



**HAL**  
open science

## An $O(n.m)$ algorithm for calculating the closure of lca-type operators

Vincent Ranwez, Stefan Janaqi, Sylvie Ranwez

► **To cite this version:**

Vincent Ranwez, Stefan Janaqi, Sylvie Ranwez. An  $O(n.m)$  algorithm for calculating the closure of lca-type operators. *Ars Combinatoria*, 2012, 104, pp.107-128. hal-00797153

**HAL Id: hal-00797153**

**<https://hal.science/hal-00797153>**

Submitted on 5 Mar 2013

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# An $O(n \cdot m)$ algorithm for calculating the closure of *lca*-type operators

Vincent Ranwez<sup>1</sup>, Stefan Janaqi<sup>2</sup>, Sylvie Ranwez<sup>2</sup>

<sup>1</sup> Institut des Sciences de l'Evolution de Montpellier (ISE-M), UMR 5554 CNRS,  
Université Montpellier II, place E. Bataillon, CC 064, 34 095 Montpellier cedex 05, France.  
E-mail: vincent.ranwez@univ-montp2.fr

<sup>2</sup> LGI2P/EMA Research Centre, Site EERIE, Parc scientifique G. Besse, 30 035 Nîmes cedex 1, France.  
E-mail {sylvie.ranwez, stefan.janaqi}@mines-ales.fr}

**Abstract**— The least common ancestor on two vertices, denoted  $lca(x, y)$ , is a well defined operation in a directed acyclic graph (*dag*)  $G$ . We introduce  $U_{lca}(S)$ , a natural extension of  $lca(x, y)$  for any set  $S$  of vertices. Given such a set  $S_0$ , one can iterate  $S_{k+1} = U_{lca}(S_k)$  in order to obtain an increasing set sequence.  $G$  being finite, this sequence has always a limit which defines a closure operator. Two equivalent definitions of this operator are given and their relationships with abstract convexity are shown. The good properties of this operator permit to conceive an  $O(n \cdot m)$  time complexity algorithm to calculate its closure. This performance is crucial in applications where *dags* of thousands of vertices are employed. Two examples are given in the domain of life-science: the first one concerns genes annotations understanding by restricting Gene Ontology, the second one deals with identifying taxonomic group of environmental DNA sequences.

**Keywords**—Directed acyclic graph, Least common ancestor, Greatest common descendant, Closure operator, Abstract Convexity.

## 1 INTRODUCTION

In this paper we address the problem of efficiently computing the closure of *lca*-type operators in directed acyclic graphs (*dag*)  $G = (V, E)$ . Such graphs appear in numerous applications such as: ontologies (semantic representation), phylogeny networks (speciation histories) or inheritance graphs (object programming languages). A *least common ancestor* of two vertices  $x$  and  $y$ , denoted  $lca(x, y)$ , is an ancestor of both vertices, that has no proper descendant that is also an ancestor of  $x$  and  $y$ . Now, let  $S$  be a set of vertices of interest of  $G$ . On one side, the set  $V$  of all vertices contains all  $lca(x, y)$  for any couple  $x, y \in S$  but, this does not help to focus on relevant parts of  $G$  containing  $S$ . On the other side, filtering  $G$  to keep only vertices of  $S$  gives few insight about the relationships between vertices of  $S$ . In order to preserve those relationships, one can consider the *least overset*  $\bar{S}$  of  $S$ , that contains all  $lca(x, y)$  for any  $x, y \in \bar{S}$ . For people used to convexity concepts, this sounds like: "... for any two points in  $\bar{S}$ , the segment relying them lies in  $\bar{S}$ ". Actually, we show that it does not just "sounds as" and we define a set  $\bar{S}$  that really satisfies this property. First we define the operator:

$$U_{lca}(S) = \bigcup_{x,y \in S} lca(x, y).$$

Then, we show that the closure of this operator, denoted by  $\bar{S}$  verifies the four axioms of convex hull (see [1]):

- (U.1)  $\bar{\emptyset} = \emptyset, S \subseteq \bar{S}$ ;
- (U.2) (monotonicity)  $S_1 \subseteq S_2, \bar{S}_1 \subseteq \bar{S}_2$ ;
- (U.3) (idempotence)  $\overline{\bar{S}} = \bar{S}$ ;
- (U.4) (finiteness) if  $x \in \bar{S}$ , then there is a finite set  $F \subseteq S$  such that  $x \in U_{lca}(F)$ .

The sets  $S$  that are equal to their closure ( $S = \bar{S}$ ) are called convex and form a convex space verifying the following properties (this is a classical result of convexity theory):

- (C.1)  $\emptyset, V$  are convex;
- (C.2) if  $A, B$  are convex, then  $A \cap B$  is convex;
- (C.3) if  $A_i$  are convex and  $A_i \subseteq A_{i+1}$  for  $i = 1, 2, \dots$  then  $\bigcup_{i \geq 1} A_i$  is convex;

Thus,  $U_{lca}(S)$  and its closure have nice mathematical structures that are exploited in our greedy algorithm to reach a low time complexity of order  $O(n \cdot m)$ . Starting with a set  $S_0$  of vertices and the topological order of  $V$ , the algorithm decides once for all if a new vertex  $v$  is in the  $U_{lca}$  - closure of  $S_0$  or not. It is

easy to define and calculate similarly the  $U_{gcd}$  – closure (Greatest Common Descendant). One has just to reverse all the edges of  $G$  and apply the  $U_{lca}$  results and algorithm.

Of course, the operator  $lca(x, y)$  is not new and there are several good algorithms to calculate it. To the best of our knowledge, all the efficient approaches to calculate  $lca(x, y)$  pass through the computation of shortest paths. The main result of [2] is that, for any couple of vertices  $x, y$ , a *representative lca* can be computed with time complexity  $O(|V|^\omega)$  with  $\omega = 2.688$  (see [2, 3]). We stressed the word ‘representative’ because a couple of vertices can have more than one *lca* and, as shown further, one of the main characteristics of our algorithm is that it identifies *all* of them. Yet, the construction of [2] is interesting on its own, since it transforms the *lca* searching to a shortest path problem. An improved version of the “one representative *lca*” algorithm is given with  $\omega = 2.575$  (see [4]). This optimization relies on a novel reduction of all-pairs *lca* problem to the problem of finding maximum witnesses for Boolean matrix product. As the domain is active, actually [5] have given an algorithm that calculates *all lca(x, y)* for *all* pairs of vertices with a mean time complexity  $O(|V|^3 \log \log(|V|))$  and worst time complexity  $O(|V|^{3.3399})$ .

Remind that we need the  $U_{lca}$  – closure of a set  $S$  (denoted by  $\bar{S}$ ) and a straightforward way to use the above subroutines would have a complexity of at least  $O(|V|^{3.3399})$  for computation time and  $O(|V|^2)$  for memory space (in order to store pre-computed *lca*). Our algorithm doesn’t need to calculate *lca(x, y)* for any couple of vertices  $x, y$ . It constructs  $\bar{S}$  by using the closure and convexity axioms above, in particular (U.2), (U.3) and (C.2), (C.3). This solution has lower time –  $O(|\bar{S}||E|)$  – and space –  $O(|\bar{S}||V|)$  – complexity. The advantage of this solution is even more relevant in practice, since for most real cases  $|\bar{S}| \ll |V|$  and for most *dag*  $|E| \ll |V|^2$ .

