# Unique Least Common Ancestors and Clusters in Directed Acyclic Graphs

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Abstract. We investigate the connections between clusters and least common ancestors (LCAs) in directed acyclic graphs (DAGs). We focus on the class of DAGs having unique least common ancestors for certain subsets of their minimal elements since these are of interest, particularly as models of phylogenetic networks. Here, we use the close connection between the canonical k-ary transit function and the closure function on a set system to show that pre-k-ary clustering systems are exactly those that derive from a class of DAGs with unique LCAs. Moreover, we show that k-ary  $\mathscr{T}$ -systems and k-weak hierarchies are associated with DAGs that satisfy stronger conditions on the existence of unique LCAs for sets of size at most k.

**Keywords:** Monotone transit function; closure function; clustering system; *k*-weak hierarchy

### 1 Introduction

Directed acyclic graphs (DAGs) play an increasing role in mathematical phylogenetics as models of more complex evolutionary relationships that are not adequately represented by rooted trees. The set X of minimal vertices of a DAG G = (V, E) corresponds to the extant taxa and thus generalizes the leaf set of

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a phylogenetic tree. Inner vertices  $u \in V$  are interpreted as ancestral states and are naturally associated with the sets C(u) of the descendant genes. These sets are often called the "hardwired clusters" [12,11]. A least common ancestor of a set A of taxa is a minimal vertex v in G such that  $A \subseteq C(v)$ , i.e., all taxa in Aare descendants of v. In phylogenetics, least common ancestors play a key role in understanding evolutionary relationships and processes. The clusters of G, on the other hand, are often accessible from data. Basic relations between clustering systems of (rooted) DAGs and the uniqueness of least common ancestors were explored recently in [10]. Here, we elaborate further on this theme, making use in particular of the fact that the canonical transit function of set systems is a restriction of the closure function to small spanning sets.

Section 2 contains basic definitions, some useful properties of DAGs, and a characterization of k-weak hierarchies. Section 3 is about lca and k-lca-property, and the connection of the latter with the pre-k-ary clustering systems. Section 4 discusses the correspondence of the strict and the strong k-lca properties to the k-ary  $\mathscr{T}$ -systems and the k-weak hierarchies, respectively.

### 2 Background and Preliminaries

**Transit functions and k-ary transit functions.** Let X be a non-empty, finite set. We write  $X^k$  for the k-fold Cartesian set product of X and  $X^{(k)}$  for the set of all non-empty subsets of X with cardinality at most k.

Following [6], a k-ary transit function on X is a function  $R: X^k \mapsto 2^X$  satisfying the axioms

(t1)  $u_1 \in R(u_1, u_2, \ldots, u_k);$ 

(t2)  $R(u_1, u_2, ..., u_k) = R(\pi(u_1, u_2, ..., u_k))$  for all  $u_i \in X$  and all permutations  $\pi$  of  $(u_1, u_2, ..., u_k)$ ;

(t3)  $R(u, u, ..., u) = \{u\}$  for all  $u \in X$ .

The "symmetry" axiom (t2) allows us to interpret a k-ary transit function also as a function over subsets  $U \in X^{(k)}$ . Then axiom (t2) becomes void, (t3) becomes  $R(\{x\}) = \{x\}$  for all  $x \in X$ , and condition (t1) reads " $u \in U$  implies  $u \in R(U)$  for all  $U \in X^{(k)}$ ".

Given a k-ary transit function R on X, we denote its system of *transit sets* by  $\mathscr{C}_R := \{R(U) \mid U \in X^{(k)}\}$ . A set system  $\mathscr{C} \subset 2^X$  is identified by a k-ary transit function if  $\mathscr{C} = \mathscr{C}_{R_{\mathscr{C}}}$  where  $R_{\mathscr{C}} : X^{(k)} \to 2^X$  defined by  $R_{\mathscr{C}}(U) := \bigcap \{C \in \mathscr{C} \mid U \subseteq C\}$  for all  $U \in X^{(k)}$ . As shown in [3,7], a system of non-empty sets  $\mathscr{C} \subset 2^X$  is identified by a k-ary transit function,  $k \geq 2$ , if and only if  $\mathscr{C}$  is a (k-ary)  $\mathscr{T}$ -system, satisfying the following three axiom

**(KS)**  $\{x\} \in \mathscr{C}$  for all  $x \in X$ 

**(KR)** For all  $C \in \mathscr{C}$  there is a set  $T \subseteq C$  with  $|T| \leq k$  such that  $T \subseteq C'$  implies  $C \subseteq C'$  for all  $C' \in \mathscr{C}$ .

**(KC)** For every  $U \subseteq X$  with  $|U| \leq k$  holds  $\bigcap \{C \in \mathscr{C} \mid U \subseteq C\} \in \mathscr{C}$ .

Conversely, a k-ary transit function R identifies a set system if and only if it satisfies the *monotone* axiom

(m) For every  $w_1, \ldots, w_k \in R(u_1, \ldots, u_k)$  holds  $R(w_1, \ldots, w_k) \subseteq R(u_1, \ldots, u_k)$ .

