On Complexity of Minimum Leaf Out-Branching
Problem

Peter Dankelmann∗ Gregory Gutin† Eun Jung Kim‡

March 30, 2009

Abstract
Given a digraph $D$, the Minimum Leaf Out-Branching problem (MinLOB) is the problem of finding in $D$ an out-branching with the minimum possible number of leaves, i.e., vertices of out-degree 0. Gutin, Razgon and Kim (2008) proved that MinLOB is polynomial time solvable for acyclic digraphs which are exactly the digraphs of directed path-width (DAG-width, directed tree-width, respectively) 0. We investigate how much one can extend this polynomiality result. We prove that already for digraphs of directed path-width (directed tree-width, DAG-width, respectively) 1, MinLOB is NP-hard. On the other hand, we show that for digraphs of restricted directed tree-width (directed path-width, DAG-width, respectively) and a fixed integer $k$, the problem of checking whether there is an out-branching with at most $k$ leaves is polynomial time solvable.

Keywords: Out-branchings, leaves, directed tree-width, DAG-width, computational complexity

1 Introduction

A digraph $T$ is an out-tree if $T$ is an oriented tree with only one vertex $s$ of in-degree zero (called the root). The vertices of $T$ of out-degree zero are called leaves and all other vertices of $T$ are called nonleaves. The vertex of in-degree zero is called the root of $T$ and all vertices of out-degree at least 2

∗School of Mathematical Sciences, University of KwaZulu-Natal, Durban 4041, South Africa, dankelma@ukzn.ac.za
†Corresponding author. Department of Computer Science, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK, gutin@cs.rhul.ac.uk
‡Department of Computer Science, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK, E.J.Kim@cs.rhul.ac.uk
are called *branching vertices*. If an out-tree $T$ is a spanning subgraph of a digraph $D$, i.e. $V(T) = V(D)$, then $T$ is called an *out-branching* of $D$.

Given a digraph $D$, the *Minimum Leaf Out-Branching* problem (MinLOB) is the problem of finding in $D$ an out-branching with the minimum possible number of leaves. Notice that not every digraph $D$ has an out-branching. It is not difficult to see that $D$ has an out-branching if and only if $D$ has just one strong connectivity component without incoming arcs [2]. Since the last condition can be checked in linear time [2], we may often assume that a digraph $D$ has an out-branching.

The MinLOB problem on acyclic digraphs has applications in the area of database systems, see the patent [6], where a heuristic to solve the MinLOB problem on acyclic digraphs was suggested. Gutin, Razgon and Kim [7] showed that the MinLOB problem for acyclic digraphs is, in fact, polynomial time solvable. Since MinLOB extends the Hamilton path problem, MinLOB for all digraphs is NP-hard, but standard dynamic programming techniques allow one to have a polynomial time algorithm for digraphs whose underlying graph is of bounded tree-width [7].

In this paper we investigate how much we can extend the polynomiality result for acyclic digraphs. Notice that acyclic digraphs are the digraphs of directed path-width (directed tree-width, DAG-width, respectively) 0. We prove that already for digraphs of directed path-width (directed tree-width, DAG-width, respectively) 1, MinLOB is NP-hard. This is in sharp contrast to the fact that the Hamilton path problem (the most important special case of MinLOB) is polynomial time solvable for digraphs of bounded directed path-width (directed tree-width, DAG-width, respectively). This fact follows from Theorem 2.3 and the inequalities on the width parameters used in the proof of Theorem 3.2.

On the other hand, we show that for digraphs of bounded directed tree-width (directed path-width, DAG-width, respectively) and a fixed integer $k$, the problem of checking whether there is an out-branching with at most $k$ leaves is polynomial time solvable.