The paper is organized as follows: section 2 gives the definitions and properties of  $U_{lca}$  – closure; section 3 gives the algorithm to efficiently compute this closure and its proof of correctness; applications of our results are provided in section 4; concluding remarks are given in section 5.

## 2 LEAST COMMON ANCESTOR OPERATOR AND ITS CLOSURE

### 2.1 Preliminary definitions

In this section, we give the definitions of two generalized common operators: *least common ancestor (lca)* and *greatest common descendant (gcd)* for a *direct acyclic graph (dag)*. The following definitions are provided to make the paper self-contained. For further definitions on graphs see [6]. Given a *dag*  $G = (V, E)$  and an edge  $(x, y)$  we say that  $x$  is the *child* and  $y$  is the *father*. The *indegree*  $d_G^-(v)$  (*outdegree*  $d_G^+(v)$ ) of a vertex  $v$  is the number of edges with head  $v$  (tail  $v$ ). When  $G$  contains a directed  $(v, u)$ -path, the vertex  $u$  is said to be an *ancestor* of  $v$  and the vertex  $v$  is a *descendant* of  $u$ . For a non-empty subset  $W$  of  $V$ , the subgraph of  $G$  whose vertex set is  $W$  and whose edge set is the set of edges of  $G$  that have both ends in  $W$  is called the subgraph of  $G$  *induced* by  $W$  and is denoted  $G[W]$ .

Given a vertex  $v$  of the *dag*  $G = (V, E)$ , the set  $A_G(v)$  denotes the subset of *ancestors* of  $v$  in  $G$ . The generalization of this definition to a set  $S \subseteq V$  of vertices is straightforward, i.e.  $A_G(S) = \bigcap_{v \in S} A_G(v)$ . For simplicity, we will omit index  $G$  from the notations whenever there is no ambiguity.

**Definition 2.1.1. [2]** The *least common ancestors*  $lca(S)$  of a vertex subset  $S \subseteq V$  with respect to a *dag*  $G = (V, E)$  are the vertices  $u \in A(S)$ , such that  $d_H^-(u) = 0$  in the graph  $H = G[A(S)]$  induced by  $A(S)$ .

This definition generalizes the widely known concept of least common ancestor (see [2, 3]) for a couple of vertices, i.e.  $lca(\{x, y\}) = lca(x, y)$ . This is sometimes called *least common semi-strict ancestors* [7]. It follows immediately from Definition 2.1.1 that  $x = lca(x, y)$  if there is a directed  $(y, x)$ -path. By extension, we define  $lca(x, x) = x$  for all  $x$ .

Note that, unless the *dag*  $G$  is a tree,  $lca(x, y)$  may contain several nodes and the existence of a pair of nodes  $x, y \in S$  such that  $lca(x, y) = lca(S)$  is not guaranteed. For instance, in the example presented in Fig. 1,  $lca(\{C1, C2, C3\}) = \{A1, A2\}$  while  $lca(C1, C2) = \{B1, A2\}$ ,  $lca(C1, C3) = B2$  and  $lca(C2, C3) = \{A1, B3\}$ .

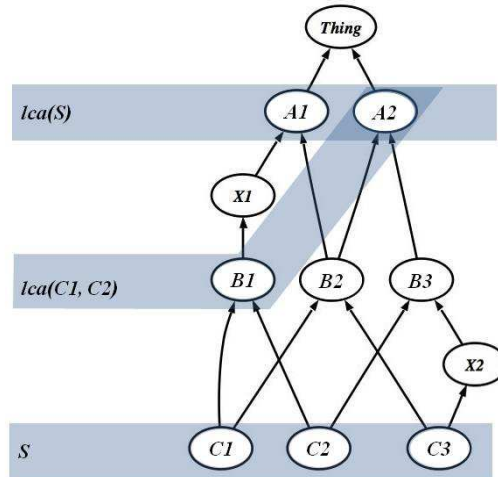


Fig. 1. Illustration<sup>1</sup> of the  $lca$  operator

An alternative definition of the  $lca$  in terms of partially ordered sets, has been proposed by [8].

## 2.2 Two equivalent definitions of $U_{lca}$ -closure in a dag

Closure operators are widely used in mathematics, especially in geometry. The best known example comes from convexity in a Euclidian space. A lot of properties follow from the fact that a convex set, for example a convex polygon, can be obtained by giving a *finite* set of points and the segment operator  $s(x, y)$ . A natural question is whether these geometric properties are preserved when extending convexity definition to graphs. It turns out that with a little set of axioms, a lot of good properties of convexity ([1, 9, 10]) can be transposed in discrete structures like graphs. The richest transposition is obtained for graphs endowed with interval convexities where the notion of segment  $s(x, y)$  is replaced by that of interval  $I(x, y)$  that is the bunch of the shortest paths between  $x$  and  $y$  in the given graph (see [10]). It is out of the scope of this paper to explore these properties. Nevertheless, the definition of closure and its properties show clearly that these objects are convex.

In the previous section, we provided an intuitive and natural definition of the least common ancestors of a set of vertices denoted as  $lca(S)$ . Yet, in applications, when considering a set of vertices  $S$ , every least common ancestor of a pair of vertices of  $S$  is a key vertex to gain insight into relationships among vertices of  $S$ . We thus now introduce a new operator that makes use of the  $lca$  operator and generalizes it to a well defined closure operator.

**Definition 2.2.1.** Let  $S$  be a subset of vertices of  $G$ . The  $U_{lca}$  - operator on  $S$  is defined as:

$$U_{lca}(S) = \bigcup_{x, y \in S} lca(x, y) \quad (1)$$

It follows from this definition that  $S \subseteq U_{lca}(S)$  and that the  $U_{lca}$  - operator is monotonous, i.e.:

$$A \subseteq B \Rightarrow U_{lca}(A) \subseteq U_{lca}(B).$$

The Fig. 2 below illustrates the definition of the  $U_{lca}$  - operator and emphasizes its difference with the standard  $lca$  operator. In this example, given the set  $S = \{C1, C2, C3\}$ ,  $U_{lca}(S) = \{B1, B2, B3, C1, C2, C3\}$ , while  $lca(S) = \{A1, A2\}$ .

In some cases, having only  $U_{lca}(S)$  and/or  $lca(S)$  is not enough to understand all relationships among vertices of  $S$ . Such a case is depicted in Fig. 3, where the vertex  $A$  is helpful for understanding

<sup>1</sup> Figures were created using GraphViz, version 2.26 <http://www.graphviz.org/>

$C1$  and  $C2$  relationships but is neither included in  $U_{lca}(S)$  nor in  $lca(S)$ . Vertex  $A$  is of interest since  $A$  is the  $lca$  of  $B1$  and  $B2$ , which in turn are  $lca$  of two vertices of  $S$ . This leads us to the following definition of the  $U_{lca}$  - closure of  $S$ .