That is, for all  $U, W \in X^{(k)}$  holds:  $W \subseteq R(U)$  implies  $R(W) \subseteq R(U)$ . The correspondence of monotone k-ary transit functions and k-ary  $\mathscr{T}$ -systems is then mediated by the *canonical transit function*  $R_{\mathscr{C}}$  and  $\mathscr{C}_R$ , respectively.

For a general set system  $\mathscr{C}$  on X, the *closure* function  $\operatorname{cl} : 2^X \to 2^X$ , sometimes also called the "convex hull", is defined as  $\operatorname{cl}(A) := \bigcap \{C \in \mathscr{C} \mid A \subseteq C\}$ for all  $A \in 2^X$ . The canonical k-ary transit function  $R_{\mathscr{C}}$  of a set system is the restriction of its closure function to small sets as arguments:  $R_{\mathscr{C}}(U) = \operatorname{cl}(U)$  for all non-empty sets U with  $|U| \leq k$ .

A set system is closed if for all non-empty set  $A \in 2^X$  holds  $A \in \mathscr{C} \iff$ cl(A) = A. By [10, L. 16], this is equivalent to the condition that for all  $A, B \in \mathscr{C}$ with  $A \cap B \neq \emptyset$  we have  $A \cap B \in \mathscr{C}$ , i.e.,  $\mathscr{C}$  is closed under pairwise intersection. A set system  $\mathscr{C}$  consisting of non-empty subsets of X is called a clustering system if it satisfies (KS) and (K1):  $X \in \mathscr{C}$ . Note that axiom (KS) translates to  $R_{\mathscr{C}}$  satisfying (t3). A k-ary  $\mathscr{T}$ -system is thus a clustering system if and only it satisfies (K1) or, equivalently [7], if its canonical transit function  $R = R_{\mathscr{C}}$ satisfies

(a') there is  $U \in X^{(k)}$  such that R(U) = X.

A set system is called *pre-k-ary* if it satisfies (**KC**) for a given parameter k. The 2-ary case has received considerable attention in the literature for the special case of clustering systems, see [3]. A 2-ary transit function is called a *transit function*. A clustering system  $\mathscr{C}$  is called pre-binary in [3] if (**KC**) with k = 2 is satisfied, i.e., if  $R_{\mathscr{C}}(x, y) \in \mathscr{C}$  for all  $x, y \in X$ , and *binary* if in addition (**KR**) holds with k = 2. Binary clustering systems are therefore identified by monotone (2-ary) transit function satisfying (a') with k = 2; that is, there is  $p, q \in X$  such that R(p,q) = X.

Weak and k-weak hierarchies. Generalizations of hierarchies are important in the clustering literature. Recall that a clustering system  $\mathscr{C}$  is a

weak hierarchy if for any three sets  $A, B, C \in \mathscr{C}$  holds  $A \cap B \cap C \in \{A \cap B, A \cap C, B \cap C\}$  [1];

*k-weak hierarchy* if for any k+1 sets  $A_1, A_2, \ldots, A_{k+1} \in \mathscr{C}$  there is  $1 \leq j \leq k+1$ 

 $k+1 \text{ such that } \bigcap_{i=1}^{k+1} A_i = \bigcap_{i=1, i \neq j}^{k+1} A_i \ [2].$ 

We write  $A \[0.5mm] B$  if  $A \cap B \notin \{A, B, \emptyset\}$  and say that A and B overlap. It is well known that weak hierarchy = 2-weak hierarchy  $\implies k$ -weak hierarchy  $\implies (k+1)$ -weak hierarchy for all  $k \ge 3$ . As outlined in [9], weak hierarchies always satisfy (**KR**) for k = 2. More generally, Lemma 6.3 of [7] ensures that k-weak hierarchies satisfy (**KR**) for the parameter k. For weak hierarchies, furthermore, axiom (**KC**) with k = 2 is equivalent to  $\mathscr{C}$  being closed under pairwise intersection.

The characterization of k-weak hierarchies by condition (**kW'**) in [5], together with the fact that every k-weak hierarchy is also a k'-weak hierarchy for all  $k' \ge k$ , can be rephrased as follows:

**Observation 1.** A set system  $\mathscr{C}$  is a k-weak hierarchy if and only if for every  $A \in 2^X$  with |A| > k there is  $z \in A$  such that  $z \in cl(A \setminus \{z\})$ .

For our purposes, the following characterization of k-weak hierarchies in terms of their closure functions will be particularly useful:

**Proposition 1.** A set system  $\mathscr{C}$  on X is a k-weak hierarchy if and only if for every  $\emptyset \neq A \subseteq X$  there exists  $U \subseteq A$  with  $|U| \leq k$  such that cl(A) = cl(U).

*Proof.* First, assume that  $\mathscr{C}$  is a k-weak hierarchy. If  $|A| \leq k$ , then A = U trivially satisfies cl(A) = cl(U). Hence, assume |A| > k. By Obs. 1, there is  $z \in A$  such that  $z \in cl(A \setminus \{z\})$ , which implies  $A \subseteq cl(A \setminus \{z\})$ . Together with isotony and idempotency of the closure function, we obtain

$$cl(A \setminus \{z\}) \subseteq cl(A) \subseteq cl(cl(A \setminus \{z\})) = cl(A \setminus \{z\}).$$

Thus, there is  $z \in A$  such that  $cl(A) = cl(A \setminus \{z\})$ . Repeating this argument for  $A' \coloneqq A \setminus \{z\}$ , we observe that we can stepwisely remove elements of A while preserving cl(A) until we arrive a residual set  $U \subset A$  with |U| = k that still satisfies cl(U) = cl(A).