We consider directed path-width, directed tree-width and DAG-width as they appear to be the most studied directed width parameters, but our results hold for other width parameters such as elimination width and Kelly-width [8] (the results for Kelly-width have to be modified by 1 taking into consideration that Kelly-width equals elimination-width plus 1).
2 Three Directed Decompositions

DAG-width was introduced independently by Berwanger et al. [4] and Obdrzalek [12]. A DAG-decomposition (DAGD) of a digraph $D$ is a pair $(H, \chi)$ where $H$ is an acyclic digraph and $\chi = \{W_h : h \in V(H)\}$ is a family of subsets (called bags) of $V(D)$ satisfying the following three properties: (a) $V(D) = \bigcup_{h \in V(H)} W_h$, (b) if $(u, v) \in A(D)$, then there exist $h_1, h_2 \in V(H)$ (it is possible that $h_1 = h_2$) such that $u \in W_{h_1}, v \in W_{h_2}$ and there is a directed $(h_1, h_2)$-path in $H$, (c) for all $h, h', h'' \in V(H)$, if $h'$ lies on a directed path from $h$ to $h''$, then $W_h \cap W_{h''} \subseteq W_{h'}$. The width of a DAGD $(H, \chi)$ is $\max_{h \in V(H)} |W_h| - 1$. The DAG-width of a digraph $D$ (dagw($D$)) is the minimum width over all possible DAGDs of $D$.

A directed path decomposition (DPD) [3] is a special case of DAGD when $H$ is a directed path. The directed path-width of a digraph $D$ (dpw($D$)) is defined as the DAG-width above, but DAGDs are replaced by DPDs.

Directed tree-width was introduced by Johnson, Robertson, Seymour and Thomas [9]. Let $Z$ be a set of vertices of a digraph $D$. A set $S \subseteq V(D) - Z$ is $Z$-normal if every directed walk that leaves and again enters $S$ must traverse a vertex of $Z$. For vertices $r, r'$ of an out-tree $T$ we write $r \leq r'$ if there is a path from $r$ to $r'$ or $r = r'$. An arboreal decomposition of a digraph $D$ is a triple $(R, X, W)$, where $R$ is an out-tree (not a subgraph of $D$), $X = \{X_e : e \in A(R)\}$ and $W = \{W_r : r \in V(R)\}$ are families of sets of vertices of $D$ that satisfy two conditions: (1) $\{W_r : r \in V(R)\}$ is a partition of $V(D)$ into nonempty sets, and (2) for each $e = (r', r'') \in A(R)$ the set $\bigcup_{r \in V(R), r \geq r''} W_r$ is $X_e$-normal. The width of $(R, X, W)$ is the least integer $w$ such that for all $r \in V(R)$, $|W_r \cup \bigcup_{e \sim r} X_e| \leq w + 1$, where $e \sim r$ means that $r$ is head or tail of $e$. The directed tree-width of $D$, dtw($D$), is the least integer $w$ such that $D$ has an arboreal decomposition of width $w$.

The following lemma is well-known [3, 4, 9, 12] and easy to prove using just the definitions above.

**Lemma 2.1** Let $D$ be a digraph. For $d \in \{\text{dag, dt, dp}\}$, we have dw($D$) = 0 if and only if $D$ is acyclic.

**Lemma 2.2** For a digraph $D$, we have dtw($D$) $\leq$ dpw($D$).

**Proof:** Let $Y_1, Y_2, \ldots, Y_k$ be the bags in a DPD of $D$. We may assume that all bags are distinct. Define an arboreal decomposition of $D$, where the arborescence is the directed path $12 \ldots k$, as follows: $W_1 = Y_1, W_i = Y_i \setminus Y_{i-1}$
for each $i = 2, 3, \ldots, k$ and if $e = (i, i+1)$ we let $X_e = Y_i \cap Y_{i+1}$. This arboreal decomposition is of the same width as the DPD and we are done. □