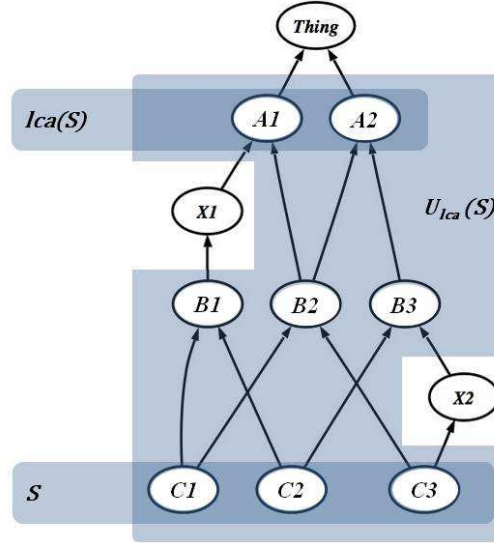


Fig. 2.  $U_{lca}$  and  $lca$  are two different operators.

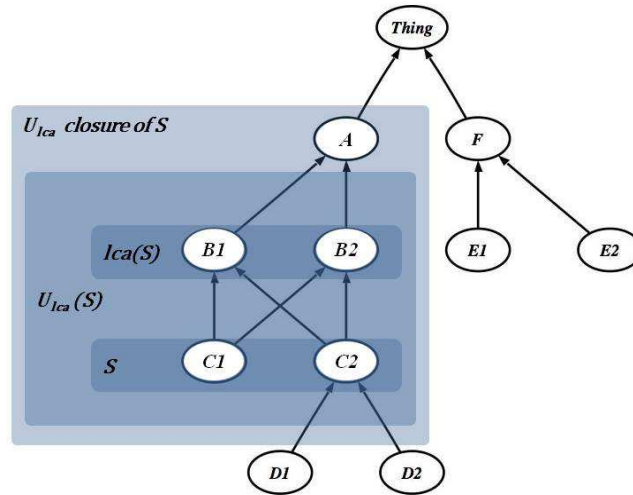


Fig. 3. Illustration of  $U_{lca}$  - closure

Let  $S$  be a subset of vertices of  $G$  and let consider the increasing set sequence defined by:

$$S_0 = S \text{ and } S_{i+1} = U_{lca}(S_i), i = 0, 1, \dots$$

Since  $G$  is finite and  $\forall i S_i \subseteq S_{i+1}$ , there is a number  $c, 0 \leq c \leq |V|$  such that  $\forall k \geq c, S_k = U_{lca}(S_k)$ . This fixpoint (or fixset) is reached because of the monotonicity of  $U_{lca}$  - operator. In fact, once this relation holds for a given  $k$  it holds for all greater values. So,  $c$  and  $S_c$  are well defined.

**Definition 2.2.2.** The number  $c$  is the *closure index* and the set  $S_c$  is called the  $U_{lca}$  - closure of  $S$  and is denoted by  $\bar{S}$ .

It is clear from the **Definition 2.2.1** that  $U_{lca}(\emptyset) = \emptyset$  and  $S \subseteq U_{lca}(S)$ . Also,  $U_{lca}$  is monotonous and it verifies the finiteness property because  $G$  is finite. Since U.1, U.2 and U.4 hold for the  $U_{lca}$  – operator, they also hold for its closure. Moreover, by definition of the closure,  $\bar{S} = S_c = U_{lca}(S_c) = U_{lca}(\bar{S})$ , therefore the idempotence axiom U.3 is also satisfied.

This definition provides a simple (and inefficient!) iterative algorithm to compute  $U_{lca}$  – closure. The time complexity of this algorithm is related to the closure index. In the simple case when  $G$  is a tree, the closure index cannot be greater than 1. The following lemma shows that this is no longer true in the general case.

**Lemma 2.2.1.** For a dag  $G = (V, E)$  and a set  $S \subseteq V$ , the number of iterations needed to obtain  $\bar{S}$  is  $O(|V|)$ .

**Proof.** It is clear that  $S_k$  increases with at least one vertex at each iteration, hence proving that  $c \leq (|V| - |S|)$ . On the other hand, as shown by the example below,  $c$  can be as large as  $(|V| - |S|)/2$ . It follows that the number of iterations needed to obtain  $\bar{S}$  is  $O(|V|)$ .

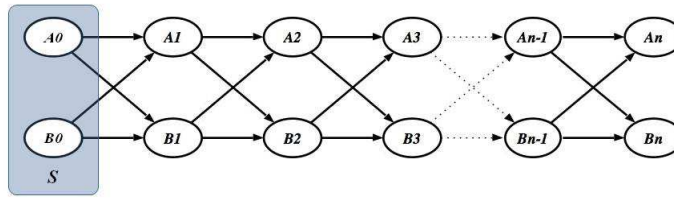


Fig. 4. The closure index can be proportional to  $|V|$ .  
 $S_0 = \{A_0, B_0\}$ , at iteration  $k$  two vertices  $\{A_k, B_k\}$  are added so that  $S_k = \{A_0, \dots, A_k, B_0, \dots, B_k\}$ .

There is an alternative (descending) way to define  $U_{lca}$  – closure. For this, let the family of  $U_{lca}$  – closed sets containing  $S$  be denoted by:

$$\mathcal{L}(S) = \{L \subseteq V \mid S \subseteq L \text{ and } L = U_{lca}(L)\} \quad (2)$$

Now, we show that the family  $\mathcal{L}(S)$  verifies the axioms C.1, C.2 and C.3. The axiom C.1 is obvious from the definition. The axiom C.3 is conceived originally in order to treat the case of infinite increasing set sequences in continuous spaces. As we are dealing with finite graphs, this axiom is obviously verified. Nevertheless, it is the basis of our greedy algorithm because, when treating the increasing set sequence of  $U_{lca}$  – closed sets, only the last one has to be stored for further treatment. The following lemma gives the proof of axiom C.2.

**Lemma 2.2.2.**  $\mathcal{L}(S)$  is non-empty and closed for the intersection, i.e.  $M, N \in \mathcal{L}(S) \Rightarrow M \cap N \in \mathcal{L}(S)$ .

**Proof.**  $\mathcal{L}(S)$  is non-empty since  $V$  obviously belongs to  $\mathcal{L}(S)$ . Let us now prove that  $M, N \in \mathcal{L}(S) \Rightarrow M \cap N \in \mathcal{L}(S)$ .

