Out-branchings with Extremal Number of Leaves

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Abstract

A subdigraph T of a digraph D is called an out-tree if T is an oriented tree with just one vertex s of in-degree zero. A spanning out-tree is called an out-branching. A vertex x of an out-branching B is called a leaf if $d^+_B(x) = 0$.

This is mainly a survey paper on out-branchings with minimum and maximum number of leaves. We give short proofs of some well-known theorems.

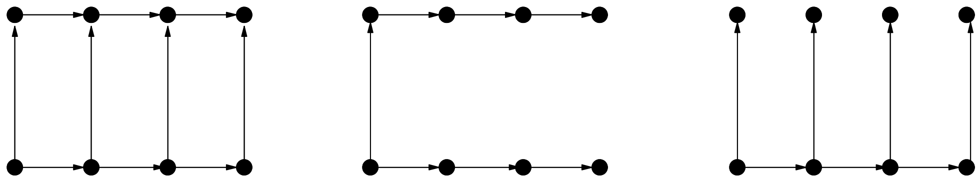
1 Introduction

This is mainly a survey paper on out-branchings with minimum and maximum number of leaves. Nevertheless, we prove some new results: Theorems 3.5 and Lemma 4.3. We also give short proofs to some well-known theorems.

The reader will see, in what follows, that out-branchings with minimum and maximum number of leaves are of great interest to graph theory, algorithms and applications.

A subdigraph T of a digraph D is called an **out-tree** if T is an oriented tree with just one vertex s of in-degree zero. The vertex s is the **root** of T. If an out-tree B is a spanning subdigraph of D, B is called an **out-branching**. A vertex x of an out-branching B is called a **leaf** if $d^+_B(x) = 0$. Figure 1 shows out-branchings with minimum and maximum number of leaves.

The problem of finding an out-branching with extremal number of leaves is of interest in applications; e.g., the problem of finding an out-branching



(a) D (b) Q (c) R

Figure 1: A digraph D and its out-branchings with minimum and maximum number of leaves (Q and R, respectively).

with minimum number of leaves was considered in the US patent [9] by Demers and Downing, where its application to the area of database systems was described.

For general digraphs, the problems of finding an out-branching with minimum/maximum number of leaves are $\mathcal{NP}$-hard: the problem of verifying the existence of an out-branching with just one leaf is the same as the hamiltonian path problem and the problem of finding a spanning tree with maximum number of leaves in an undirected graph is $\mathcal{NP}$-hard [12] (we may transform a undirected graph to the corresponding directed graph by replacing each edge xy by two arcs xy and yx). Thus, it is natural to consider parameterized complexities of the two problems. Let k be a parameter. The problem of checking whether a digraph D has an out-branching with at most k leaves (k non-leaves) is fixed-parameter tractable which was proved by Bonsma and Dorn [6] (by Gutin, Razgon and Kim [14]). This means that each of the two parameterized problems can be solved in time $O(f(k) \cdot n^{O(1)})$, where $f(k)$ is a computable function dependent on k but not on n and n is the order of D. We would like to note, in passing, that the problem of checking whether a digraph D has an out-tree with at most k leaves is also fixed-parameter tractable [1].

Note that restricted to acyclic digraphs the problems of finding an out-branching with minimum and maximum number of leaves are of different complexity (provided $\mathcal{P} \neq \mathcal{NP}$): while the former is polynomial time solvable (see Section 3), the latter is $\mathcal{NP}$-hard (see Section 4).

Our paper is organized as follows. In the next section, we will provide additional terminology and notation. Sections 3 and 4 are devoted to out-branchings with minimum and maximum number of leaves, respectively.

2 Terminology and Notation

For an out-branching B, let $\boldsymbol{L(B)}$ denote the set of leaves of B. For a digraph D containing an out-branching, let $\boldsymbol{\ell_{\min}(D)}$ and $\boldsymbol{\ell_{\max}(D)}$ denote the minimum and maximum number of leaves in an out-branching of D. If D has no out-branching we will write $\ell_{\min}(D) = 0$ or $\ell_{\max}(D) = 0$; it is well-known and easy to prove that a connected digraph D contains an out-branching if and only if D has only one initial strong component [4].

