierarchy collapses to third level, using a breakthrough lower bound result by Bodlaender et al [3]. A linear kernel for the acyclic subcase of ROOTED MAXIMUM LEAF OUTBRANCHING and an  $O^*(3, 72^k)$  algorithm for ROOTED MAXIMUM LEAF OUTBRANCHING were exhibited in [6].

This paper is organized as follows. In Section 2 we exhibit combinatorial bounds on the problem of finding an outbranching with many leaves. We use the notion of  $s-t$  numbering introduced in [18]. We next present our reduction rules, which are independent of the parameter, and in the following section we prove that these rules give a quadratic kernel. We finally present a constant factor approximation algorithm in Section 5 for finding directed trees with many leaves.

## 2 Combinatorial Bounds

Let  $D$  be a directed graph. For an arc  $(u, v)$  in  $D$ , we say that  $u$  is an *in-neighbour* of  $v$ , that  $v$  is an *outneighbour* of  $u$ , that  $(u, v)$  is an *in-arc* of  $v$  and an *out-arc* of  $u$ . The *outdegree* of a vertex is the number of its outneighbours, and its *indegree* is the number of its in-neighbours. An outbranching with a maximum number of leaves is said to be *optimal*. Let us denote by  $\text{maxleaf}(D)$  the number of leaves in an optimal outbranching of  $D$ .

Without loss of generality, we restrict ourselves to the following. We exclusively consider loopless digraphs with a distinguished vertex of indegree 0, denoted by  $r$ . We assume that there is no arc  $(u, r)$  in  $D$  with  $u \in V(D)$ , and no arc  $(x, y)$  with  $x \neq r$  and  $y$  an outneighbour of  $r$ , and that  $r$  has outdegree at least 2. Throughout this paper, we call such a digraph a *rooted digraph*. Definitions will be made exclusively with respect to rooted digraphs, hence the notions we present, like connectivity and resulting concepts, do slightly differ from standard ones. Let  $D$  be a rooted digraph with a specified vertex  $r$ .

The rooted digraph  $D$  is *connected* if every vertex of  $D$  is reachable by a directed path starting at  $r$  in  $D$ . A *cut* of  $D$  is a set  $S \subseteq V(D) - r$  such that there exists a vertex  $z \notin S$  endpoint of no directed path from  $r$  in  $D - S$ . We say that  $D$  is *2-connected* if  $D$  has no cut of size at most 1. A cut of size 1 is called a *cutvertex*. Equivalently, a rooted digraph is 2-connected if there are two internally vertex-disjoint paths from  $r$  to any vertex besides  $r$  and its outneighbours.

We will show that the notion of  $s-t$  numbering behaves well with respect to outbranchings with many leaves. It has been introduced in [18] for 2-connected undirected graphs, and generalized in [5] by Cheriyan and Reif for digraphs which are 2-connected in the usual sense. We adapt it in the context of rooted

digraphs.

Let  $D$  be a 2-connected rooted digraph. An  $r - r$  numbering of  $D$  is a linear ordering  $\sigma$  of  $V(D) - r$  such that, for every vertex  $x \neq r$ , either  $x$  is an outneighbour of  $r$  or there exist two in-neighbours  $u$  and  $v$  of  $x$  such that  $\sigma(u) < \sigma(x) < \sigma(v)$ . An equivalent presentation of an  $r - r$  numbering of  $D$  is an injective embedding  $f$  of the graph  $D$  where  $r$  has been duplicated into two vertices  $r_1$  and  $r_2$ , into the  $[0, 1]$ -segment of the real line, such that  $f(r_1) = 0$ ,  $f(r_2) = 1$ , and such that the image by  $f$  of every vertex besides  $r_1$  and  $r_2$  lies inside the convex hull of the images of its in-neighbours. Such *convex embeddings* have been defined and studied in general dimension by Lovász, Linial and Wigderson in [19] for undirected graphs, and in [5] for directed graphs.