- $S \subseteq M \cap N$ . As  $S \subseteq M$  and  $S \subseteq N$ ,  $S \subseteq M \cap N$ .
- $M \cap N = U_{lca}(M \cap N)$ .
  - $M \cap N \subseteq U_{lca}(M \cap N)$ , by the  $U_{lca}$  definition.
  - $U_{lca}(M \cap N) \subseteq M \cap N$ . This comes from the fact that the  $U_{lca}$  preserves monotonicity:
$$M \cap N \subseteq M \Rightarrow U_{lca}(M \cap N) \subseteq U_{lca}(M) = M$$

$$M \cap N \subseteq N \Rightarrow U_{lca}(M \cap N) \subseteq U_{lca}(N) = N$$

$$U_{lca}(M \cap N) \subseteq M \text{ and } U_{lca}(M \cap N) \subseteq N \Rightarrow U_{lca}(M \cap N) \subseteq M \cap N. \quad \square$$

**Definition 2.2.3.** The  $U_{lca}$  – closure of  $S$  is the set  $\bar{S} = \bigcap_{M \in \mathcal{L}(S)} M$ .

**Lemma 2.2.3.** The two above definitions of  $U_{lca}$  - closure are equivalent.

**Proof.** One need to show that  $\bar{\bar{S}} = \bar{S}$ .

- $\bar{\bar{S}} \subseteq \bar{S}$ . By definition,  $\bar{S} = U_{lca}(\bar{S})$ , furthermore the monotonicity of the set sequence  $S_0, S_1, \dots, \bar{S}$  ensures that  $S \subseteq \bar{S}$ . Therefore  $\bar{S} \in \mathcal{L}(S)$ , thus proving that  $\bar{\bar{S}} \subseteq \bar{S}$ .
- $\bar{S} \subseteq \bar{\bar{S}}$ . By definition,  $S$  is included in every set of  $\mathcal{L}(S)$  and thus in their intersections. It follows that  $S_0 \subseteq \bar{\bar{S}}$ , and therefore  $U_{lca}(S_0) \subseteq U_{lca}(\bar{\bar{S}})$ , which can be rewritten  $S_1 \subseteq \bar{\bar{S}}$ . Applying the  $U_{lca}$  operator to both terms leads to  $S_2 \subseteq \bar{\bar{S}}$ ,  $S_3 \subseteq \bar{\bar{S}}$  and so on until  $S_c \subseteq \bar{\bar{S}}$ , thus proving that  $\bar{S} \subseteq \bar{\bar{S}}$ .  $\square$

These definitions and properties provide the framework for our algorithm.

### 3 AN EFFICIENT ALGORITHM TO COMPUTE $U_{lca}$ - CLOSURE

In our applications, we have encountered *dag*s that may contain several thousand of vertices. Thus, efficient algorithms are needed to compute the  $U_{lca}$  - closure. As mentioned in introduction, several good algorithms exist to retrieve all the vertices  $v \in lca(x, y)$ . When calculating the  $U_{lca}$  - closure, one could use one of these algorithms as a subroutine. This approach, detailed below, provides a straightforward solution to calculate the  $U_{lca}$  - closure and a (high) upper bound on time complexity. Then, we introduce an optimized solution that takes advantages of convexity properties and topological vertex order. The main result is an algorithm with a worst time complexity of order  $O(|\bar{S}||E|)$ .

#### 3.1 Straightforward algorithm to compute $U_{lca}$ - closure

```

Name: Straightforward_  $U_{lca}$ _closure
Input: a dag  $G$  and a set of nodes  $S$  of  $G$ .
Result:  $\bar{S}$ .
 $S_k \leftarrow S; S_{new} \leftarrow S;$ 
do
   $S_{tmp} \leftarrow S_k;$ 
  for each  $(x, y) \in S_k \times S_{new}$ 
     $S_{tmp} \leftarrow S_{tmp} \cup lca(x, y);$ 
  end
   $S_{new} \leftarrow S_{tmp} - S_k;$ 
   $S_k \leftarrow S_{tmp};$ 
while  $S_{new} \neq \emptyset$ 
return  $S_k$ 

```

Algorithm 1. A straightforward  $U_{lca}$  - closure algorithm

In Algorithm 1 the  $lca$  of each couple of vertices of  $\bar{S}$  is computed once leading to  $O(|V|^2)$  calls of the  $lca(x, y)$  subroutine. It follows that the time complexity of this algorithm is bounded by the preprocessing of the *dag* that allows obtaining the  $lca$  of two nodes in constant time. As mentioned in the introduction, the best known solution to this pre-process problem has a  $O(|V|^{3.3399})$  worst time complexity and requires  $O(|V|^2)$  memory space.

#### 3.2 Optimized algorithm to compute $U_{lca}$ - closure in $O(|\bar{S}||E|)$

This subsection details an optimized algorithm that determines  $\bar{S}$  for a *dag*  $G = (V, E)$  in  $O(|\bar{S}||E|)$  time complexity. The key idea of this greedy algorithm is that, though there are  $O(|V|^2)$  couples of vertices, at most  $O(|V|)$  nodes can be added to  $S$ . Rather than computing  $lca$  for each pair of vertices, our greedy algorithm considers each node and decide whether or not it must be added to  $\bar{S}$ . This can

be done efficiently by taking a topological vertex order induced by the *dag*.

<p><b>Name:</b> postOrder  <b>Input:</b> a <i>dag</i> <math>G</math>  <b>Result:</b> the list of nodes of <math>G</math> in postOrder  <math>G.postOrder \leftarrow</math> empty list  <b>for</b> <math>root</math> <b>in</b> <math>G.nodes()</math>              <b>if</b> <math>root</math> has no parent                  postOrderRec(<math>root</math>)  <b>end</b>  <b>return</b> <math>G.postOrder</math></p>	<p><b>Name:</b> postOrderRec  <b>Input:</b> a <i>dag</i> <math>G</math>, a node <math>n</math> of <math>G</math>  <b>Result:</b> add the list of desc(<math>n</math>), in post order, to the postOrder list of <math>G</math>              mark <math>n</math> as visited              <b>for</b> <math>s</math> <b>in</b> children(<math>n</math>)                  <b>if</b> <math>s</math> has not been visited                      postOrderRec(<math>s</math>)  <b>end</b>              append <math>n</math> to the postOrder list of <math>G</math></p>
--	---

Algorithm 2. Post order implementation.

Our  $U_{lca}$  - closure algorithm considers vertices in *post order*, i.e. a vertex is never considered before considering all of its descendants. Indeed, vertices of a *dag* can be ordered along a horizontal line such that all descendants of a vertex are placed to its left. We call this a *post order* since, as shown in [11], one can be efficiently obtained using the post-order indices of a depth-first search. We give this classical ordering algorithm (Algorithm 2) below to make the paper self-content.

<p><b>Name:</b> <math>U_{lca}</math> - closure  <b>Input:</b> a <i>dag</i> <math>G</math>, a set <math>S</math> of vertices.  <b>Result:</b> <math>S^{AL} = \bar{S}</math>.  <math>S^{AL} \leftarrow \emptyset</math>  <math>P = postOrder(G)</math>  <b>for</b> <math>n</math> <b>in</b> <math>P</math>              <math>S^D(n) \leftarrow \emptyset</math> // <math>S^D(n)</math> is the set of descendants of <math>n</math> present in <math>\bar{S}</math>              <math>maxS^D(n) \leftarrow 0</math> // <math>maxS^D(n)</math> is the maximal value <math> S^D(s) </math> with <math>s</math> a child of <math>n</math>              <b>for</b> <math>s</math> <b>in</b> children(<math>n</math>)                  <math>S^D(n) \leftarrow S^D(n) \cup S^D(s)</math> (*)                  <math>maxS^D(n) \leftarrow \max( S^D(s) , maxS^D(n))</math>              <b>end</b>              <b>if</b> ( <math>(n \in S)</math> OR ( <math> S^D(n)  &gt; maxS^D(n)</math> ) ) (**)                  <math>S^D(n) \leftarrow S^D(n) \cup \{n\}</math>                  <math>S^{AL} \leftarrow S^{AL} \cup \{n\}</math>              <b>end</b>  <b>end</b>  <b>return</b> <math>S^{AL}</math></p>
---

Algorithm 3. Computation of  $U_{lca}$  - closure

**Proposition 3.2.1.** (*Proof of correctness*). Given the inputs  $G = (V, E)$  and  $S$ , the set  $S^{AL}$  returned by Algorithm 3 is the closure of  $S$  with respect to  $G$ , that is  $S^{AL} = \bar{S} = \bar{S}$ .