For a digraph D, $\boldsymbol{\alpha(D)}$ denotes the **independence number** of D, i.e., the maximum size of a vertex set X of D such that there is no arc between any pair of vertices of X. A vertex x of a digraph D is called a **source**, if the in-degree of x equals zero. The **path covering number pc($\boldsymbol{D}$)** of a digraph D is the minimum number of disjoint directed paths needed to cover $V(D)$. A digraph D is called **transitive** if the existence of arcs xy, yz implies the existence of the arc xz, where x, y and z are distinct vertices of D. The underlying (undirected) graph of a digraph D will be denoted by $\boldsymbol{UG(D)}$.

For more terminology and notation on digraphs, see Chapter 1 of [4].

3 Minimum Leaf Out-branchings

In this subsection, we give upper bounds on $\ell_{\min}(D)$ for general and strong digraphs D (Subsection 3.1) and a polynomial algorithm for computing $\ell_{\min}(D)$ for acyclic digraphs D (Subsection 3.2).

3.1 Upper Bounds on $\ell_{\min}(D)$

Las Vergnas [18] proved the following upper bound on $\ell_{\min}(D)$ for general digraphs.

Theorem 3.1 (Las Vergnas' theorem)**.** *For a digraph D, we have $\ell_{\min}(D) \leq \alpha(D)$.*

We will prove the following proposition which immediately implies the theorem.

Proposition 3.2. *[18] Let B be an out-branching of D with more than $\alpha(D)$ leaves. Then D contains an out-branching B' such that $L(B')$ is a proper subset of $L(B)$.*

Proof: We will prove this claim by induction on the number n of vertices in D. For $n \leq 2$ the result holds; thus, we may assume that $n \geq 3$ and consider an out-branching B of D with $|L(B)| > \alpha(D)$. Clearly, D has an arc xy such that x, y are leaves of B. If the in-neighbor p of y in B is of out-degree at least 2, then $L(B') \subset L(B)$, where $B' = B + xy - py$. So, we may assume that $d^+_B(p) = 1$. Observe that $\alpha(D - y) \leq \alpha(D) < |L(B)| = |L(B - y)|$. Hence by the induction hypothesis, $D - y$ has an out-branching B'' such that $L(B'') \subset L(B - y)$. Notice that $L(B - y) = L(B) \cup \{p\} \setminus \{y\}$. If $p \in L(B'')$, then observe that $L(B'' + py) \subset L(B)$. Otherwise, $L(B'' + xy) \subseteq L(B) \setminus \{x\} \subset L(B)$. □

The bound of Las Vergnas' theorem is tight as there are many digraphs D for which $\ell_{\min}(D) = \alpha(D)$, see, e.g., Theorem 3.5. It would be interesting to find other tight upper bounds on $\ell_{\min}(D)$.

While it is easy to show that the problem of checking whether a digraph has an out-branching with at most k leaves is $\mathcal{NP}$-hard for each fixed natural number k, Gutin, Razgon and Kim [14] proved that the problem of checking whether a digraph D of order n has an out-branching with at most $n - k$ leaves (or, equivalently, at least k non-leaves) is fixed-parameter tractable. Their proof uses a polynomial algorithm obtained from the proof of Proposition 3.2.

It is easy to show that Las Vergnas' theorem implies the well-known Gallai-Millgram theorem, Theorem 3.4. However, first we need the following simple result.