Now assume that  $\mathscr{C}$  is *not* a *k*-weak hierarchy. Hence, there are k + 1 sets  $A_1, A_2, \ldots, A_{k+1} \in \mathscr{C}$  such that for all  $1 \leq j \leq k+1$  it holds that  $\bigcap_{i=1}^{k+1} A_i \subsetneq \bigcap_{i=1, i \neq j}^{k+1} A_i$ . Thus, there are k+1 (distinct) elements  $x_1, \ldots, x_{k+1} \in X$  such that  $x_i \in A_j$  if and only  $i \neq j$ . Set  $A = \{x_1, x_2, \ldots, x_{k+1}\}$  and consider any subset  $U \subset A$  with  $|U| \leq k$ . Then there is at least one set  $A_h, 1 \leq h \leq k+1$ , such that  $U \subseteq A_h$ . By the previous arguments,  $x_h \notin A_h$ . Since  $A_h \in \mathscr{C}$ , we have  $cl(U) \subseteq A_h$ , and thus  $x_h \notin cl(U)$ . Since  $x_h \in A$  and  $A \subseteq cl(A)$ , we have  $x_h \in cl(A)$  and, thus,  $cl(U) \neq cl(A)$ .

Clusters, LCA and lca in DAGs. Let G be a directed acyclic graph (DAG) with an associated partial order  $\preceq$  on its vertex set V(G) defined by  $v \preceq_G w$  if and only if there is a directed path from w to v. In this case, we say that w is an ancestor of v and v is a descendant of w. If the context is clear, we may drop the subscript and write  $\preceq$ . Two vertices  $u, v \in V(G)$  are *incomparable* if neither  $u \preceq v$  nor  $v \preceq u$  is true. We denote by  $X = L(G) \subseteq V(G)$  the  $\preceq$ -minimal vertices of G and we call  $x \in X$  a leaf of G. For every  $v \in V(G)$ , the set of its descendant leaves

$$C(v) \coloneqq \{x \in X \mid x \preceq v\}$$
(1)

is a cluster of G. We write  $\mathscr{C}_G := \{\mathsf{C}(v) \mid v \in V(G)\}$ . By construction  $\mathsf{C}(x) = \{x\}$  for  $x \in X$ , hence  $\mathscr{C}_G$  satisfies **(KS)**. For  $v \in V(G)$ , we write  $\operatorname{Anc}(v) = \{w \in V(G) \mid v \leq w\}$  for the ancestors of v. For every leaf  $x \in X$  we have  $\operatorname{Anc}(x) = \{v \mid x \in \mathsf{C}(v)\}$ . We write  $\operatorname{Anc}(Y) := \bigcap_{w \in Y} \operatorname{Anc}(w)$  for the set of common ancestors of all  $w \in Y$ . In general, not every set  $Y \subseteq V$  has a common ancestor in a DAG: Consider the DAG with three leaves  $\{x, y, z\}$ , two maximal vertices  $\{p, q\}$ ,  $\mathsf{C}(p) = \{x, y\}$ , and  $\mathsf{C}(q) = \{x, z\}$ . Then  $\operatorname{Anc}(\{x, z\}) = \emptyset$ . A *(rooted) network* G is a DAG such that there is a unique vertex  $\rho \in V(G)$ , called the root, with indegree 0. In a network, we have  $x \leq \rho$  for all  $x \in V(G)$  and, thus, in particular,  $\mathsf{C}(\rho) = X$ , i.e.,  $X \in \mathscr{C}_G$ , and thus  $\mathscr{C}_G$ , satisfying **(K1)**, is a clustering system.

**Definition 1.** [4] If G is a DAG then w is a least common ancestor (LCA) of  $Y \subseteq V(G)$  if it is a  $\preceq$ -minimal element in Anc(Y). The set LCA(Y) comprises all LCAs of Y in G.

An LCA of Y thus is an ancestor of all vertices in Y that is  $\leq$ -minimal w.r.t. this property. Clearly, LCA( $\{v\}$ ) =  $\{v\}$  for all  $v \in V(G)$  and LCA(Y) =  $\emptyset$  if and only if Anc(Y) =  $\emptyset$ . In a network, the root vertex is a common ancestor for any set of vertices, and thus LCA(Y)  $\neq \emptyset$ .

We will, in particular, be interested in situations where the LCA of certain sets of leaves is uniquely defined. More precisely, we are interested in DAGs where |LCA(Y)| = 1 holds for certain subsets  $Y \subseteq X$ ; the most obvious examples are DAGs that satisfy the 2-lca-property (also known as the *pairwise lca-property* [10]), i.e., for every pair of leaves  $x, y \in L(G)$  there is a unique least common ancestor |LCA(Y)| = 1 and say that |ca(Y)| = q instead of  $\text{LCA}(Y) = \{q\}$  whenever |LCA(Y)| = 1 and say that |ca(Y)| is defined; otherwise, we leave |ca(Y)| undefined.