Given a linear order  $\sigma$  on a finite set  $V$ , we denote by  $\bar{\sigma}$  the linear order on  $V$  which is the reverse of  $\sigma$ . An arc  $uv$  of  $D$  is a *forward* arc if  $u = r$  or if  $u$  appears before  $v$  in  $\sigma$ ;  $uv$  is a *backward* arc if  $u = r$  or if  $u$  appears after  $v$  in  $\sigma$ . A spanning out-tree  $T$  is *forward* if all its arcs are forward. Similar definition for *backward* out-tree.

The following result and proof is just an adapted version of [5], given here for the sake of completeness.

**Lemma 1** *Let  $D$  be a 2-connected rooted digraph. There exists an  $r - r$  numbering of  $D$ .*

*Proof:* By induction over  $D$ . We first reduce to the case where the indegree of every vertex besides  $r$  is exactly 2. Let  $x$  be a vertex of indegree at least 3 in  $D$ . Let us show that there exists an in-neighbour  $y$  of  $x$  such that the rooted digraph  $D - (y, x)$  is 2-connected. Indeed, there exist two internally vertex disjoint paths from  $r$  to  $x$ . Consider such two paths intersecting  $N^-(x)$  only once each, and denote by  $D'$  the rooted digraph obtained from  $D$  by removing one arc  $(y, x)$  not involved in these two paths. There are two internally disjoint paths from  $r$  to  $x$  in  $D'$ . Consider  $z \in V(D) - r - x$ . Assume by contradiction that there exists a vertex  $t$  which cuts  $z$  from  $r$  in  $D'$ . As  $t$  does not cut  $z$  from  $r$  in  $D$  and the arc  $(y, x)$  alone is missing in  $D'$ ,  $t$  must cut  $x$  and not  $y$  from  $r$  in  $D'$ . Which is a contradiction, as there are two internally disjoint paths from  $r$  to  $x$  in  $D'$ . By induction,  $D'$  has an  $r - r$  numbering, which is also an  $r - r$  numbering for  $D$ .

Hence, let  $D$  be a rooted digraph, where every vertex besides  $r$  has indegree 2. As  $r$  has indegree 0, there exists a vertex  $v$  with outdegree at most 1 in  $D$  by a counting argument. If  $v$  has outdegree 0, then let  $\sigma$  be an  $r - r$  numbering of  $D - v$ , let  $u_1$  and  $u_2$  be the two in-neighbours of  $v$ . Insert  $v$  between  $u_1$  and  $u_2$  in  $\sigma$  to obtain an  $r - r$  numbering of  $D$ . Assume now that  $v$  has a single outneighbour  $u$ . Let  $w$  be the second in-neighbour of  $u$ . Let  $D'$  be the graph obtained from  $D$  by contracting the arc  $(v, u)$  into a single vertex  $uv$ . As  $D'$  is 2-connected, consider by induction an  $r - r$  numbering  $\sigma$  of  $D'$ . Replace  $uv$  by  $u$ . It is now possible to insert  $v$  between its two in-neighbours in order to make it so that  $u$  lies between  $v$  and  $w$ . Indeed, assume without loss of generality that  $w$  is after  $uv$  in  $\sigma$ . Consider the in-neighbour  $t$  of  $v$  smallest in  $\sigma$ . As  $\sigma$

is an  $r - r$  numbering of  $D'$ ,  $t$  lies before  $uv$  in  $\sigma$ . We insert  $v$  just after  $t$  to obtain an  $r - r$  numbering of  $D$ .  $\square$

Note that an  $r - r$  numbering  $\sigma$  of  $D$  naturally gives two acyclic covering subdigraphs of  $D$ , the rooted digraph  $D|_{\sigma}$  consisting of the forward arcs of  $D$ , and the rooted digraph  $D|_{\bar{\sigma}}$  consisting of the backward arcs of  $D$ . The intersection of these two acyclic digraphs is the set of out-arcs of  $r$ .

**Corollary 1** *Let  $D$  be a 2-connected rooted digraph. There exists an acyclic connected spanning subdigraph  $A$  of  $D$  which contains at least half of the arcs of  $D - r$ .*

Let  $G$  be an undirected graph. A *vertex cover* of  $G$  is a set of vertices covering all edges of  $G$ . A *dominating set* of  $G$  is a set  $S \subseteq V$  such that for every vertex  $x \notin S$ ,  $x$  has a neighbour in  $S$ . A *strongly dominating set* of  $G$  is a set  $S \subseteq V$  such that every vertex has a neighbour in  $S$ .