Lemma 3.3. *[15] Let $D = (V, A)$ be a digraph and let $\hat{D}$ be the digraph obtained from D by adding a new vertex s and all possible arcs from s to V. Then $\mathrm{pc}(D) = \ell_{\min}(\hat{D})$.*

Proof: Since a collection of p disjoint directed paths in D covering $V(D)$ corresponds to an out-branching of $\hat{D}$ with p leaves, we have $\mathrm{pc}(D) \geq \ell_{\min}(\hat{D})$. Let B be an out-branching of $\hat{D}$ with p leaves. We say that a vertex x of B is **branching** if $d^+_B(x) > 1$. Consider a maximal directed path Q of B not containing branching vertices. Observe that $B - V(Q)$ has $p - 1$ leaves. Thus, we can decompose the vertices of B into p disjoint directed paths. Deleting the vertex s from this collection of paths, we see that $\mathrm{pc}(D) \leq \ell_{\min}(\hat{D})$. Thus, $\mathrm{pc}(D) = \ell_{\min}(\hat{D})$. □

Theorem 3.4 (Gallai-Milgram theorem)**.** *[11] For every digraph D, $\mathrm{pc}(D) \leq \alpha(D)$.*

Proof: Consider the digraph $\hat{D}$ defined in Lemma 3.3. By Lemma 3.3 and Las Vergnas' theorem, $\mathrm{pc}(D) = \ell_{\min}(\hat{D}) \leq \alpha(\hat{D}) = \alpha(D)$. □

The bound of Las Vergnas' theorem is sharp as one can see from the following:

Theorem 3.5. *If D is a transitive acyclic digraph with a unique source s, then $\ell_{\min}(D) = \alpha(D)$.*

Proof: By Las Vergnas' theorem, D contains an out-branching B with $k \leq \alpha(D)$ leaves. Observe that B is rooted at s and the vertices of every path in B starting at s and terminating at a leaf induce a clique in $UG(D)$. Thus, the vertices of $UG(D)$ can be covered by k cliques and, hence, $\alpha(UG(D)) \leq k$. We conclude that $\ell_{\min}(D) = \alpha(D)$. □

The next theorem is equivalent to Theorem 3.5. Indeed, by Theorem 3.5 and Lemma 3.3, we have $\mathrm{pc}(D) = \ell_{\min}(\hat{D}) = \alpha(\hat{D}) = \alpha(D)$ for every transitive acyclic digraph D which implies Dilworth's theorem. Since $\mathrm{pc}(D) \leq \ell_{\min}(D) \leq \alpha(D)$ for each transitive acyclic digraph with a unique source, Dilworth theorem implies Theorem 3.5.

Theorem 3.6 (Dilworth's theorem)**.** *[10] Every transitive acyclic digraph D has* $\mathrm{pc}(D) = \alpha(D)$.

Theorems 3.5 and 3.6 give raise to the following natural research problem.

Problem 3.7. *Find other non-trivial digraph classes for which the equalities of Theorem 3.5 and/or Theorem 3.6 hold.*

Las Vergnas proved another upper bound on $\ell_{\min}(D)$.

Theorem 3.8. *[18] Let D be a digraph on n vertices such that any two distinct non-adjacent vertices have degree sum at least $2n - 2h - 1$, where $1 \leq h \leq n - 1$. Then $\ell_{\min}(D) \leq h$.*

Settling a conjecture of Las Vergnas [18], Thomassé [20] proved the following:

Theorem 3.9. *If D is a strong, then $\ell_{\min}(D) \leq \max\{\alpha(D) - 1, 1\}$.*

3.2 Acyclic Digraphs

Demers and Downing [9] suggested a heuristic approach for finding, in an acyclic digraph, an out-branching with minimum number of leaves. However, no argument or assertion has been made to provide the validity of their approach and to investigate its computational complexity. Using another approach, Gutin, Razgon and Kim [14] showed that a minimum leaf out-branching in an acyclic digraph can be found in polynomial time.

The following algorithm MINLEAF introduced by Gutin, Razgon and Kim [14] returns an out-branching with minimum number of leaves in an acyclic digraph. Observe that an acyclic digraph D has an out-branching if and only if it has exactly one source. It is not difficult to prove that MINLEAF is correct and of running time $O(n^{1.5}\sqrt{m})$, where n (m) is the order (size) of the input digraph.

MINLEAF
Input: An acyclic digraph D with vertex set V.
Output: A minimum leaf out-branching T of D if $\ell_{\min}(D) > 0$ and "NO", otherwise.

Step 1 Find a source r in D. If there is another source in D, return "no out-branching". Let $V' = \{v' : \ v \in V\}$.