The following result for networks [10, L. 17] remains valid for all DAGs.

**Lemma 1.** Let G be a DAG. Then  $v \preceq_G w$  implies  $C(v) \subseteq C(w)$  for all  $v, w \in V(G)$ .

Consequently, [10, Obs. 12 & 13] also hold for DAGs in general:

**Observation 2.** Let G be a DAG with leaf set X,  $\emptyset \neq A \subseteq X$ , and suppose lca(A) is defined. Then the following is satisfied:

(i)  $\operatorname{lca}(A) \preceq_G v$  for all v with  $A \subseteq C(v)$ .

(ii) C(lca(A)) is the unique inclusion-minimal cluster in  $C_G$  containing A.

(*iii*)  $\operatorname{lca}(\operatorname{C}(\operatorname{lca}(A))) = \operatorname{lca}(A)$ .

Note that the existence of lca(A) for all  $A \subseteq X$  does not imply that G is a network since we could expand any network "upward" for  $\rho$  by attaching an arbitrary DAG that has  $\rho$  as its unique leaf. Clearly, the vertices "above"  $\rho$  cannot be least common ancestors of any leaves.

Consider a set system  $\mathscr{Q} \subseteq 2^X$ . Then the Hasse diagram  $\mathfrak{H}(\mathscr{Q})$  is the DAG with vertex set  $\mathscr{Q}$  and directed edges from  $A \in \mathscr{Q}$  to  $B \in \mathscr{Q}$  if (i)  $B \subsetneq A$  and (ii) there is no  $C \in \mathscr{Q}$  with  $B \subsetneq C \subsetneq A$ . As we shall see later, Hasse diagrams are of interest here because they guarantee well-behaved least common ancestors.

The correspondence between Hasse diagrams that are networks and k-ary transit function is summarized in the following

**Lemma 2.** Let R be a k-ary transit function. Then  $\mathfrak{H}(\mathscr{C}_R)$  is a network if and only if R satisfies (a') for k.

*Proof.* If  $N := \mathfrak{H}(\mathscr{C}_R)$  is a network, it contains a unique vertex  $\rho$  with indegree 0; the root of N. Since R satisfies **(t3)**, all singletons  $\{x\}$  with  $x \in X$  are contained as vertices of N. Since N has a unique root, it follows that X is a vertex of N and, in particular,  $C(\rho) = X \in \mathscr{C}_R$ . This implies that there must be a subset  $U \in X^{(k)}$  such that R(U) = X. Hence, R satisfies **(a')**. Conversely, if **(a')** with parameter k holds, there is a subset  $U \in X^{(k)}$  with R(U) = X and thus  $X \in \mathscr{C}_R$ .

Let  $v_X$  be the vertex in  $\mathfrak{H}(\mathscr{C}_R)$  for which  $C(v_X) = X$  holds. Since  $v \leq v_X$  for every vertex v in  $\mathfrak{H}(\mathscr{C}_R)$ , this is in particular true for the singletons, and thus  $v_X$  serves as the unique root of  $\mathfrak{H}(\mathscr{C}_R)$ .  $\Box$ 

Following [10], we say that a DAG G = (V, E) has the *path-cluster-comparability* (**PCC**) property if it satisfies, for all  $u, v \in V$ : u and v are  $\leq_G$ -comparable if and only if  $C(u) \subseteq C(v)$  or  $C(v) \subseteq C(u)$ . By [10, Cor. 11 & Prop. 3], the Hasse diagram G of a clustering system  $\mathscr{C}$  satisfies (**PCC**) and [10, Prop. 2] implies that  $\mathscr{C}_G = \mathscr{C}$ .

### 3 DAGs with lca- and k-lca-property

In the following, we consider the generalization of lca-networks introduced in [10] for arbitrary (not necessarily rooted) DAGs.

**Definition 2.** A DAG with leaf set X has the lca-property if lca(A) is defined for all non-empty  $A \subseteq X$ .

By definition, every DAG with the lca-property also has the pairwise lcaproperty. The converse is, in general, not satisfied. An example of a network (rooted DAG) that satisfies the pairwise lca-property but that is not an lcanetwork, can be found in [10, Fig. 13(A)].

**Lemma 3.** If a DAG G has the lca-property then its clustering system  $\mathcal{C}_G$  is closed.

*Proof.* To show that  $\mathscr{C}_G$  is closed, we use the equivalent condition that  $\mathscr{C}_G$  is closed under pairwise intersection. Thus, let  $C(u), C(v) \in \mathscr{C}_G$  for some  $u, v \in V(G)$ . If  $C(u) \subseteq C(v), C(v) \subseteq C(u)$  or  $C(u) \cap C(v) = \emptyset$ , there is nothing to show. Hence, assume that  $C(u) \not \in C(v)$  and set  $A := C(u) \cap C(v) \neq \emptyset$ . Since G has the lca-property, there is  $w \in V(G)$  such that w = lca(A), and thus  $A \subseteq C(w)$ . The contraposition of Lemma 1 shows that u and v are two incomparable common ancestors of A. Since w is the unique  $\preceq$ -minimal common ancestor of A, we have  $w \preceq u$  and  $w \preceq v$ , which – together with Lemma 1 – implies  $C(w) \subseteq C(u)$  and  $C(w) \subseteq C(v)$ . Therefore  $C(w) \subseteq A$ . Hence  $A = C(w) \in \mathscr{C}_G$  and thus,  $\mathscr{C}_G$  is closed.