Let  $D$  be a rooted digraph. A *strongly dominating set* of  $D$  is a set  $S \subseteq V$  such that every vertex besides  $r$  has an in-neighbour in  $S$ . We need the following folklore result:

**Lemma 2** *Any undirected graph  $G$  on  $n$  vertices and  $m$  arcs has a vertex cover of size  $\frac{n+m}{3}$ .*

*Proof:* By induction on  $n + m$ . If there exists a vertex of degree at least 2 in  $G$ , choose it in the vertex cover, otherwise choose any non-isolated vertex.  $\square$

**Lemma 3** *Let  $G$  be a bipartite graph over  $A \cup B$ , with  $d(a) = 2$  for every  $a \in A$ . There exists a subset of  $B$  dominating  $A$  with size at most  $\frac{|A|+|B|}{3}$ .*

*Proof:* Let  $G'$  be the graph which vertex set is  $B$ , and where  $(b, b')$  is an arc if  $b$  and  $b'$  share a common neighbour in  $A$ . The result follows from Lemma 2 since  $G'$  has  $|A|$  arcs and  $|B|$  vertices.  $\square$

**Corollary 2** *Let  $D$  be an acyclic rooted digraph with  $l$  vertices of indegree at least 2 and with a root of outdegree  $d(r) \geq 2$ . Then  $D$  has an outbranching with at least  $\frac{l+d(r)-1}{3} + 1$  leaves.*

*Proof:* Denote by  $n$  the number of vertices of  $D$ . For every vertex  $v$  of indegree at least 3, delete incoming arcs until  $v$  has indegree exactly 2. Since  $D$  is acyclic, it has a vertex  $s$  with outdegree 0.

Let  $Z$  be the set of vertices of indegree 1 in  $D$ , of size  $n - 1 - l$ . Let  $Y$  be the set of in-neighbours of vertices of  $Z$ , of size at most  $n - 1 - l$ . Let  $A'$  be the set of vertices of indegree 2 dominated by  $Y$ . Let  $B = V(D) - Y - s$ . Let  $A$  be the set of vertices of indegree 2 not dominated by  $Y$ . Note that  $Y$  cannot have the same size as  $Z \cup A'$ . Indeed,  $Z$  contains the outneighbours of  $r$ , and hence  $Y$  contains  $r$ , which has outdegree at least 2. More precisely,  $|Y| + d(r) - 1 \leq |Z \cup A'|$ . As  $B = V(D) - Y - s$  and  $A = V(D) - A' - Z - r$ ,

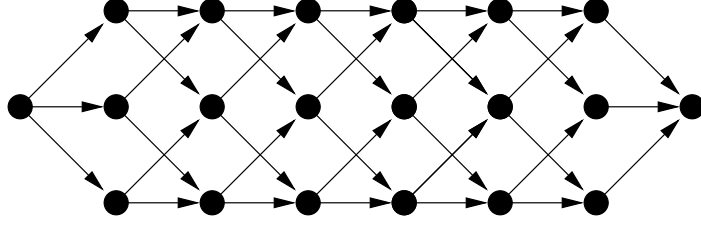


Figure 1: The "boloney" graph  $D_6$

we have that  $|B| \geq |A| + d(r) - 1$ . Moreover, as  $Y$  has size at most  $n - 1 - l$ , we have that  $|B| \geq l$ . Consider a copy  $A_1$  of  $A$  and a copy  $B_1$  of  $B$ . Let  $G$  be the bipartite graph with vertex bipartition  $(A_1, B_1)$ , and where  $(b, a)$ , with  $a \in A_1$  and  $b \in B_1$ , is an edge if  $(b, a)$  is an arc in  $D$ . By Lemma 3 applied to  $G$ , there exists a set  $X \subseteq B$  of size at most  $\frac{|A|+|B|}{3} \leq \frac{2|B|-(d(r)-1)}{3}$  which dominates  $A$  in  $D$ . The set  $C = X \cup Y$  strongly dominates  $V(D) - r$  in  $D$ , and has size at most  $|X| + |Y| \leq \frac{2|B|-(d(r)-1)}{3} + |Y| = |B| + |Y| - \frac{|B|+d(r)-1}{3}$ . As  $|Y| + |B| = n - 1$  and  $|B| \geq l$ , this yields  $|X \cup Y| \leq n - 1 - \frac{l+d(r)-1}{3}$ . As  $D$  is acyclic, any set strongly dominating  $V - r$  contains  $r$  and is a connected dominating set. Hence there exists an outbranching  $T$  of  $D$  having a subset of  $C$  as internal vertices.  $T$  has at least  $\frac{l+d(r)-1}{3} + 1$  leaves.