**Proof.** Let  $P$  denote the array of nodes of  $G$  sorted by the postOrder function. The  $U_{lca}$  - closure algorithm goes through  $P[1], \dots, P[k], \dots, P[|V|]$  gathering, for each  $k$ , a subset of  $S^{AL}$  denoted  $S^{AL}(k)$ . It is clear that  $S^{AL} = S^{AL}(|V|)$ . We show by induction that:

$$S^{AL}(k) = \bar{S} \cap P[1..k] \text{ and} \\ S^D(P[k]) = \bar{S} \cap desc(P[k]), k = 1, 2, \dots, |V|. \quad (3)$$

In other words we want to show that  $\bar{S}$  is constructed as an increasing sequence. Each term  $S^{AL}(k)$  of this sequence is closed in the subgraph of  $G$  induced by the nodes  $\{P[1], \dots, P[k]\}$ . In fact, it cannot contain vertices that are in  $\{P[k+1], \dots, P[|V|]\}$ . The axiom C.3 says that when taking the union of



these terms, the result is the last one.

**The statement (3) holds for  $k = 1$ .**

Node  $P[1]$  has no descendant. It is kept in  $S^{AL}$  if and only if  $P[1] \in S \subseteq \bar{S}$  (the line (\*\*)) of the algorithm.) Thus,  $S^{AL}(1) = \bar{S} \cap P[1..1]$  and  $S^D(P[1]) = \bar{S} \cap desc(P[1])$ .

**Assuming that (3) holds for  $1, \dots, (k - 1)$ , then it also holds for  $k$ .**

Let  $n = P[k]$  be the current node and  $\{s_1, \dots, s_p\}$  be the set of immediate descendants (children) of  $n$ . Since nodes are considered in post order, all children of  $n$  are at the left of  $n$  in array  $P$ . When the algorithm is considering  $n$ , all of its children  $s_1, \dots, s_p$  have already been treated and set  $S^D(s_i)$  has been recorded for each  $s_i \in \{s_1, \dots, s_p\}$ . At the point (\*\*), the current recorded set for node  $n$  (see point (\*\*)) is:

$$S^D(n) = S^D(s_1) \cup \dots \cup S^D(s_p) \quad (4)$$

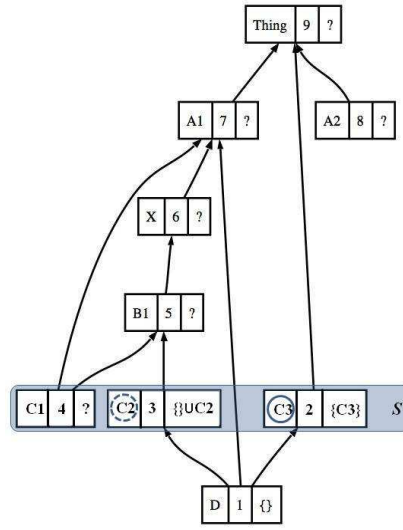


Fig. 5.  $U_{lca}$  - closure algorithm: considering a node of  $S$ .

For each node  $n$ , the 3 following characteristics are displayed: its label, its rank in the postOrder vector and its current set  $S^D(n)$ . This figure shows the information available at the point (\*\*) when processing the node  $C2$  (dotted circle). At this step the two sets  $S^D(D)$  and  $S^D(C3)$  have already been computed. The other  $S^D$  sets are not yet initialized (marked with '?').  $C3$  has been identified as part of  $\bar{S}$  (represented by a circle around it) and the algorithm is considering whether or not  $C2$  belongs to  $\bar{S}$ . Since  $C2 \in S$  the test line (\*\*) returns true and  $C2$  will be included into  $\bar{S}$ .

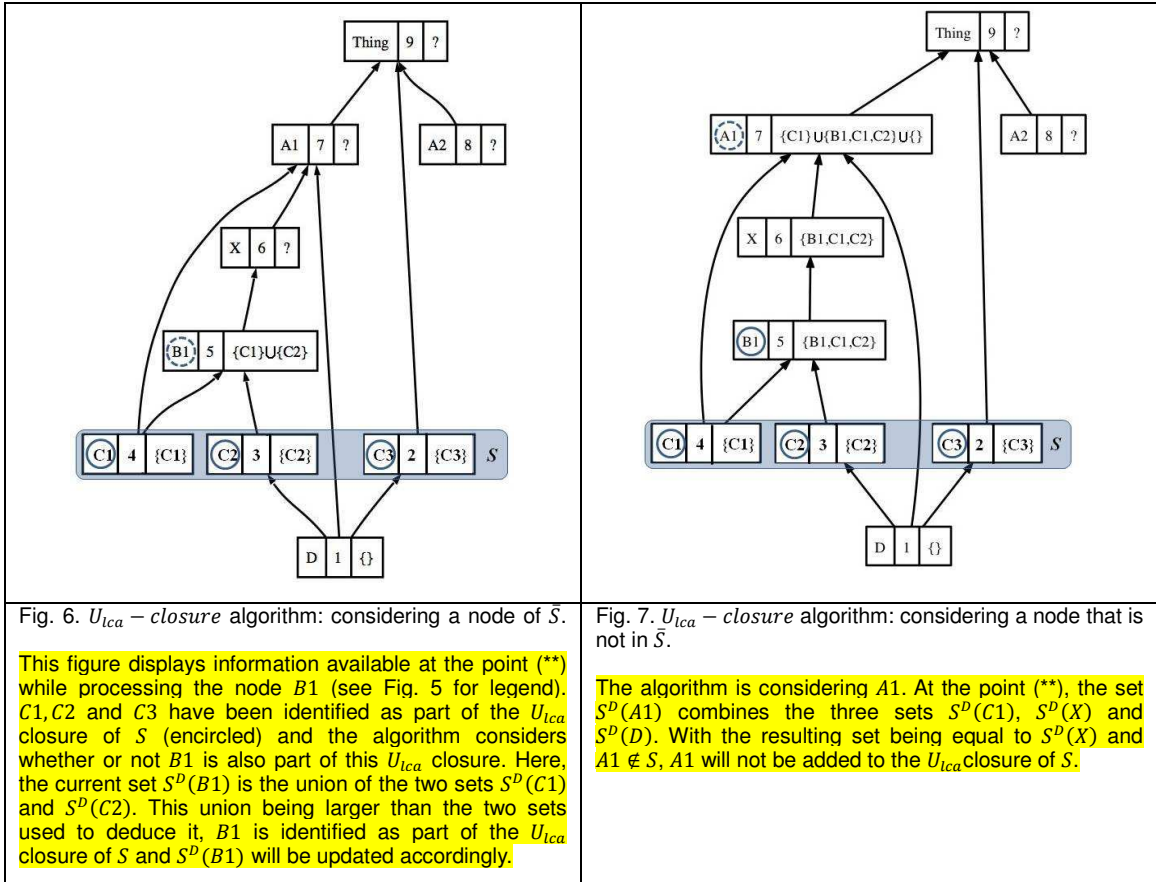
The test at the point (\*\*) of the algorithm is used to decide whether or not  $n$  is in the closure and should be added to  $S^D(n)$  and to  $S^{AL}$ .