The converse of Lemma 3 is not true. A counter-example can be found in Fig. 1. The following connection between the clusters, the least common ancestors, and the closure function will be useful in the remainder of this contribution:

**Observation 3.** If G is a DAG with leaf set X and lca-property, then C(lca(Y)) = cl(Y) for all  $\emptyset \neq Y \subseteq X$ .

*Proof.* The argument follows the proof of [10, L. 41], observing that [10, L.17] remains true for arbitrary DAGs, and substituting Obs. 2(i) and Lemma 3 for [10, Cor. 18] and [10, P. 11], respectively.



Fig. 1. The cluster system  $\mathscr{C}_G = \{\{w\}, \{x\}, \{y\}, \{x\}, \{x, y\}, \{w, x, y\}, \{x, y, z\}, \{w, x, y, z\}\}\$  of the network G is closed and satisfies (KC) for every  $k \in \{1, 2, 3, 4\}$ . However, we have  $\operatorname{LCA}(\{x, y\}) = \{p, v, q\}\$  and thus G does not have the pairwise lca-property. By Prop. 2, if G has the pairwise lca-property, then  $\mathscr{C}_G$  is pre-binary. The example in this Figure shows that the converse is not true. In particular, the equivalence between pre-k-ary and the k-lca-property in Prop. 3 requires (PCC), which is not satisfied by G.

The observations above can be extended to networks where more least common ancestors exist and are unique for all leaf sets of size at most k. Naturally, we start from the cluster system  $\mathscr{C} := \mathscr{C}_G := {\mathsf{C}(v); v \in V(G)}$  and consider the map  $R_{\mathscr{C}} : X^k \to 2^X$  defined by

$$R_{\mathscr{C}}(u_1, u_2, \dots, u_k) \coloneqq \bigcap \{ \mathsf{C}(v) \mid v \in V(G), u_1, u_2, \dots, u_k \in \mathsf{C}(v) \}$$

One easily verifies that  $R_{\mathscr{C}}$  satisfies (t2) and, thus, we can again interpret  $R_{\mathscr{C}}$  as a function over sets in which case we have  $R_{\mathscr{C}}(U) = \operatorname{cl}(U)$  for all  $U \in X^{(k)}$ . In this setting, we are interested in cases where  $\operatorname{lca}(U)$  is defined at least for all sets of cardinality  $|U| \leq k$ . We formalize this idea in

**Definition 3.** A DAG G with leaf set X has the k-lca-property if lca(A) is defined for all  $A \in X^{(k)}$ .

Now, we define the k-ary map  $R_G : X^k \to 2^X$  by  $R_G(u_1, \ldots, u_k) \coloneqq C(\operatorname{lca}(u_1, \ldots, u_k));$  in set notation this reads  $R_G(U) = C(\operatorname{lca}(U))$  for all  $U \in X^{(k)}$ .

**Proposition 2.** Let G be a DAG with k-lca-property. Then  $R_G$  is a monotone, k-ary transit function that satisfies  $R_G = R_{\mathscr{C}_G}$ . Moreover,  $\mathscr{C}_G$  is pre-k-ary.

Proof. Let G be a DAG with k-lca-property and leaf set X. It follows directly from the definition and uniqueness of lca(U) for  $U \in X^{(k)}$  that  $R_G$  satisfies (t1), (t2) and (t3), i.e,  $R_G$  is a k-ary transit function. If  $u_1, \ldots, u_k \in$  $R_G(x_1, \ldots, x_k) = \mathbb{C}(\operatorname{lca}(x_1, \ldots, x_k))$ , then  $\{u_1, \ldots, u_k\} \subseteq \mathbb{C}(\operatorname{lca}(x_1, \ldots, x_k))$ and we can apply Obs.2(i) to conclude that  $\operatorname{lca}(u_1, \ldots, u_k) \preceq \operatorname{lca}(x_1, \ldots, x_k)$ . Applying Lemma 1 yields  $\mathbb{C}(\operatorname{lca}(u_1, \ldots, u_k)) \subseteq \mathbb{C}(\operatorname{lca}(x_1, \ldots, x_k))$ , and thus  $R_G(u_1, \ldots, u_k) \subseteq R_G(x_1, \ldots, x_k)$ , i.e.,  $R_G$  is monotone. It follows from Obs. 2(ii) that  $\mathbb{C}(\operatorname{lca}(U))$  is the unique inclusion minimal cluster in  $\mathscr{C}_G$  containing U, i.e.,  $\operatorname{cl}(U) = \mathbb{C}(\operatorname{lca}(U))$  for all  $U \in X^{(k)}$ . Consequently,  $R_G = R_{\mathscr{C}_G}$ .