One of the main algorithmic results in [9] is on the following linkage problem. Let

$$\sigma = (s_1, t_1, s_2, t_2, \ldots, s_p, t_p)$$

be a sequence of $2p$ vertices of a digraph $D$, (vertices in $\sigma$ are not necessarily distinct). A hamiltonian $\sigma$-linkage of $D$ is a collection of $p$ directed paths $P_1, P_2, \ldots, P_p$ such that $V(P_1) \cup \ldots \cup V(P_p) = V(D)$, $P_i$ starts at $s_i$ and terminates at $t_i$, $1 \leq i \leq p$, and $(V(P_i) \setminus \{s_i, t_i\}) \cap (V(P_j) \setminus \{s_j, t_j\}) = \emptyset$ for all $1 \leq i < j \leq p$. In the hamiltonian linkage problem, given $\sigma$ we are to check whether there is a hamiltonian $\sigma$-linkage of $D$.

**Theorem 2.3** [9] For every fixed positive integer $p$ and every fixed nonnegative integer $w$ the hamiltonian linkage problem with input sequence $\sigma$ of $2p$ vertices for digraphs of directed tree-width at most $w$ is polynomial time solvable.

### 3 New Results on MinLOB

If $P$ is a directed path and vertices $a, b$ are, in that order, on $P$, then we denote the $a - b$-segment of $P$ by $P[a, b]$, and by $P[b, *]$ we mean the $b - t$-segment of $P$, where $t$ is the terminal vertex of $P$.

**Theorem 3.1** MinLOB is NP-hard for digraphs of directed path-width (directed tree-width, DAG-width, respectively) 1.

**Proof:** We prove the theorem by reduction of 3SAT to MinLOB. We use the following gadget $H$, the digraph with vertex set $V(H) = \{x_1, y_1, z_1, x_2, y_2, z_2\}$ and arc set $A(H) = \{x_1y_1, y_1z_1, z_1x_1, x_1x_2, y_1y_2, z_1z_2, x_2z_2, z_2y_2, y_2x_2\}$. It is easy to verify that $H$ has the following properties:

(i) there exists a hamiltonian $(x_1, x_2)$-linkage $P_x$ of $H$,
(ii) there exists a hamiltonian $(x_1, x_2, y_1, y_2)$-linkage of $H$,
(iii) there exists an hamiltonian $(x_1, x_2, y_1, y_2, z_1, z_2)$-linkage of $H$,
(iv) if $P_x$ is a hamilton path of $H$ starting at $x_1$ then $P_x$ ends in $x_2$,
(v) if $P_x$ and $P_y$ are vertex disjoint paths in $H$ starting at $x_1$ and $y_1$, respectively, which go through all vertices of $H$, then either $P_x$ ends in $x_2$ and $P_y$ ends in $y_2$, or $P_x$ ends in $y_2$ and $P_y$ ends in $z_1$.

Analogous statements hold for each permutation of $x, y, z$. 

4
Consider an instance $I$ of 3SAT with variables $v_1, v_2, \ldots, v_k$ and clauses $C_1, C_2, \ldots, C_p$. Construct a digraph $D = D(I)$ as follows: For each clause $C_j$ let $H_j$ be a copy of $H$. If $C = \alpha + \beta + \gamma$, where $\alpha, \beta$, and $\gamma$ are literals, denote the vertices of $H_j$ by $\alpha_1(H_j), \beta_1(H_j), \gamma_1(H_j), \alpha_2(H_j), \beta_2(H_j), \gamma_2(H_j)$. (Occasionally, when we do not wish to specify the variables $\alpha, \beta, \gamma$, we denote the vertices simply by $x_1(H_j), \ldots, z_2(H_j)$.) We also introduce a vertex $u_i$ for each variable $v_i$ and a root vertex $r$. So $V(D) = \{r, u_1, u_2, \ldots, u_k\} \cup \bigcup_{j=1}^{p} V(H_j)$, and $D$ is a graph of order $6p + k + 1$.