□

This bound is tight up to one leaf. The rooted digraph  $D_k$  depicted in Figure 1 is 2-connected, has  $3k - 2$  vertices of indegree at least 2,  $d(r) = 3$  and  $\text{maxleaf}(D_k) = k + 2$ .

Finally, the following combinatorial bound is obtained:

**Theorem 1** *Let  $D$  be a 2-connected rooted digraph with  $l$  vertices of indegree at least 3. Then  $\text{maxleaf}(D) \geq \frac{l}{6}$ .*

*Proof:* Apply Corollary 2 to the rooted digraph with the larger number of vertices of indegree 2 among  $D_\sigma$  and  $D_{\bar{\sigma}}$ . □

An arc is *simple* if does not belong to a 2-circuit. A vertex  $v$  is *nice* if it is incident to a simple in-arc.

The second combinatorial bound is the following:

**Theorem 2** *Let  $D$  be 2-connected rooted digraph. Assume that  $D$  has  $l$  nice vertices. Then  $D$  has an outbranching with at least  $\frac{l}{24}$  leaves.*

*Proof:* By Lemma 1, we consider an  $r - r$  numbering  $\sigma$  of  $D$ . For every nice vertex  $v$  (incident to some in-arc  $a$ ) with indegree at least three, delete incoming arcs of  $v$  different from  $a$  until  $v$  has only one incoming forward arc and one incoming backward arc. For every other vertex of indegree at least 3 in  $D$ , delete

incoming arcs of  $v$  until  $v$  has only one incoming forward arc and one incoming backward arc. At the end of this process,  $\sigma$  is still an  $r - r$  numbering of the digraph  $D$ , and the number of nice vertices has not decreased.

Denote by  $T_f$  the set of forward arcs of  $D$ , and by  $T_b$  the set of backward arcs of  $D$ . As  $\sigma$  is an  $r - r$  numbering of  $D$ ,  $T_f$  and  $T_b$  are spanning trees of  $D$  which partition the arcs of  $D - r$ .

The crucial definition is the following: say that an arc  $uv$  of  $T_f$  (resp. of  $T_b$ ), with  $u \neq r$ , is *transverse* if  $u$  and  $v$  are *incomparable* in  $T_b$  (resp. in  $T_f$ ), that is if  $v$  is not an ancestor of  $u$  in  $T_b$  (resp. in  $T_f$ ). Observe that  $u$  cannot be an ancestor of  $v$  in  $T_b$  (resp. in  $T_f$ ) since  $T_b$  is backward (resp.  $T_f$  is forward) while  $uv$  is forward (resp. backward) and  $u \neq r$ .

Assume without loss of generality that  $T_f$  contains more transverse arcs than  $T_b$ . Consider now any planar drawing of the rooted tree  $T_b$ . We will make use of this drawing to define the following: if two vertices  $u$  and  $v$  are incomparable in  $T_b$ , then one of these vertices is to the left of the other, with respect to our drawing. Hence, we can partition the transverse arcs of  $T_f$  into two subsets: the set  $S_l$  of transverse arcs  $uv$  for which  $v$  is to the left of  $u$ , and the set  $S_r$  of transverse arcs  $uv$  for which  $v$  is to the right of  $u$ . Assume without loss of generality that  $|S_l| \geq |S_r|$ .

The digraph  $T_b \cup S_l$  is an acyclic digraph by definition of  $S_l$ . Moreover, it has  $|S_l|$  vertices of indegree two since the heads of the arcs of  $|S_l|$  are pairwise distinct. Hence, by Corollary 2,  $T_b \cup S_l$  has an outbranching with at least  $\frac{|S_l|+d(r)-1}{3} + 1$  leaves, hence so does  $D$ .

