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Conditional Separation as a Binary Relation. A Coq Assisted Proof

Jean-Philippe Chancelier[†], Michel De Lara
, Benjamin Heymann[†]

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Abstract

The concept of d-separation holds a pivotal role in causality theory, serving as a fundamental tool for deriving conditional independence properties from causal graphs. Pearl defined the d-separation of two subsets conditionally on a third one. In this study, we present a novel perspective by showing i) how the d-separation can be extended beyond acyclic graphs, possibly infinite, and ii) how it can be expressed and characterized as a binary relation between vertices. Compared to the typical perspectives in causality theory, our equivalence opens the door to more compact and computational proofing techniques, because the language of binary relations is well adapted to equational reasoning. Additionally, and of independent interest, the proofs of the results presented in this paper are checked with the Coq proof assistant.

1 Introduction

In an era increasingly driven by data-informed decision-making, the significance of causal inference has grown substantially across applied sciences, statistics, and machine learning. Pioneering this field, Pearl's seminal work [Pea95, PM18] leverages graphical models [CDLS06] to introduce the do-calculus and the concept of d-separation on directed acyclic graphs (DAGs). This concept plays a pivotal role in causality theory by providing a tool for deducing conditional independence properties from causal graphs.

This study introduces a novel perspective by handling graphs as binary relations — hence what we call graph is a directed simple graph permitting loops in graph theory, and we allow for infinite such graphs — and, from there, move in two successive directions. First, we extend the d-separation beyond acyclic graphs, to general, possibly infinite, graphs. Second, we characterize the d-separation property as a binary relation among the vertices of the graph. Compared to the typical perspectives in causality theory, our equivalence opens the door to more compact and computational proofing techniques, because the language of

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binary relations is well adapted to equational reasoning. Additionally, and of independent interest, the proofs of the results presented in this paper are checked with the Coq proof assistant. Last but not least, the characterization presented in this work serves as a building block for two concurrently developed works.¹

As far as we know, this is the first attempt to formalize d-separation in a proof assistant. However, some works can be found in the literature on probabilistic conditional independence and proof assistants. For example, in [AGT20], the authors introduce a formalism for reasoning with conditional probabilities and joint distributions in Coq. In [YKS⁺16], the authors introduce a formalism for reasoning on probabilistic conditional independence (PCI) in Coq based on universal algebraic structure suitable for studying PCI relations called cains (derived from *ca*usal *in*ference) and developed in [Wan10]. What we present in this work could be a starting point to make a link between [Wan10] and Pearl's d-separation in Coq. The Coq code developed by J.P. Chancelier for proving the results exposed in this paper is publicly available on GitHub² and counts around 7000 lines of code using Mathcomp/SSReflect [ABC⁺22, GMT16].

The paper is organized as follows. In Sect. 2, we revisit graphs as binary relations and define extended-oriented paths; then, we present our extended definitions of active extended-oriented paths and of d-separation. In Sect. 3, we state and sketch the proof of our main result, the characterization of the d-separation relation as the complementary of the conditional active relation. The main body of the proof is to be found in the Appendices, which follow its sketch. In Appendix A, we comment on how Coq is used in parallel to mathematical proofs. In Appendix B, we show that the conditional active relation can be replaced by the star conditional active relation in the statement of our main result. In Appendix C, we show that the star conditional active relation is included in the complementary of the d-separation relation. In Appendix D, we show the reverse inclusion.

2 A formal Pearl's d-separation definition

In §2.1, we deal with graphs but using the concepts of binary relations. In §2.2, we formally define what we call extended-oriented paths in a graph and discuss the Coq implementation used to formalize extended-oriented paths. Thus equipped, in §2.3, we formally adapt Pearl's definition of active (and blocked) extended-oriented paths in a graph, from which we deduce the (conditional) d-separation binary relation.

¹The mathematical side of the present paper was written in [CDH21] in parallel to two other papers [DCH21, HDC21], all of which aimed at providing another perspective on conditional independence (and do-calculus). The first paper [CDH21] was a prerequisite for [DCH21] and both [CDH21, DCH21] were a prerequisite for [HDC21]. In order to facilitate the reading of [CDH21, DCH21], which were quite long and technical, we have implemented Coq proofs for them. The aim of the present paper is to provide a version of the mathematical results of the preprint [CDH21] complemented with the description of the Coq formalization used for the proofs. The aim is thus twofold, as it gives the proof of yet unpublished results together with their Coq assisted proof.

²at URL https://github.com/jpc-cermics/relations.git

2.1 Binary relations and graphs

We employ the vocabulary and concepts both of binary relations and of graph theory. We denote by \mathbb{N} the set of natural numbers (including zero), and $\mathbb{N}^* = \mathbb{N} \setminus \{0\}$. We use the notation $[r, s] = \{r, r+1, \ldots, s-1, s\}$ for two natural numbers $r \leq s$.