- **Case  $n \in S$ .**  $n$  is added to  $S^{AL}(k)$  as well as to  $S^D(n)$  and evidently  $n \in \bar{S} \cap P[1..k]$  and  $S^D(P[k]) = \bar{S} \cap desc(P[k])$  (see Fig. 5 for an example).
- **Case  $n \notin S$ .** In this case, assuming the induction hypothesis, at the point (\*\*), all the nodes of  $S^D = S^D(s_1) \cup \dots \cup S^D(s_p)$  are in  $\bar{S}$  and  $S^D = S^D(n) - \{n\} = \bar{S} \cap desc(n)$ . The only thing remaining to prove is that  $n$  will be included in  $S^{AL}(k)$  and in  $S^D(n)$  if, and only if, it is the least common ancestor of two nodes of  $S^D$ .
  - **If  $(|S^D(n)| > \max S^D(n))$  then there are at least two nodes  $z, t$  of  $S^D$ , such that  $n = lca(z, t)$  and  $n$  should be added to  $S^{AL}(k)$  as well as to  $S^D(n)$ .** (see Fig. 6 for an example.)  
**As  $|S^D(n)| > \max S^D(n)$ , there are at least two nodes  $z, t \in S^D$  such that  $\{z, t\} \not\subseteq S^D(s_i)$ ,  $i =$**

1, ..., p. It follows that there are two distinct children  $s_i, s_j$  of  $n$  such that  $z \in S^D(s_i)$ ,  $t \in S^D(s_j)$ . By definition of the  $lca$ ,  $n \in lca(z, t)$  if and only if,  $n \in A(z, t)$  and  $n$  has no descendant in the ancestors set  $A(z) \cap A(t)$ . The former assertion is obvious, let us prove the latter by supposing that this is not the case (*reductio ad absurdum*). So, there is a node  $n' \in A(z) \cap A(t)$  and a  $(n, n')$  directed path in  $G$ . This path necessarily goes through a child  $s_m$  of  $n$  and, according to the induction hypothesis,  $S^D(s_m) = \bar{S} \cap desc(s_m)$ . It follows that  $\{z, t\} \subseteq S^D(s_m)$ , which is impossible.

- **If the test (\*\*) is not true, then  $n$  is not in the closure and is added neither to  $S^D$  nor to  $S^{Al}$ .** (see Fig. 7 for an example.)

The main thing to prove is that when  $|S^D(n)| = \max S^D(n)$ , there are not two nodes  $z, t$  of  $S^D(n)$  such that  $n = lca(z, t)$ . (see Fig. 7 for an example). **As  $|S^D(n)| = \max S^D(n)$  then there is some  $i \in \{1, \dots, p\}$  such that  $S^D(n) = S^D(s_i)$ .** In this case,  $n$  cannot be the  $lca$  of a couple of nodes  $(z, t)$  because the node  $s_i$  is (by construction) an ancestor of  $z, t$  and a descendant of  $n$ . It follows that  $n \notin \bar{S}$  and the proof is complete.  $\square$



**Proposition 3.2.2.** (Time complexity of  $U_{lca}$  - closure algorithm) For a node set  $S$  in a dag  $G = (V, E)$ , the  $U_{lca}$  - closure algorithm runs in  $O(|\bar{S}||E|) = O(|V||E|)$ .

**Proof.** Obtaining the postorder vector of nodes is done through a classical depth first search traversal of the graph in  $O(|E|)$ . The complexity of the remaining part of the algorithm, made of two nested for loops, is obviously determined by the number of executions of line (\*). This line computes the union of two sets of at most  $|\bar{S}|$  elements and is executed for every child of every node, i.e.  $O(|E|)$  times. It follows that the overall complexity of this algorithm is  $O(|\bar{S}||E|)$ .  $\square$

**Proposition 3.2.3.** (Space complexity of  $U_{lca}$  - closure algorithm) For a node set  $S$  in a dag  $G = (V, E)$ ,

the  $U_{lca} - closure$  algorithm requires  $O(|\bar{S}||V|) = O(|V|^2)$  memory space.

**Proof.** For each node, a subset of  $\bar{S}$  is stored. In the worst case,  $|\bar{S}| = |V|$  leading to a complexity of  $O(|V|^2)$ .

Note that in most real cases  $|\bar{S}| \ll |V|$ . Moreover, when all the parents of a node  $n$  have been treated, the subset of  $\bar{S}$  attached to  $n$  becomes useless. As a consequence, some memory space can be freed. This can be easily done by maintaining a counter for each node initialized to its number of parents. When treating a node, the counters of all of its children are decreased by one, and when a child reaches a zero value its memory is freed. This does not reduce the worst case complexity, since this optimization is useless when the *dag* is made of one node that has  $|V| - 1$  children, but it significantly reduces the memory space needed in real applications.

### 3.3 Building a relevant excerpt of a *dag* from a subset of its vertices

When searching for the least relevant overset  $\bar{S}$ , the  $U_{lca} - closure$  algorithm described above provide an efficient solution to identify them. Our set of relevant nodes is  $S_r = \bar{S}$ .

Then, one may need to extract the corresponding excerpt of the *dag*. This reduced *dag* can be seen as a dedicated “view” of the largest *dag* and can be used to speed up further analysis or to allow end user interaction/visualization related to the task. This “relevant *dag* excerpt” must preserve the partial order among vertices of  $S_r$  that is induced by the whole original *dag* even though some intermediary nodes have not been kept in  $S_r$ . More formally, given the *dag*  $G = (V, E)$  and a subset  $S_r$  of  $V$ , we define the relevant *sub-dag*  $G_r = (V_r, E_r)$  as:

- $V_r = S_r$
- $(u, v) \in E_r$  iff there is a directed path in  $G$  going from  $u$  to  $v$  without crossing any nodes of  $V_r$ .

The set  $E_r$  of edges can be efficiently computed thanks to the topological order induced by the *dag*. This time we will consider a vertex  $u$  only after having considered all of its ascendants. Such an order, that we will call a *pre order*, can be obtained by considering the post order vector from tail to head.