Step 2 Construct a bipartite graph $B = B(D)$ of D with partite sets $V, V' - r'$ and edge xy' for each arc $xy \in A(D)$.

Step 3 Find a maximum matching M in B.

Step 4 $M^* := M$. For all $y' \in V'$ not covered by M, set $M^* := M^* \cup \{$an arbitrary edge incident with $y'\}$.

Step 5 $A(T) := \emptyset$. For all $xy' \in M^*$, set $A(T) := A(T) \cup \{xy\}$.

Step 6 Return T.

Figure 2 illustrates MINLEAF. There $M = \{rx', xy', zt'\}$ and $T = D - zy$.

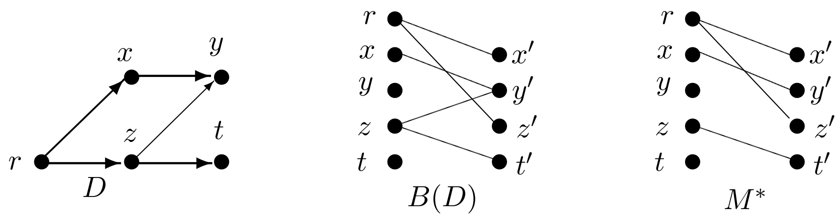


Figure 2: Illustration for MINLEAF

The parameters directed tree-width, directed path-width and DAG-width of digraphs are analogs of tree-width of undirected graphs; for definitions, see [8]. Acyclic digraphs are of directed tree-width, directed path-width and DAG-width equal zero. It follows from one of the main results of the paper [16] by Johnson, Robertson, Seymour and Thomas that there is a polynomial-time algorithms for verifying whether a digraph of bounded directed tree-width (directed path-width, DAG-width, respectively) has a Hamilton directed path. In contrast, Dankelmann, Gutin and Kim [8] proved that the problem of finding the minimum number of leaves in an out-branching of a digraph of directed tree-width (directed path-width, DAG-width, respectively) equal one is NP-hard.

4 Maximum Leaf Out-branchings

Alon, Fomin, Gutin, Krivelevich and Saurabh [3] proved the following complexity result.

Proposition 4.1. *The problem of finding an out-branching of maximum number of leaves in an acyclic digraph is $\mathcal{NP}$-hard.*

Proof: Consider a bipartite graph G with bipartition X, Y and a vertex $s \notin V(G)$. To obtain an acyclic digraph D from G and s, orient the edges of G from X to Y and add all arcs sx, $x \in X$. Let B be an out-branching in D. Then the set of leaves of B is $Y \cup X'$, where $X' \subset X$, and for each $y \in Y$ there is a vertex $z \in Z = X \setminus X'$ such that $zy \in A(D)$. Observe that B has maximum number of leaves if and only if $Z \subseteq X$ is of minimum size among all sets $Z' \subseteq X$ such that $N_G(Z') = X$. However, the problem of finding Z' of minimum size such that $N_G(Z') = X$ is equivalent to the Set Cover problem ($\{N_G(y) : y \in Y\}$ is the family of sets to cover), which is $\mathcal{NP}$-hard. □

Bonsma and Dorn [6, 7] showed that the problem of checking whether a digraph has an out-branching with at least k leaves is fixed-parameter tractable. In [7], they presented an algorithm for the problem of running time $2^{O(k \log k)} \cdot n^{O(1)}$. Kneis, Langer and Rossmanith [17] designed an algorithm of running time $4^k \cdot n^{O(1)}$.

Lower bounds on the maximum number of leaves in an out-branching of a digraph were investigated by Alon, Fomin, Gutin, Krivelevich and Saurabh [1, 2] and Bonsma and Dorn [7].

For a digraph D let $\ell^t_{\max}(D)$, denote the maximum possible number of leaves in an out-tree of D. Notice that $\ell^t_{\max}(D) \geq \ell_{\max}(D)$ for every digraph D. Let $\mathcal{L}$ be the family of digraphs D for which either $\ell_{\max}(D) = 0$

or $\ell^t_{\max}(D) = \ell_{\max}(D)$. It is easy to see that $\mathcal{L}$ contains all strong and acyclic digraphs.