The arc set of $D$ consists of $\bigcup_{j=1}^{p} E(H_j)$, arcs $ru_i$ for $i = 1, 2, \ldots, k$ and the arcs in the sets $\text{Arc}(v^1), \text{Arc}(v^2), \ldots, \text{Arc}(v^k)$, $\text{Arc}(\overline{v}^1), \text{Arc}(\overline{v}^2), \ldots, \text{Arc}(\overline{v}^k)$ defined as follows.

Consider a variable $v^i$. Let $C_{j_1}, C_{j_2}, \ldots, C_{j_s}$, with $j_1 < j_2 < \ldots < j_s$, be the clauses containing $v^i$ as literal. Then the set $\text{Arc}(v^i)$ contains the arcs $u_i v^i_1(H_{j_1}), v^i_2(H_{j_2}) v^i_1(H_{j_2}), v^i_2(H_{j_3}) v^i_1(H_{j_3}), \ldots, v^i_2(H_{j_{s-1}}) v^i_1(H_{j_s})$. Similarly let $C_{h_1}, C_{h_2}, \ldots, C_{h_t}$, with $h_1 < h_2 < \ldots < h_t$, be the clauses containing $\overline{v}^i$ as literal. Then the set $\text{Arc}(\overline{v}^i)$ contains the arcs $u_i \overline{v}^i_1(H_{h_1}), \overline{v}^i_2(H_{h_2}) \overline{v}^i_1(H_{h_2}), \overline{v}^i_2(H_{h_3}) \overline{v}^i_1(H_{h_3}), \ldots, \overline{v}^i_2(H_{h_{t-1}}) \overline{v}^i_1(H_{h_t})$. This completes the construction of $D$. 

Figure 1: The gadget $H$ and construction of $D = D(I)$ from 3-SAT instance.
We prove that
\[ \text{dtw}(D) = \text{dagw}(D) = \text{dpw}(D) = 1 \]  
(1)

Since $D$ is not acyclic, by Lemma 2.1, every width parameter in (1) is positive and, by Lemma 2.2, it is enough to show that $\text{dpw}(D) \leq 1$. It can be easily checked that the following bags form a DPD of $D$ of width 1:

\[
\{r\}, \{u_1\}, \{u_2\}, \ldots, \{u_k\},
\{z_1(H_1), y_1(H_1)\}, \{y_1(H_1), x_1(H_1)\}, \{x_2(H_1), y_2(H_1)\}, \{y_2(H_1), z_2(H_1)\},
\ldots, \{z_1(H_p), y_1(H_p)\}, \{y_1(H_p), x_1(H_p)\}, \{x_2(H_p), y_2(H_p)\}, \{y_2(H_p), z_2(H_p)\}.
\]

We now show that $D$ has an out-branching with exactly $k$ leaves if and only if $I$ is satisfiable.

Given a valid truth assignment to $v^1, \ldots, v^k$ we construct an out-branching $B$ of $D$ with $k$ leaves as follows. Root $B$ at $r$. Let $ru_1, ru_2, \ldots, ru_k \in E(B)$. If variable $v^i$ has truth value TRUE then add all arcs in $\text{Arc}(v^i)$ to $A(B)$. Then these arcs, together with suitably (i.e., according to properties (i), (ii) and (iii) of $H$) chosen $v^i_1(H_j) - v^i_2(H_j)$ paths through those $H_j$ which correspond to the $C_j$ containing $v^i$ as a literal, yield a path $P(v^i)$ starting at $u_i$.

Similarly, if variable $v^i$ has truth value FALSE then add all arcs in $\text{Arc}(\overline{v^i})$ and suitably chosen $\overline{v^i_1(H_j)} - \overline{v^i_2(H_j)}$ paths to $A(B)$ and obtain a path $P(\overline{v^i})$ starting at $u_i$. Since these $k$ paths, attached to the vertices $u_1, \ldots, u_k$, go through all vertices in $V(D)$, $B$ is an out-branching of $D$ with exactly $k$ leaves.