<p><b>Name:</b> relevantDagExcerpt</p> <p><b>Input:</b> a <i>dag</i> <math>G = (V, E)</math> a set <math>S_r</math> of relevant nodes</p> <p><b>Result:</b> <math>G_r = (V_r, E_r)</math> the relevant <i>dag</i> excerpt.</p> <p><math>V_r \leftarrow S_r; G_r \leftarrow (V_r, \emptyset)</math></p> <p><b>for each</b> <math>u</math> <b>in</b> reverse(postOrder(<math>G</math>))</p> <p>    <math>V_{RRA}(u) \leftarrow \emptyset</math></p> <p>    <b>for each</b> <math>f</math> <b>in</b> parents(<math>u</math>)</p> <p>        <b>if</b> (<math>f \notin V_r</math>)</p> <p>            <math>V_{RRA}(u) \leftarrow V_{RRA}(u) \cup V_{RRA}(f)</math> (*)</p> <p>        <b>else</b></p> <p>            <math>V_{RRA}(u) \leftarrow V_{RRA}(u) \cup f</math></p> <p>    <b>if</b> (<math>u \in V_r</math>)</p> <p>        <b>for each</b> <math>v</math> <b>in</b> <math>V_{RRA}(u)</math></p> <p>            <math>E_r \leftarrow E_r \cup (u, v)</math></p> <p><b>return</b> <math>G_r</math></p>
---

Algorithm 4. Relevant *dag* excerpt algorithm

Let  $V_{RRA}(u)$  be the set of *Relevant Reachable Ancestors* of  $u$  containing vertices that are present in  $V_r$  and can be reached from  $u$  through a path crossing no other nodes of  $V_r$ . When considering vertices in *pre order*, the set  $V_{RRA}(u)$  of the current node  $u$  is the union of the sets  $V_{RRA}(f)$  of all its parent nodes that are not in  $V_r$ , plus all its parent nodes that are in  $V_r$ . The set  $E_r$  is then constructed by adding, for each node  $u$  of  $V_r$ , the edges  $(u, v)$  between  $u$  and any node  $v$  of  $V_{RRA}(u)$  as detailed in Algorithm 4.

The complexity of this algorithm is similar to that of the  $U_{lca}$  - closure (Algorithm 3). As for this latter algorithm, the key instruction, line (\*), computes the union of two sets of at most  $|V_r|$  elements and is executed for every parent of every node of the initial *dag*  $G$  i.e.  $O(|E|)$  times.

## 4 BUILDING RELEVANT SUB-DAG VIEWS BASED ON CLOSURE: TWO CASE STUDIES

This section illustrates the usefulness of our approach for two biological applications. The first one is related to ontology based annotation while the second one is related to species identification for metagenomic analysis.

### 4.1 Building sub-ontology to apprehend gene annotations

Ontologies are successfully used as semantic guides when navigating through the huge and ever increasing quantity of digital documents [12]. They are a graph based representation of domain semantics where nodes represent concepts of the fields and labeled edges represent concept relationships. The *is-a* relationship is central in ontology for it is the sole one that appears in formal ontology definition [13]; it is the sole that is present in all ontologies; and it is by far the most widely used relationship used to link concepts. When restricted to *is-a* edges the ontology graph is a *dag* that is often referred to as the backbone of the ontology [13, 14].

The need for sub-ontology extraction is clearly exposed in [15], where authors point out the fact that an application focuses only on particular aspects of the whole ontology. Having concise and meaningful sub-ontology is also crucial in any computer assisted ontology operation needing a human expert, such as ontology design and evolution or visual filtering within conceptual maps. When focusing on a subset of concepts (e.g. those indexing a given document or those over represented in the index of a set of documents) a graphical representation of their *is-a* relationships is very helpful. The most widespread solution is to display those concepts of interest with *all* their ancestors. This rough solution is (manually) used in many publications (e.g. [16, 17]) as well as within Web based tools (<http://www.informatics.jax.org/GOgraphs/OrthoDisease>). The  $U_{lca}$  - closure provides a more concise excerpt of the *is-a* *dag* by keeping only ancestors that highlight relation among the concept of interests. Indeed this ontology problematic was at the origin of our work on  $U_{lca}$  - closure and we have developed a dedicated tool called OntoFocus.

To illustrate the relevance and scalability of this approach, OntoFocus has been used to restrict the Gene Ontology (containing about 30,000 terms) to the 50 concepts of the BRCA1 gene associated with BReast CANcer susceptibility according to the European Bioinformatics Institute (<http://www.ebi.ac.uk/GOA/>.) The corresponding sub-ontology inferred by OntoFocus in about one minute contains 92 relevant concepts.

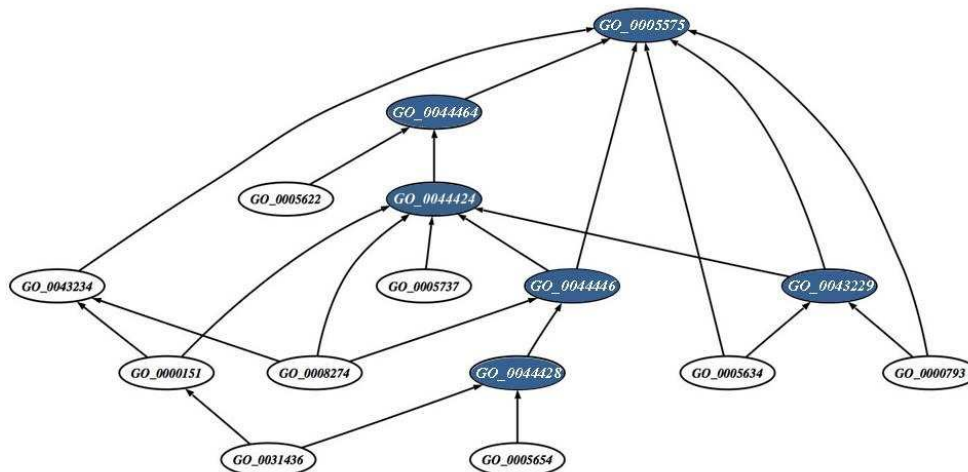


Fig. 8. Visualization of cellular component (GO\_0005575).

GO-sub-ontologies constructed by OntoFocus using BRCA1 annotation (white colored concepts). Blue colored concepts were added by OntoFocus to explicit semantic relationships among white ones.

In Fig. 8 one of the three connected parts of the sub-ontology is presented, that corresponds to *cellular components*. As one may see, the visualization is very comfortable and within human cognitive and perceptive limits. The two other parts, not shown here, contain 15 and 63 terms, which also allow a comfortable visualization.

Several applications may be underlined. First of all, the user-centered sub-ontology may be useful for biological users in exploiting annotations. This highlights, for example, that several annotations are refinements of the *intracellular part* (GO\_0044424.) The same approach may be used to simultaneously consider the annotation of several genes that share some biological characteristics (e.g. genes having similar expression profiles in microarray experiments.)