The following assertion from [1] shows that $\mathcal{L}$ includes a large number of digraphs including all strong digraphs, acyclic digraphs, semicomplete multipartite digraphs and quasi-transitive digraphs.

Proposition 4.2. *Suppose that a digraph D satisfies the following property: for every pair R and Q of distinct strong components of D, if there is an arc from R to Q then each vertex of Q has an in-neighbor in R. Then $D \in \mathcal{L}$.*

Let $P = u_1u_2 \dots u_q$ be a directed path in a digraph D. An arc u_iu_j of D is a **forward** (**backward**) **arc for** P if $i \leq j - 2$ ($j < i$, respectively). Every backward arc of the type $v_{i+1}v_i$ is called **double**.

The following assertion is a slight refinement of a result by Alon, Fomin, Gutin, Krivelevich and Saurabh [1]. Better bounds were proved in [2] and [7] (the bound of Bonsma and Dorn [7] is optimal in a sense, see Remark 4.5), but our proof is significantly shorter than the proofs of the corresponding results in [1], [2] and [7].

Lemma 4.3. *Let D be an oriented graph of order n with every vertex of in-degree 2 and let D have an out-branching. If D has no out-tree with k leaves, then $n \leq k^5$.*

Proof: Assume that D has no out-tree with k leaves. Consider an out-branching T of D with p leaves so that this is the maximum number of leaves over all out-branchings in D. By the assumption $p < k$.

First observe that if $Q = v_1v_2 \dots v_s$ is an arbitrary path in T from the root to a leaf and v_iv_j is a forward arc, then, by the maximality of p, T must branch at v_{j-1}, that is, $d^+_T(v_{j-1}) \geq 2$. Since T has at most $k-1$ leaves and no two forward arcs end in the same vertex, this implies that Q has at most $(k-2)$ forward arcs.

Now fix a path $P = u_1u_2 \dots u_q$ from the root to a leaf in T which has $q \geq n/p$ vertices. When we delete all vertices of P from T we obtain a collection of out-trees covering $V(D) - V(P)$. It is easy to show by induction on the number of leaves that T can be decomposed into a collection $\mathcal{P} = \{P_1, P_2, \dots, P_p\}$ of vertex-disjoint directed paths covering all vertices of D so that $P = P_1$.

Let $P' \in \mathcal{P} \setminus \{P\}$ be arbitrary. There are at most $k-1$ vertices on P with in-neighbors on P' since otherwise we could choose a set X of at least k vertices on P for which there were in-neighbors on P'. The vertices of X would be leaves of an out-tree formed by the vertices $V(P') \cup X$. Thus, there are $m \leq (k-1)(p-1) \leq (k-1)(k-2)$ vertices of P with in-neighbors outside P and at least $q-(k-2)(k-1)$ vertices of P have both in-neighbors on P.

Let f be the number of forward arcs for P. By the argument above $f \leq k-2$. Let uv be an arc of $A(D) \setminus A(P)$ such that $v \in V(P)$. There are three possibilities: (i) $u \notin V(P)$, (ii) $u \in V(P)$ and uv is forward for P, (iii) $u \in V(P)$ and uv is backward for P. By the inequalities above for m and f, we conclude that there are at most $k(k-2)$ vertices on P which are not terminal vertices (i.e., heads) of a backward arc. Consider a path $R = v_0v_1 \dots v_r$ formed by backward arcs. Observe that the arcs $\{v_iv_{i+1} : 0 \leq i \leq r-1\} \cup \{v_jv_j^+ : 1 \leq j \leq r\}$ form an out-tree with r leaves, where v_j^+ is the successor of v_j on P. Thus, there is no path of backward arcs of length more than $k-1$.