We now give a lower bound on the number of transverse arcs in  $D$  to bound  $|S_l|$ . Consider a nice vertex  $v$  in  $D$ , which is not an outneighbour of  $r$ , and with a simple in-arc  $uv$  belonging to, say,  $T_f$ . If  $uv$  is not a transverse arc, then  $v$  is an ancestor of  $u$  in  $T_b$ . Let  $w$  be the outneighbor of  $v$  on the path from  $v$  to  $u$  in  $T_b$ . Since  $uv$  is simple, the vertex  $w$  is distinct from  $u$ . No path in  $T_f$  goes from  $w$  to  $v$ , hence  $vw$  is a transverse arc. Therefore, we proved that  $v$  (and hence every nice vertex) is incident to a transverse arc (either an in-arc, or an out-arc). Thus there are at least  $\frac{l-d(r)}{2}$  transverse arcs in  $D$ .

Finally, there are at least  $\frac{l-d(r)}{4}$  transverse arcs in  $T_f$ , and thus  $|S_l| \geq \frac{l-d(r)}{8}$ . In all,  $D$  has an outbranching with at least  $\frac{l}{24}$  leaves.  $\square$

As a corollary, the following result holds for oriented graphs (digraphs with no 2-circuit):

**Corollary 3** *Every 2-connected rooted oriented graph on  $n$  vertices has an outbranching with at least  $\frac{n-1}{24}$  leaves.*

### 3 Reduction Rules

We say that  $P = \{x_1, \dots, x_l\}$ , with  $l \geq 3$ , is a *bipath of length  $l - 1$*  if the set of arcs adjacent to  $\{x_2, \dots, x_{l-1}\}$  in  $D$  is exactly  $\{(x_i, x_{i+1}), (x_{i+1}, x_i) | i \in \{1, \dots, l - 1\}\}$ .

To exhibit a quadratic kernel for ROOTED MAXIMUM LEAF OUTBRANCHING, we use the following four reduction rules:

- (0) If there exists a vertex not reachable from  $r$  in  $D$ , then reduce to a trivially FALSE instance.
- (1) Let  $x$  be a cutvertex of  $D$ . Delete vertex  $x$  and add an arc  $(v, z)$  for every  $v \in N^-(x)$  and  $z \in N^+(x) - v$ .
- (2) Let  $P$  be a bipath of length 4. Contract two consecutive internal vertices of  $P$ .
- (3) Let  $x$  be a vertex of  $D$ . If there exists  $y \in N^-(x)$  such that  $N^-(x) - y$  cuts  $y$  from  $r$ , then delete the arc  $(y, x)$ .

Note that these reduction rules are not parameter dependent. Rule (0) only needs to be applied once.

**Observation 1** *Let  $S$  be a cutset of a rooted digraph  $D$ . Let  $T$  be an outbranching of  $D$ . There exists a vertex in  $S$  which is not a leaf in  $T$ .*

**Lemma 4** *The above reduction rules are safe and can be checked and applied in polynomial time.*

*Proof:*

- (0) Reachability can be tested in linear time.
- (1) Let  $x$  be a cutvertex of  $D$ . Let  $D'$  be the graph obtained from  $D$  by deleting vertex  $x$  and adding an arc  $(v, z)$  for every  $v \in N^-(x)$  and  $z \in N^+(x) - v$ . Let us show that  $\text{maxleaf}(D) = \text{maxleaf}(D')$ . Assume  $T$  is an outbranching of  $D$  rooted at  $r$  with  $k$  leaves. By Observation 1,  $x$  is not a leaf of  $T$ . Let  $f(x)$  be the father of  $x$  in  $T$ . Let  $T'$  be the tree obtained from  $T$  by contracting  $x$  and  $f(x)$ .  $T'$  is an outbranching of  $D'$  rooted at  $r$  with  $k$  leaves.