Since G has the k-lca-property, lca(U) is defined for all  $U \in X^{(k)}$ . Thus C(lca(U)) is the unique inclusion minimal cluster in  $\mathscr{C}_G$  containing U for all  $U \in X^{(k)}$  by Obs. 2(ii); hence  $\mathscr{C}_G$  satisfies **(KC)** for k, i.e.,  $\mathscr{C}_G$  is pre-k-ary.  $\Box$ 

Note that a DAG G for which  $\mathscr{C}_G$  is pre-k-ary does not necessarily have the k-lca-property, see Fig. 2 and Fig. 1 for a counter-example. Moreover, **(KR)** with

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**Fig. 2.** Consider the DAG *G* with leaf set X = L(G) where  $\mathscr{C}_G = \{\{x\}, \{y\}, \{z\}, \{w\}, \{x, y, z\}, X\}$ . Here,  $\mathscr{C}_G$  satisfies **(KS)** and **(KC)** for k = 2. By definition,  $\mathscr{C}_G$  is thus pre-binary. However, *G* is not a pairwise lca-network since lca(x, y), lca(x, z), and lca(y, z) are not defined. Moreover,  $\mathscr{C}_G$  also satisfies **(KC)** for k = 3 but *G* is not a 3-lca-network since lca(x, y, z) is not defined.

parameter k is not necessarily satisfied since the k-lca-property does not claim the existence of clusters that are not associated with least common ancestors of a set  $U \in X^{(k)}$ . Therefore,  $R_G$  need not identify  $\mathscr{C}_G$ . At least for an important subclass of DAGs there is a simple correspondence between the uniqueness of LCAs and a property of the  $\mathscr{T}$ -system.

# **Proposition 3.** Let G be a DAG that satisfies (PCC). Then, G satisfies the k-lca-property if and only if $\mathcal{C}_G$ is pre-k-ary.

*Proof.* Suppose that G is a DAG with leaf set X that satisfies (PCC). If G satisfies the k-lca-property, then Prop. 2 implies that  $\mathscr{C}_G$  is pre-k-ary. Assume now that  $\mathscr{C}_G$  is pre-k-ary. Hence, for all  $U \in X^{(k)}$  we have  $R_{\mathscr{C}_G}(U) = \bigcap \{C \in \mathcal{C}\}$  $\mathscr{C}_G \mid U \subseteq C \in \mathscr{C}_G$ . Therefore, Anc $(\{U\}) \neq \emptyset$  and thus, LCA $(\{U\}) \neq \emptyset$ . Assume, for contradiction, that there are two distinct vertices  $v, w \in LCA(U)$ . Note that  $U \subseteq R_{\mathscr{C}_{\mathcal{C}}}(U) \subseteq \mathsf{C}(v) \cap \mathsf{C}(w)$ . By Def. 1, both v and w are  $\prec$ -minimal ancestors of the vertices in U and, therefore, v and w are incomparable in G. This, together with the fact that G satisfies (PCC) implies that neither  $C(v) \subseteq C(w)$  nor  $C(w) \subseteq C(v)$  can hold. This and  $C(v) \cap C(w) \neq \emptyset$  implies that  $C(v) \notin C(w)$ . Since  $\mathscr{C}_G$  is pre-k-ary,  $R_{\mathscr{C}_G}(U) \in \mathscr{C}_G$ , i.e., there is a vertex  $z \in V(G)$  such that  $C(z) = R_{\mathscr{C}_G}(U)$ . Hence,  $C(z) \subseteq C(w) \cap C(v)$ . Since  $C(v) \notin C(w)$  it must hold that  $C(z) \subseteq C(w)$  and  $C(z) \subseteq C(v)$ . Since G satisfies (PCC), z and v must be  $\leq$ -comparable. If, however,  $v \leq z$ , then Lemma 1 implies that  $C(v) \subseteq C(z)$ ; a contradiction. Hence,  $z \prec v$  and, by similar arguments,  $z \prec w$  must hold. This, however, contradicts the fact that v and w are  $\prec$ -minimal ancestors of all the vertices in U. Hence, |LCA(U)| = 1 must hold for all  $U \in X^{(k)}$ . Consequently, G satisfies the k-lca-property. 

Consequently, we obtain a characterization of pre-k-ary clustering systems in terms of the DAGs from which they derive.

**Theorem 1.** A clustering system  $\mathscr{C}$  is pre-k-ary if and only if there is a DAG G with  $\mathscr{C} = \mathscr{C}_G$  and k-lca-property.

*Proof.* Suppose that  $\mathscr{C}$  is a pre-*k*-ary clustering system and consider the Hasse diagram  $G \coloneqq \mathfrak{H}(\mathscr{C})$ . It satisfies **(PCC)** and  $\mathscr{C}_G = \mathscr{C}$ . Consequently,  $\mathscr{C}_G$  is pre-*k*-ary. Thus, we can apply Prop. 3 to conclude that G satisfies the *k*-lca-property. Conversely, suppose that G is a DAG with the *k*-lca-property and  $\mathscr{C} = \mathscr{C}_G$ . By Prop. 2,  $\mathscr{C}$  is pre-*k*-ary.

Next, we show that k-ary transit functions give rise to DAGs with the k-lcaproperty in a rather natural way:

**Lemma 4.** Let R be a monotone k-ary transit function. Then, the Hasse diagram of its transit sets  $\mathfrak{H}(\mathscr{C}_R)$  satisfies the k-lca-property.