In §2.1.1, we provide background on binary relations. In §2.1.2, we list tools that will be useful to navigate between vertices, edges and pair of edges representations in a graph, as defined in §2.1.3.

2.1.1 Background on binary relations

Let \mathcal{V} be a nonempty set (finite or not). We recall that a *(binary)* relation \mathcal{R} on \mathcal{V} is a subset $\mathcal{R} \subset \mathcal{V} \times \mathcal{V}$ and that $\gamma \mathcal{R} \lambda$ means $(\gamma, \lambda) \in \mathcal{R}$. For any subset $\Gamma \subset \mathcal{V}$, the *(sub)diagonal relation* is $\Delta_{\Gamma} = \{(\gamma, \lambda) \in \mathcal{V} \times \mathcal{V} \mid \gamma = \lambda \in \Gamma\}$ and the diagonal relation is $\Delta = \Delta_{\mathcal{V}}$. A relation is reflexive if $\Delta \subset \mathcal{R}$. A foreset of a relation \mathcal{R} is any set of the form $\mathcal{R} \lambda = \{\gamma \in \mathcal{V} \mid \gamma \mathcal{R} \lambda\},\$ where $\lambda \in \mathcal{V}$, or, by extension, of the form $\mathcal{R}\Lambda = \{\gamma \in \mathcal{V} \mid \exists \lambda \in \Lambda, \gamma \mathcal{R}\lambda\}$, where $\Lambda \subset \mathcal{V}$. An afterset of a relation \mathcal{R} is any set of the form $\gamma \mathcal{R} = \{\lambda \in \mathcal{V} \mid \gamma \mathcal{R} \lambda\}$, where $\gamma \in \mathcal{V}$, or, by extension, of the form $\Gamma \mathcal{R} = \{\lambda \in \mathcal{V} \mid \exists \gamma \in \Gamma, \gamma \mathcal{R} \lambda\}$, where $\Gamma \subset \mathcal{V}$. The opposite or complementary \mathcal{R}^{c} of a binary relation \mathcal{R} is the relation $\mathcal{R}^{c} = \mathcal{V} \times \mathcal{V} \setminus \mathcal{R}$, that is, defined by $\gamma \mathcal{R}^{\mathsf{c}} \lambda \iff \neg(\gamma \mathcal{R} \lambda)$. The converse \mathcal{R}^{-1} of a binary relation \mathcal{R} is defined by $\gamma \mathcal{R}^{-1} \lambda \iff \lambda \mathcal{R} \gamma$ (and \mathcal{R} is symmetric if $\mathcal{R}^{-1} = \mathcal{R}$). The composition $\mathcal{R}\mathcal{R}'$ of two binary relations $\mathcal{R}, \mathcal{R}'$ on \mathcal{V} is defined by $\gamma(\mathcal{R}\mathcal{R}')\lambda \iff \exists \delta \in \mathcal{V}, \gamma \mathcal{R} \delta$ and $\delta \mathcal{R}' \lambda$; then, by induction we define³ $\mathcal{R}^{n+1} = \mathcal{R}\mathcal{R}^n$ for $n \in \mathbb{N}^*$. The transitive closure of a binary relation \mathcal{R} is $\mathcal{R}^+ = \bigcup_{k=1}^{\infty} \mathcal{R}^k$ (and \mathcal{R} is transitive if $\mathcal{R}^+ = \mathcal{R}$) and the reflexive and transitive closure is $\mathcal{R}^* = \mathcal{R}^+ \cup \Delta = \bigcup_{k=0}^{\infty} \mathcal{R}^k$ with the convention $\mathcal{R}^0 = \Delta$. A partial equivalence relation is a symmetric and transitive binary relation (generally denoted by \sim or \equiv). An equivalence *relation* is a reflexive, symmetric and transitive binary relation.

Binary relations are implemented as sets on a product space using the classical sets implemented in classical_sets.v from the Coq mathcomp library [ABC⁺22] using SS-Reflect tactics [GMT16]

```
Definition relation (T: Type) := set (T * T). .<sup>4</sup>
```

As described in more details below, we have developed a library for relations taking into account all the definitions recalled at the beginning of §2.1.1.

³In what follows, when we consider a binary relation as a subset $\mathcal{R} \subset \mathcal{V} \times \mathcal{V}$, we will use the notation $\prod_{i=1}^{n} \mathcal{R} \subset \prod_{i=1}^{n} \mathcal{V} \times \mathcal{V}$, where *n* is a positive integer, to denote a product subset of the product set \mathcal{V}^{2n} , thus making the distinction with the binary relation $\mathcal{R}^n \subset \mathcal{V} \times \mathcal{V}$ obtained by *n* compositions.