Given an out-branching $B$ with exactly $k$ leaves of $D$, we derive an assignment of truth values to the variables $v^1, \ldots, v^k$ that satisfies each clause $C_j$ and thus $I$. We note that $B$ must be rooted at $r$ since $d^+_{\overline{P_i}}(r) = 0$ and that $ru_i \in A(B)$ for $i = 1, 2, \ldots, k$ since $d^+_{\overline{P_i}}(u_i) = 1$. So $d^+_{\overline{P_i}}(r) = k$, hence the subtree of $T$ rooted at $u_i$ is a path $P_i$ for $i = 1, 2, \ldots, k$.

Consider a subgraph $H_j$ of $D$. A path $P_i$ that intersects with $H_j$ is said to be $H_j$-compatible if $P_i$ enters $H_j$ at $x_1$ and leaves at $x_2$, or it enters $H_j$ at $y_1$ and leaves at $y_2$, or it enters $H_j$ at $z_1$ and leaves at $z_2$. We now show that $B$ can be modified, without changing the number of leaves, so that whenever a path $P_i$ and a gadget $H_j$ intersect, $P_i$ is $H_j$-compatible. Consider a fixed $H_j$. First assume that $P_i$ is the only path that intersects $H_j$. By property (iv) $P_i$ is $H_j$-compatible. Next assume that two paths, $P_h$ and $P_i$, say, intersect $H_j$ and that they enter $H_j$ in, say, $x_1$ and $y_1$, respectively. By property (v) either $P_h$ and $P_i$ are $H_j$-compatible, or $P_i$ ends in $z_1$ and $P_h$ ends in $y_2$. In the latter case let $P'_h$ be the union of $P_h[u_h, x_1]$ and the path $x_1, x_2,$
and let $P_i'$ be the union of $P_i[u_i, y_1]$, the path $y_1, z_1, z_2, y_2$ and $P_h[y_2, \ast]$, and replace $P_i$ and $P_i$ by $P_i'$ and $P_i'$. Finally assume that three paths $P_g, P_h, P_i$ intersect $H_j$. Then a similar construction yields $H_j$-compatible paths $P_g', P_h', P_i'$. Clearly, replacing $P_g, P_h, P_i$ by $P_g', P_h', P_i'$ if necessary does not change the number of leaves of $B$, nor does it create any incompatibilities. Hence repeating this step for all $H_j$ eventually yields an out-branching in which every path $P_i$ that intersects a gadget $H_j$ is $H_j$-compatible.

Note that vertex $u_i$ has two out-neighbors in $D$, $v_i'(H_{j_1})$ and $v_i'(H_{h_1})$, where $C_{j_1}$ ($C_{h_1}$) is the first clause to contain $v^i$ ($v^i$) as a literal, and that $T$ contains at most one of these arcs. If the first arc of $P_i$ is $u_i, v_i'(H_{j_1})$ then we assign the value TRUE to $v^i$, if the first arc of $P_i$ is $u_i, v_i'(H_{h_1})$ then we assign the value FALSE to $v^i$, and if $P_i$ has no arc we assign an arbitrary truth value to $v^i$. It remains to show that this satisfies $I$.

Fix an arbitrary clause $C_j$ and consider $H_j$. There is at least one path $P_i$ of the out-branching $B$ that intersects with $H_j$. Assume that the first arc of $P_i$ is, say, $u_i, v_i'(H_{j_1})$ (for $u_i, v_i'(H_{h_1})$ the proof is analogous) and that $P$ passes through $H_{j_1}, H_{j_2}, \ldots$ before reaching $H_j$. Since $P_i$ is compatible with $H_{j_1}, H_{j_2}, \ldots, H_j$, it enters $H_{j_1}, H_{j_2}, \ldots, H_j$ in $v_i'(H_{j_1}), v_i'(H_{j_2}), \ldots, v_i'(H_j)$. Hence clauses $C_{j_1}, C_{j_2}, \ldots, C_j$ contain $v^i$ as a literal. But since we assigned the value TRUE to $v^i$ clause $C_j$ is satisfied. Since $C_j$ was arbitrary, all clauses and thus $I$ are satisfied.

\[\square\]

**Theorem 3.2** Let $d \in \{\text{dag}, \text{dt}, \text{dp}\}$. For every fixed positive integer $k$ and every fixed nonnegative integer $w$, we can check, in polynomial time, whether a digraph $D$ with $\text{dw}(D) \leq w$ has an out-branching with at most $k$ leaves.