Let  $T'$  be an outbranching of  $D'$  rooted at  $r$  with  $k$  leaves.  $N^-(x)$  is a cut in  $D'$ , hence by Observation 1 there is a non-empty collection of vertices  $y_1, \dots, y_l \in N^-(x)$  which are not leaves in  $T'$ . Choose  $y_i$  such that  $y_j$  is not an ancestor of  $y_i$  for every  $j \in \{1, \dots, l\} - \{i\}$ . Let  $T$  be the graph obtained from  $T'$  by adding  $x$  as an isolated vertex, adding the arc  $(y_i, x)$ , and for every  $j \in \{1, \dots, l\}$ , for every arc  $(y_j, z) \in T$  with  $z \in N^+(x)$ , delete the arc  $(y_j, z)$  and add the arc  $(x, z)$ . As  $y_i$  is not reachable in  $T'$  from any vertex  $y \in N^-(x) - y_i$ , there is no cycle in  $T$ . Hence  $T$  is an outbranching of  $D$  rooted at  $r$  with at least  $k$  leaves. Moreover, deciding the existence of a cut vertex and finding one if such exists can be done in polynomial time.



- (2) Let  $P$  be a bipath of length 4. Let  $u, v, w, x$  and  $z$  be the vertices of  $P$  in this consecutive order. Let  $z$  be an outbranching of  $D$ . Note that either  $u$  is the father of  $w$  or  $w$  is the father of  $u$  in  $T$ . Let  $D'$  be the rooted digraph obtained from  $D$  by contracting  $v$  and  $w$ . The rooted digraph obtained from  $T$  by contracting  $w$  with its father in  $T$  is an outbranching of  $D'$  with as many leaves as  $T$ .

Let  $T'$  be an outbranching of  $D'$ . If the father of  $vw$  in  $T'$  is  $x$ , then  $T' - (x, vw) \cup (x, v) \cup (v, u)$  is an outbranching of  $D$  with at least as many leaves as  $T'$ . If the father of  $vw$  in  $T'$  is  $u$ , then  $T' - (u, vw) \cup (u, v) \cup (v, w)$  is an outbranching of  $D$  with at least as many leaves as  $T'$ .

- (3) Let  $x$  be a vertex of  $D$ . Let  $y \in N^-(x)$  be a vertex such that  $N^-(x) - y$  cuts  $y$  from  $r$ . Let  $D'$  be the rooted digraph obtained from  $T$  by deleting the arc  $(y, x)$ . Every outbranching of  $D'$  is an outbranching of  $D$ . Let  $T$  be an outbranching of  $D$  containing  $(y, x)$ . There exists a vertex  $z \in N^-(x) - y$  which is an ancestor of  $x$ . Thus  $T - (y, x) \cup (z, x)$  is an outbranching of  $D'$  with at least as many leaves as  $T$ .

□

We apply these rules iteratively until reaching a *reduced instance*, on which none can be applied.

**Lemma 5** *Let  $D$  be a reduced rooted digraph with a vertex of indegree at least  $k$ . Then  $D$  is a TRUE instance.*

*Proof:* Assume  $x$  is a vertex of  $D$  with in-neighbourhood  $N^-(x) = \{u_1, \dots, u_l\}$ , with  $l \geq k$ . For every  $i \in \{1, \dots, l\}$ ,  $N^-(x) - u_i$  does not cut  $u_i$  from  $r$ . Thus there exists a path  $P_i$  from  $r$  to  $u_i$  outside  $N^-(x) - u_i$ . The rooted digraph  $D' = \cup_{i \in \{1, \dots, l\}} P_i$  is connected, and for every  $i \in \{1, \dots, l\}$ ,  $u_i$  has outdegree 0 in  $D'$ . Thus  $D'$  has an outbranching with at least  $k$  leaves, and such an outbranching can be extended into an outbranching of  $D$  with at least as many leaves. □

## 4 Quadratic kernel

In this section and the following, a vertex of a 2-connected rooted digraph  $D$  is said to be *special* if it has indegree at least 3 or if one of its incoming arcs is simple. A non special vertex is a vertex  $u$  which has exactly two in-neighbours, which are also outneighbours of  $u$ . A *weak bipath* is a maximal connected set of non special vertices. If  $P = \{x_1, \dots, x_l\}$  is a weak bipath, then the in-neighbours of  $x_i$ , for  $i = 2, \dots, l - 1$  in  $D$  are exactly  $x_{i-1}$  and  $x_{i+1}$ . Moreover,  $x_1$  and  $x_l$  are each outneighbour of a special vertex. Denote by  $s(P)$  the in-neighbour of  $x_1$  which is a special vertex.