Proof. Let R be a monotone transit function on X and  $U \in X^{(k)}$ . Considering R as a function over subsets, conditions (t1) and (t2) imply that  $U \subseteq R(U)$ . In the following, let  $v_C$  denote the unique vertex in  $\mathfrak{H}(\mathscr{C}_R)$  that corresponds to the cluster  $C \in \mathscr{C}_R$ . For all  $W \in X^{(k)}$  with  $U \subseteq R(W)$  it holds, by condition (m), that  $R(U) \subseteq R(W)$ . This, together with the definition of the Hasse diagram implies that  $v_{R(U)} \preceq v_{R(W)}$  for all  $W \in X^{(k)}$  with  $U \subseteq R(W)$ . Thus,  $v_{R(U)}$  is the unique  $\preceq$ -minimal vertex in  $\mathfrak{H}(\mathscr{C}_R)$  satisfying  $x \preceq v_{R(U)}$  for all  $x \in U$ , and thus  $v_{R(U)} = \operatorname{lca}(U)$ .

As an immediate consequence of the correspondence between monotone k-ary transit functions and k-ary  $\mathscr{T}$ -systems, we also conclude that the Hasse diagram of k-ary  $\mathscr{T}$ -systems has the k-lca-property.

The converse of Lemma 4, however, need not be true: A Hasse diagram  $\mathfrak{H}(\mathscr{C}_R)$  with the k-lca-property for some k is not sufficient to imply that R is monotone:

Example 1. Let R on  $X = \{a, b, c, d\}$  be symmetric and defined by R(a, b) = X,  $R(a, c) = \{a, b, c\}$  and all other sets are singletons or X in such a way that (t1) and (t3) is satisfied. One easily verifies that R is a transit function satisfying (a') and that  $\mathfrak{H}(\mathscr{C}_R)$  is a network with root X. In fact,  $\mathfrak{H}(\mathscr{C}_R)$  is a rooted tree having pairwise lca-property. However, R is not monotone since  $R(a, b) = X \nsubseteq R(a, c)$ .

**Theorem 2.** Let R be a k-ary transit function. Then R is monotone if and only if there is a DAG G with k-lca-property and that satisfies  $\mathscr{C}_G = \mathscr{C}_R$  and  $R_{\mathscr{C}_G} = R$ .

*Proof.* If R is a monotone k-ary transit function, then  $G = \mathfrak{H}(\mathscr{C}_R)$  satisfies  $\mathscr{C}_G = \mathscr{C}_R$ . By Lemma 4, G has the k-lca-property. Moreover, since  $\mathscr{C}_G = \mathscr{C}_R$  it follows that  $R_{\mathscr{C}_G} = R_{\mathscr{C}_R}$ . Since R is monotone,  $R = R_{\mathscr{C}_R} = R_{\mathscr{C}_G}$ .

Conversely, let G be a DAG with  $\mathscr{C}_G = \mathscr{C}_R$  and k-lca-property. By Prop. 2,  $R_G = R_{\mathscr{C}_G}$  is monotone. Therefore, R is a monotone k-ary transit function.

### 4 DAGs with strict and strong k-lca-property.

In general,  $lca(\mathbf{C}(w))$  is not necessarily defined for all  $w \in V(G)$ , see e.g. the DAG in Fig. 2. As discussed in [10], it is, however, a desirable property: (CL) For every  $v \in V(G)$ ,  $lca(\mathbf{C}(v))$  is defined.

By definition, every DAG G that has the lca-property satisfies (CL).

**Lemma 5.** Let G be a DAG satisfying (CL). Then C(lca(C(v))) = C(v) for all  $v \in V(G)$ .

*Proof.* Since lca(C(v)) is defined, Obs. 2(i) implies  $lca(C(v)) \leq v$ . Then by Lemma 1,  $C(lca(C(v))) \subseteq C(v)$ . The reverse inclusion is trivial.

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**Definition 4.** Let G be a DAG with leaf set X and k-lca property. Then, G has the strict k-lca-property if G satisfies (CL) and for every  $w \in V(G)$  there is  $U \in X^{(k)}$  such that lca(C(w)) = lca(U).

**Proposition 4.** Let G be a DAG with leaf set X and k-lca-property. Then G has the strict k-lca-property if and only if  $\mathcal{C}_G$  is a k-ary  $\mathcal{T}$ -system. In this case,  $\mathcal{C}_G$  is identified by  $R_G$ .

Proof. The k-lca-property of G implies that  $\mathscr{C}_G$  is pre-k-ary, from Prop. 2. First assume that G has the strict k-lca-property. Consider  $C(w) \in \mathscr{C}_G$ . By definition, there exists  $U \in X^{(k)}$  such that lca(C(w)) = lca(U). Since G satisfies (CL), Lemma 5 implies C(w) = C(lca(C(w))) = C(lca(U)). Moreover, by Obs. 2(ii), C(lca(U)) = C(w) is the unique inclusion minimal cluster in  $\mathscr{C}_G$  containing U. This implies both  $U \subseteq C(w)$  and  $C(w) \subseteq C(v)$  for every  $v \in V(G)$  with  $U \subseteq C(v)$ . Hence,  $\mathscr{C}_G$  satisfies (KR). Hence,  $\mathscr{C}_G$  is a k-ary  $\mathscr{T}$ -system.