**Proof:** Let $D$ be a digraph. By Lemma 2.2, if $\text{dpw}(D) \leq w$ then $\text{dtw}(D) \leq w$. It is shown in [4] that if $\text{dagw}(D) \leq w$ then $\text{dtw}(D) \leq 3w + 1$.

Thus, we may assume that $D$ is of directed tree-width at most $w$, for some integer $w$, and let $B$ be an out-branching in $D$ with at most $k$ leaves. Let $X(B)$ be the set consisting of the root, the leaves and the branching vertices of $B$. It is not difficult to show that $|X(B)| \leq 2k$. Now contract each directed path of $B$ between two vertices of $X(B)$ into an arc (between the vertices of $X(B)$) and observe that we have obtained an out-tree $B'$ with exactly $|X(B)|$ vertices. We call $B'$ the contraction of $B$.

Now let $Y \subseteq V(D)$, $|Y| \leq 2k$, and let $T$ be an out-branching constructed on the vertices of $D[Y]$ with arcs $A(T) = \{(s_1, t_1), (s_2, t_2), \ldots, (s_{|Y| - 1}, t_{|Y| - 1})\}$. Notice here that the arcs of $A(T)$ may be not present in the digraph $D$. Using the algorithm of Theorem 2.3 with input $(s_1, t_1, s_2, t_2, \ldots, s_{|Y| - 1}, t_{|Y| - 1}),$
we can check, in polynomial time, whether $D$ contains an out-branching $B^*$ whose contraction is $T$.

Thus, to find an out-branching in $D$ with the minimum number of leaves, we can use the following procedure. We generate all subsets of $V(D)$ with at most $2k$ vertices and, for each such subset $Y$, we generate all out-branchings $T$ in $D[Y]$. For each $T$ we use the algorithm of Theorem 2.3 to verify whether $D$ has an out-branching whose contraction is $T$. Finally, we find a minimum leaf out-branching among all the outputs of the algorithm if one with at most $k$ leaves exists.

Observe that for each $Y$, by Cayley’s formula on the number of spanning trees in a complete graph, there are at most $|Y|^{|Y|-1}$ out-branchings of $D[Y]$ and that there are less than $|V(D)|^{2k+1}$ sets $Y$ with $|Y| \leq 2k$. Thus, in our procedure, we use the algorithm of Theorem 2.3 less than $|V(D)|^{2k+1} \cdot (2k)^{2k-1}$ times, which shows that the running time of the procedure is polynomial.

\[ \square \]

\section{Conclusions and Further Research}

The NP-hardness results of this paper and the recent papers [10, 11] allow us to conclude that only a relatively few NP-hard optimization problems on digraphs become tractable when restricted to digraphs of bounded directed width parameters. This is a sharp contrast to undirected graphs for which a relatively few NP-hard optimization problems remain NP-hard when restricted to graphs of bounded treewidth.

Moreover, the treewidth of the underlying undirected graph of a digraph appears to be a much more useful measure in algorithmic applications than directed width parameters, cf. [1, 5, 7]. This is clearly an unsatisfactory situation as the treewidth of the underlying undirected graph depends only on the underlying structure of a digraph, not on any directions of its arcs.

Certainly, development is needed of new, more algorithmically applicable width-like measures for digraphs that depend on directions of their arcs.

\textbf{Acknowledgements} We are grateful to the referees for a number of useful suggestions. The main results of this paper were obtained in summer 2008 when Dankelmann was visiting Royal Holloway, University of London. Research of Gutin and Kim was supported by an EPSRC grant.
References