This section is dedicated to the proof of the following statement:

**Theorem 3** *A digraph  $D$  of size at least  $(3k - 2)(30k - 2)$  reduced under the reduction rules of previous section has an outbranching with at least  $k$  leaves.*

*Proof:* By Theorem 1 and Theorem 2, if there are at least  $6k + 24k - 1$  special vertices, then  $D$  has an outbranching with at least  $k$  leaves. Assume that there are at most  $30k - 2$  special vertices in  $D$ .

As  $D$  is reduced under Rule (2), there is no bipath of length 4. We can associate to every weak bipath  $B$  of  $D$  of length  $t$  a set  $A_B$  of  $\lceil t/3 \rceil$  out-arcs toward special vertices. Indeed, let  $P = (x_1, \dots, x_l)$  be a weak bipath of  $D$ . For every three consecutive vertices  $x_i, x_{i+1}, x_{i+2}$  of  $P$ ,  $2 \leq i \leq l - 3$ ,  $(x_{i-1}, x_i, x_{i+1}, x_{i+2}, x_{i+3})$  is not a bipath by Rule (2), hence there exists an arc  $(x_j, z)$  with  $j = i, i + 1$  or  $i + 2$  and  $z \notin P$ . Moreover  $z$  must be a special vertex as arcs between non-special vertices lie within their own weak bipath. The set of these arcs  $(x_j, z)$  has the prescribed size.

By Lemma 5, any vertex in  $D$  has indegree at most  $k - 1$  as  $D$  is reduced under Rule (3), hence there are at most  $3(k - 1)(30k - 2)$  non special vertices in  $D$ .  $\square$

To sum up, the kernelization algorithm is as follows: starting from a rooted digraph  $D$ , apply the reduction rules. Let  $D'$  be the obtained reduced rooted digraph. If  $D$  has size more than  $(3k - 2)(30k - 2)$ , then reduce to a trivially TRUE instance. Otherwise,  $D'$  is an instance equivalent to  $D$  of size quadratic in  $k$ .

This bound is tight up to a constant factor with respect to our reduction rules (see Annex).

## 5 Approximation

Let us describe our constant factor approximation algorithm for ROOTED MAXIMUM LEAF OUTBRANCHING, being understood that this also gives an approximation algorithm of the same factor for MAXIMUM LEAF OUTBRANCHING as well as for finding an out-tree (not necessarily spanning) with many leaves in a digraph.

Our reduction rules directly give an approximation algorithm asymptotically as good as the best known approximation algorithm [10] (see Annex). Let us now describe our constant factor approximation algorithm. Given a rooted digraph  $D''$ , apply exhaustively Rule (1) of Section 3. The resulting rooted digraph  $D$  is 2-connected. By Lemma 4,  $\text{maxleaf}(D'') = \text{maxleaf}(D)$ .

Let us denote by  $D_{ns}$  the digraph  $D$  restricted to non special vertices. Recall that  $D_{ns}$  is a disjoint union of bipaths, which we call *non special components*. A vertex of outdegree 1 in  $D_{ns}$  is called an *end*. Each end has exactly one special vertex as an in-neighbour in  $D$ .

**Theorem 4** *Let  $D$  be a 2-connected rooted digraph with  $l$  special vertices and  $h$  non special components. Then  $\max(\frac{l}{30}, h - l) \leq \text{maxleaf}(D) \leq l + 2h$ .*

*Proof:* The upper bound is clear, as at most two vertices in a given non special component can be leaves of a given outbranching. The first term of the lower bound comes from Theorem 1 and Theorem 2. To establish the second term, consider the digraph  $D'$  whose vertices are the special vertices of  $D$  and  $r$ . For

every non special component of  $D$ , add an edge in  $D'$  between the special neighbours of its two ends. Consider an outbranching of  $D'$  rooted at  $r$ . This outbranching uses  $l - 1$  edges in  $D'$ , and directly corresponds to an out-tree  $T$  in  $D$ . Extend  $T$  into an outbranching  $\tilde{T}$  of  $D$ . Every non special component which is not used in  $T$  contributes to at least a leaf in  $\tilde{T}$ , which concludes the proof.  $\square$