Conversely, assume that G holds k-lca-property and  $\mathscr{C}_G$  satisfies **(KR)**. Thus, for every  $w \in V(G)$ , there is  $U \in X^{(k)}$  such that  $U \subseteq C(w)$  and  $U \subseteq C(v)$ implies  $C(w) \subseteq C(v)$  for all  $v \in V(G)$ . Hence, C(w) is an inclusion minimal set in  $\mathscr{C}_G$  containing U. Since G has the k-lca-property, lca(U) is defined and, by Obs. 2(ii), C(lca(U)) is the unique inclusion minimal set in  $\mathscr{C}_G$  containing U, and thus C(w) = C(lca(U)) must hold. By Obs. 2(iii) we have lca(C(w)) =lca(C(lca(U))) = lca(U). Therefore, G has the strict k-lca-property.

Since a set system is identified by a k-ary transit function if and only if it is a k-ary  $\mathscr{T}$ -system and its canonical transit function identifies it, we have  $\mathscr{C}_G$  is identified by  $R_{\mathscr{C}_G}$ . Moreover,  $R_{\mathscr{C}_G} = R_G$  from Prop. 2. Hence the result.  $\Box$ 

In [10], networks with the *strong* lca-*property* were introduced. These satisfy (i) the lca-property and (ii) for every non-empty subset  $A \subseteq X$ , there are  $x, y \in A$ such that lca(x, y) = lca(A). As it turns out, these networks are characterized by their clustering systems: G is a strong lca-network if and only if G has the lca-property and  $\mathscr{C}_G$  is a weak hierarchy [10, Prop. 13]. In the following, we generalize these results to DAGs in general and spanning sets for lca(A) that are larger than a pair of points:

**Definition 5.** Let G be DAG with leaf set X and lca-property. Then, G has the strong k-lca-property if, for every non-empty subset  $A \subseteq X$ , there is  $U \in X^{(k)}$  such that lca(U) = lca(A).

Fig. 3 shows that the lca property does not imply the strong k-lca-property, i.e., the uniqueness of LCAs for all  $A \subseteq X$  does not imply that these are spanned by small subsets of leaves.

**Lemma 6.** If a DAG G has the strong k-lca-property, then it has the strict k-lca-property.

*Proof.* Suppose that G is a DAG with leaf set X and that has the strong k-lcaproperty. By definition, G has the lca-property. Hence, for all non-empty  $A \in 2^X$ , lca(A) is defined. This implies that lca(A) is defined for all  $A \in X^{(k)} \subseteq 2^X$  and



thus, G has the k-lca-property. Furthermore, since  $C(v) \in 2^X$  for all  $v \in V(G)$ , the DAG G satisfies **(CL)**. Let  $w \in V(G)$ . Since  $A \coloneqq C(w) \subseteq X$  and since G has the strong k-lca-property, there exists  $U \in X^{(k)}$  such that lca(U) = lca(A) = lca(C(w)). In summary, G has the strict k-lca-property.

**Proposition 5.** Let G be a DAG with leaf set X and lca-property. Then G has the strong k-lca-property if and only if for every non-empty subset  $A \subseteq X$  there exists  $U \subseteq A$  with  $|U| \leq k$  such that cl(A) = cl(U) in  $\mathcal{C}_G$ .

*Proof.* Assume first that *G* has the strong *k*-lca-property and let  $\emptyset \neq A \subseteq X$ . Then lca(*A*) = lca(*U*) for some *U* ⊆ *X* with  $|U| \leq k$ . Applying Obs. 3, we obtain cl(*A*) = C(lca(*A*)) = C(lca(*U*)) = cl(*U*). Conversely, assume that for every non-empty subset  $A \subseteq X$ , there exists  $U \subseteq A$  with  $|U| \leq k$  such that cl(*A*) = cl(*U*) in  $\mathscr{C}_G$ . Let  $A \subseteq X$  be non-empty. Applying Obs. 2(iii) and Obs. 3 yields lca(*A*) = lca(C(lca(*A*))) = lca(cl(*A*)) = lca(cl(*U*)) = lca(C(lca(*U*))) = lca(*U*). □

Prop. 5 and 1 imply

**Theorem 3.** G is DAG with the strong k-lca-property if and only if G has the lca-property and  $\mathcal{C}_G$  is a k-weak hierarchy.

## 5 Concluding Remarks

The connection between clusters and LCAs in DAGs is not limited to the relationships discussed so far and summarized in the following diagram:



Note that there are no implications between the lca-, strict 2-lca- and strict k-lca-property.

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Weak pyramids are weak hierarchies that, in addition, satisfy a necessary (but not sufficient) condition for  $\mathscr{C}$  to comprise intervals [13] called **(WP)** in [8]. One can show, for instance, that  $\mathscr{C}_G$  is weakly pyramidal for a DAG with the strong 2-lca-property if and only if no four distinct vertices  $a, b, c, d \in X$  exist such that  $b, c \not\leq \text{lca}(a, d), a, c \not\leq \text{lca}(b, d)$ , and  $a, b \not\leq \text{lca}(c, d)$ . Results like this, which we can only mention here due to space restrictions, suggest that the connection between LCAs and clusters in DAGs remains an interesting topic for future research.

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