## 4.2 Identifying taxonomic group of environmental DNA sequences

New high-throughput sequencing techniques allow to obtain millions of short portions of DNA genomes (or transcriptome) called reads. These techniques can be used to sequence DNA of a single species. In that case the quantity of obtained information allows assembling almost the whole genome of this species. Alternatively, one can also choose to sequence the whole set of genomes available in a given environment (e.g. human guts, ocean or earth sample and so on). This is particularly useful to study the evolution of the biodiversity of the sampled environment in response to some changes (e.g. illness, climate change). In this latter case a key task is to assign the sequenced reads to a given species or taxonomic group. This is generally done based on a phylogenetic tree whose leaves represent today species and internal nodes speciation events that define taxonomic groups. To assign a taxonomic identity to a given read, the unknown DNA sequence is compared to those of the phylogeny tree leaves that are: colored in blue when similar to the read and in red otherwise. In the easiest case there is a single blue leaf and the read will be annotated with the corresponding species. For ambiguous reads, there are several blue leaves and the read is traditionally annotated based on their *lca*. A recent paper described an original approach that performed better on simulated and real datasets [18]. The idea is to identify the internal node  $n$  that best annotates a read based on the number of its blue descendants (true positives) red descendants (false positive) as well as the number of blue and red leaves that are not descendant of  $n$  (true and false negative). For doing so, it suffices to tests what they also called “relevant nodes” that are the least common ancestors of two or more blue leaves. This can be seen as a particular case of our  $U_{lca}$  – closure when the *dag* is a tree. Moreover they provide an algorithm to restrict the taxonomic tree to this relevant set of nodes which is also a particular case of our more general *dag* excerpt algorithm. Our work provides theoretical results and an algorithm that extend their read annotation approach to the case where the taxonomy is depicted by a phylogenetic network instead of a phylogenetic tree. Phylogenetic networks are *dags* whose leaves also represent extant species that received more and more attention in evolutionary biology (a recent book is entirely dedicated to them [19]). Indeed, by authorizing a node to have several parents they allow to represent phylogenetic uncertainty (it is not clear which parent is the real one) and complex biological events (such as species hybridization or lateral gene transfers).

## 5 CONCLUDING REMARKS

This paper introduced the concept of  $U_{lca}$  – closure of a set  $S$  of vertices in a *dag* and an optimized algorithm to identify it. This algorithm has the best known time complexity  $O(|S||E|)$  while using only  $O(|V|^2)$  memory space. This low complexity comes from the convexity properties of the closure of  $U_{lca}$  – operator that allows to obtain a greedy algorithm.

Many applications may benefit from such an algorithm. Two of them, developed in this paper, concern the life sciences domain. One is related to the widespread Gene Ontology while the other is related to environmental metagenomic analysis.

Future directions of our work include further study of the relationship between the closure concept and convexity and related algorithm's optimization.

## ACKNOWLEDGMENTS

This publication is the result of a collaboration between the "Institut des Sciences de l'Evolution de Montpellier" (UMR 5554 - CNRS) and the "LGI2P Research Centre from Ecole des Mines d'Alès". This work was supported by the French Agence Nationale de la Recherche 'Domaines Emergents' [ANR-08-EMER-011 'PhylAriane']. This publication is contribution No. 2011-XXX of the Institut des Sciences de l'Evolution de Montpellier (UMR 5554 - CNRS), France.

## REFERENCES

- [1] P. H. Edelman and R. E. Jamison, "The theory of convex geometries," in *Geometriae Dedicata*, vol. 19, *Mathematics and Statistics*: Springer Netherlands, 1985, pp. 247-270.
- [2] M. A. Bender, G. Pemmasani, S. Skiena, and P. Sumazin, "Finding least common ancestors in directed acyclic graphs," *Proceedings of the Twelfth Annual Acm-Siam Symposium on Discrete Algorithms*, pp. 845-854, 2001.
- [3] R. Yuster, "All-pairs disjoint paths from a common ancestor in  $O(n(\omega))$  time," *Theoretical Computer Science*, vol. 396, pp. 145-150, 2008.
- [4] A. Czumaj, M. Kowaluk, and A. Lingas, "Faster algorithms for finding lowest common ancestors in directed acyclic graphs," *Theory of Computer Science* vol. 380, pp. 37-46, 2007.
- [5] S. Eckhardt, A. M. Mühling, and J. Nowak, "Fast lowest common ancestor computations in dags," in *Proceedings of the 15th annual European conference on Algorithms*. Eilat, Israel: Springer-Verlag, 2007.
- [6] J. A. Bondy and U. S. R. Murty, *Graph Theory with Applications*. New York: American Elsevier Co., 1976.
- [7] G. Cardona, M. Lladrés, F. Rossello, and G. Valiente, "Metrics for Phylogenetic Networks I: Generalizations of the Robinson-Foulds Metric," *IEEE/ACM Trans. Comput. Biol. Bioinformatics*, vol. 6, pp. 46-61, 2009.
- [8] H. Aitkaci, R. Boyer, P. Lincoln, and R. Nasr, "Efficient Implementation of Lattice Operations," *Acm Transactions on Programming Languages and Systems*, vol. 11, pp. 115-146, 1989.
- [9] S. Janaqi and C. Payan, "Une Caractérisation des Produits d'Arbres et des Grilles," *Discrete Mathematics*, vol. 163, pp. 201-208, 1997.
- [10] H. M. Mulder and L. Nebesky, "Axiomatic characterization of the interval function of a graph," *European Journal of Combinatorics*, vol. 30, pp. 1172-1185, 2009.
- [11] Thomas H. Cormen, Charles E. Leiserson, and Ronald L. Rivest, "Graph Algorithms," in *Introduction to Algorithms*, 6 ed. Cambridge: The MIT Press, 1992.
- [12] A. Abecker and L. van Elst, "Ontologies for Knowledge Management," in *Handbook on Ontologies second edition, International handbooks on information systems*, S. S. a. R. S. (Eds.), Ed. Heidelberg: Springer, 2009, pp. 713-734.
- [13] N. Guarino, D. Oberle, and S. Staab, "What is an Ontology?," in *Handbook on ontologies, International handbooks on information systems*, S. a. S. Staab, Rudi, Ed. Heidelberg: Springer, 2009, pp. 1-17.
- [14] C. Ben Necib and J. C. Freytag, "Ontology based query processing in database management systems," *On the Move to Meaningful Internet Systems 2003: Coopis, Doa, and Odbase*, vol. 2888, pp. 839-857, 2003.
- [15] M. Bhatt, A. Flahive, C. Wouters, W. Rahayu, D. Taniar, and T. Dillon, "A distributed approach to sub-ontology extraction," *18th International Conference on Advanced Information Networking and Applications, Vol 1 (Long Papers), Proceedings*, pp. 636-641, 2004.
- [16] M. E. Dolan and J. A. Blake, "Using ontology visualization to understand annotations and reason about them," presented at KR-MED 2006 "Biomedical Ontology in Action", Baltimore, Maryland, USA, 2006.
- [17] M. E. Dolan and J. A. Blake, "Using Ontology Visualization to Coordinate Cross-species Functional Annotation for Human Disease Genes," in *Computer-Based Medical Systems, IEEE Symposium on*, vol. 0. Los Alamitos, CA, USA: IEEE Computer Society, 2006, pp. 583-587.
- [18] J. C. Clemente, J. Jansson, and G. Valiente, "Flexible taxonomic assignment of ambiguous sequencing reads," *BMC Bioinformatics*, vol. 12, pp. 8, 2011.
- [19] D. H. Huson, R. Rupp, and C. Scornavacca, *Phylogenetic Networks: Concepts, Algorithms and Applications*: Cambridge University Press, 2011.