Consider the best of the three outbranchings of  $D$  obtained in polynomial time by Theorem 1, Theorem 2 and Theorem 4. This outbranching has at least  $\max(\frac{l}{30}, h - l)$  leaves. The worst case is when  $\frac{l}{30} = h - l$ . In this case, the upper bound becomes:  $\frac{92l}{30}$ , hence we have a factor 92 approximation algorithm for ROOTED MAXIMUM LEAF OUTBRANCHING.

## 6 Conclusion

We have given a quadratic kernel and a constant factor approximation algorithm for ROOTED MAXIMUM LEAF OUTBRANCHING: reducing the gap between the problem of finding trees with many leaves in undirected and directed graphs. MAXIMUM LEAF SPANNING TREE has a factor 2 approximation algorithm, and ROOTED MAXIMUM LEAF OUTBRANCHING now has a factor 92 approximation algorithm. Reducing this 92 factor into a small constant is one challenge. The gap now essentially lies in the fact that MAXIMUM LEAF SPANNING TREE has a linear kernel while ROOTED MAXIMUM LEAF OUTBRANCHING has a quadratic kernel. Deciding whether ROOTED MAXIMUM LEAF OUTBRANCHING has a linear kernel is a challenging question. Whether long paths made of 2-circuits can be dealt with or not might be key to this respect.

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## A Appendix

In this annex we just explain two very minor points not explicited in the main body due to space constraints.

Firstly, our analysis for the quadratic kernel for ROOTED MAXIMUM LEAF OUTBRANCHING is tight up to a constant factor. Indeed, the following graph  $T_l$  is reduced under the reduction rules stated on Section 3 and has a number of vertices quadratic in its maximal number of leaves. Let  $V = \{v_{i,j} | i = 1, \dots, l, j = 1, \dots, 3(l-1)\}$ . For every  $i = 1, \dots, l$ ,  $(r, v_{i,1})$  is an arc of  $T$ . For every  $j = 1, \dots, 3l-2$ ,  $i = 1, \dots, l$ ,  $(v_{i,j}, v_{i,j+1})$  is a 2-circuit of  $T_l$ . For every  $i = 1, \dots, l$ ,  $(v_{i,3l-1}, v_{i+1[l],3l-1})$  is an arc of  $T_l$ . For every  $t = 1, \dots, l-1$ ,  $i = 1, \dots, l$ ,  $(v_{i,3t}, v_{i+t[l],1})$  is an arc of  $T_l$ . This digraph  $T_l$  is reduced under the reduction rules of Section 3, and  $\text{maxleaf}(T_l) = 2(l-1)$ . Finally,  $T_l$  has  $3l(l-1) + 1$  vertices.

Note that this graph has many 2-circuits. We are not able to deal with them with respect to kernelization. For the approximation on the contrary, we are able to deal with the 2-circuits to produce a constant factor approximation algorithm.

The second point is that the reduction rules described in Section 4 directly give an approximation algorithm asymptotically as good as the best known approximation algorithm [10]. Indeed, as these rules are independant of the parameter, and as our proof of the existence of a solution of size  $k$  when the reduced graph has size more than  $3(k-1)(30k-2)$  is constructive, this yields a  $O(\sqrt{OPT})$  approximation algorithm. Let us sketch this approximation algorithm. Start by applying the reduction rules described in Section 4 to the input rooted digraph. This does not change the value of the problem. Let  $m$  be the size of the reduced graph. Exhibit an outbranching with at least  $\sqrt{\frac{m}{90}}$  leaves as in the proof of Theorem 3. Finally, undo the sequence of contractions yield by the application of reduction rules at the start of the algorithm, repairing the tree as in the proof of Lemma 4. The tree thus obtained has at least  $\sqrt{\frac{m}{90}}$  leaves, while the tree with maximum number of leaves in the input graph has at most  $m-1$  leaves. Thus this algorithm is an  $O(\sqrt{OPT})$  approximation algorithm.