If the in-degree of u_1 in the subdigraph of D induced by $V(P)$ is 2, remove one of the backward arcs terminating at u_1. Observe that now the backward arcs for P form a vertex-disjoint collection of out-trees with roots at vertices that are not terminal vertices of backward arcs. Therefore, the number of the out-trees in the collection is at most $k(k-2)$. Observe that each out-tree in the collection has at most $k-1$ leaves and thus its arcs can be decomposed into at most $k-1$ paths, each of length at most $k-1$. Hence, the original total number of backward arcs for P is at most $k(k-2)(k-1)^2+1$ (where the last one comes from the possible extra arc into u_1). On the other hand, it is at least $q-k(k-2)$ as every vertex on P is the head of an arc not in $A(P)$. Thus, $q-k(k-2) \leq k(k-2)(k-1)^2+1$. Combining this inequality with $q \geq n/(k-1)$, we conclude that $n \leq k^5$. □

Theorem 4.4. *[1] Let D be a digraph in $\mathcal{L}$ with $\ell_{\max}(D) > 0$.*

(a) If D is an oriented graph with minimum in-degree at least 2, then $\ell_{\max}(D) \geq n^{1/5} - 1$.

(b) If D is a digraph with minimum in-degree at least 3, then $\ell_{\max}(D) \geq n^{1/5} - 1$.

Proof: (a) Let B^+ be an out-branching of D. Delete some arcs from $A(D) \setminus A(B^+)$, if needed, such that the in-degree of each vertex of D becomes 2. Now the inequality $\ell_{\max}(D) \geq n^{1/5} - 1$ follows from Lemma 4.3 and the definition of $\mathcal{L}$.

(b) Let B^+ be an out-branching of D. Let P be the path formed in the proof of Lemma 4.3. (Note that $A(P) \subseteq A(B^+)$.) Delete every double arc of P, in case there are any, and delete some more arcs from $A(D) \setminus A(B^+)$, if needed, to ensure that the in-degree of each vertex of D becomes 2. It is not difficult to see that the proof of Lemma 4.3 remains valid for the new digraph D. Now the inequality $\ell_{\max}(D) \geq n^{1/5} - 1$ follows from Lemma 4.3 and the definition of $\mathcal{L}$. □

It is not difficult to give examples showing that the restrictions on the minimum in-degrees in Theorem 4.4 are optimal. Indeed, any directed cycle C is a strong oriented graph with all in-degrees 1 for which $\ell_{\max}(C) = 1$ and any directed double cycle D is a strong digraph with in-degrees 2 for which $\ell_{\max}(D) = 2$ (a **directed double cycle** is a digraph obtained from an undirected cycle by replacing every edge xy with two arcs xy and yx).

Remark 4.5. *Bonsma and Dorn [7] proved that one can replace* $n^{1/5} - 1$ *in the bounds of Theorem 4.4 by* $\sqrt{n}/4$. *Alon et al. [1] proved that if* $D \in \mathcal{L}$, *then* $\ell_{\max}(D) \leq c \cdot \sqrt{n}$ *for some constant* c. *Thus, we may conclude that if* $D \in \mathcal{L}$ *and* $\ell_{\max}(D) > 0$, *then* $\ell_{\max}(D) = \Theta(\sqrt{n})$.

Remark 4.6. *For some subfamilies of* $\mathcal{L}$, *one can obtain better bounds on* $\ell_{\max}(D)$. *One example is the class of* **multipartite tournaments**, *i.e., orientations of complete multipartite graphs. Gutin [13] and Petrovic and Thomassen [19] proved that every multipartite tournament* M *with at most one source has a vertex* x *such that the distance from* x *to any vertex of* M *is at most 4. Thus, a BFS tree of* M *has at least* $\frac{n-1}{4}$ *leaves and, hence,* $\ell_{\max}(M) \geq \frac{n-1}{4}$. *Another example is the class of quasi-transitive digraphs. A digraph* Q *is* **quasi-transitive** *if the existence of arcs* xy *and* yz *in* Q *implies the existence of an arc between* x *and* z. *Bang-Jensen and Huang [5] proved that every quasi-transitive digraph* Q *with* $\ell_{\max}(Q) > 0$ *has a vertex* x *such that each vertex of* Q *is at distance at most 3 from* x. *This implies that* $\ell_{\max}(Q) \geq \frac{n-1}{3}$.

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