⁴At the end of a Coq statement, ended by a dot belonging to the Vernacular (the language of Coq commands) we add a dot or a comma which serve as text punctuation.

2.1.2 Sequences, sets and binary relations

Being an active extended oriented path, as defined later, involves mixed properties of vertices, oriented edges and successive pairs of oriented edges path. This is why we need to develop tools that permit to navigate between vertices, edges and pair of edges representations. This part is devoted to list these tools and some of their properties. To formalize graph paths, we use sequences (as defined in mathcomp seq.v) combined with set formalization (defined in mathcomp classical_sets.v).

• **p** $[\in]$ **X.** We consider a set T and, for any subset $D \subset T$ and $n \in \mathbb{N}$, we denote by $\mathcal{S}_n(D) = \prod_{i=1}^n D$ the set of sequences of length n of elements of the set D ($\mathcal{S}_0(D)$ being the singleton set with the empty sequence) and by $\mathcal{S}_{\geq n}(D)$ the set of finite sequences of length greater than or equal to n of elements of the set D, that is, the disjoint union⁵ $\sqcup_{k\geq n} \mathcal{S}_k(D)$. The largest set $\mathcal{S}_{>0}(D)$ will be denoted by $\mathcal{S}(D)$:

$$\mathcal{S}_{\geq n}(D) = \bigsqcup_{k \geq n} \mathcal{S}_k(D) \text{ and } \mathcal{S}(D) = \mathcal{S}_{\geq 0}(D) .$$
 (1)

The sets $S_{\geq n}(T)$ and $S_n(T)$ are formalized in Coq in the mathcomp library as sequences of elements of type T and the restriction to elements in a subset (D: set T) is obtained using the function all (in mathcomp library seq.v). As an example, the set $S_n(D)$ is implemented as follows

Notation "p [\in] X" := (all (fun x => x \in X) p). Definition Sn (n: nat) (D: set T):= [set st| st [\in] D \land size(st)=n].

• (Lift p) and (p $[L \in] R$). Then, we define a lift operator

$$\mathcal{L}: \mathcal{S}(T) \to \mathcal{S}(T \times T) ,$$

such that

• for all $n \geq 2$, the restriction of the operator \mathcal{L} to the set $\mathcal{S}_n(T)$ coincides with the following mapping $\mathcal{L}_n : \mathcal{S}_n(T) \to \mathcal{S}_{n-1}(T \times T)$, given by

$$\forall (v_1, \dots, v_n) \in \prod_{i=1}^n T , \ \mathcal{L}_n(v_1, \dots, v_n) = \left((v_1, v_2), (v_2, v_3), \dots, (v_{n-1}, v_n) \right) , \quad (2)$$

transforming a sequence of elements of T of length n into a sequence of oriented pairs in $T \times T$ of length n-1,

• the restriction of the operator \mathcal{L} on $\mathcal{S}_0(T) \cup \mathcal{S}_1(T)$ is the constant mapping giving the empty list on $T \times T$.

⁵The symbol \sqcup stands for a disjoint union.

The lift operator \mathcal{L} is implemented in Coq as a recursive mapping denoted Lift:

```
Fixpoint Lift (st: seq T): seq (T*T) :=
  match st with
  | x :: [:: y & st] as st1 => (x,y)::(Lift st1)
  | _ => Nil (T*T)
  end. .
```

We note that, thanks to Coq polymorphism, the lift mapping is parameterized by a type and thus can be used to lift a sequence of vertices into a sequences of edges, but also to lift a sequence of edges (in $T \times T$) into a sequence of ordered pairs of edges (in $(T \times T)^2$).

The notation $p [L \in] R$ is used to denote the expression (Lift p) $[\in] R$.

• **p** [Suc \in] **R.** We must be able to check that successive elements of a sequence whose elements are in T belong to a given subset R of $T \times T$, that is, satisfy a relation R on T.

This is easily implemented with the help of an inductive predicate (RPath in seq1.v)

```
Notation "s [Suc<] R" := (RPath R s). ,
```

that we do not detail here as we prove that it can be equivalently implemented with the Lift mapping (which enables more computational proofs) as we have

Lemma RPath_equiv: \forall (st: seq T), st [L \in] R \leftrightarrow st [Suc \in] R.

As a first example, consider the (chain) relation $C_{\rm H}$ – denoted by Chrel in Coq – defined by $((v_1, v_2) C_{\rm H} (v_3, v_4) \iff v_2 = v_3)$, on the product set $T \times T$

Definition Chrel {T:Type} := [set s: (T*T)*(T*T) | (s.1).2 = (s.2).1].

Now, the fact that lifted sequences are well chained sequences can be stated as proving the following Coq Lemma

Lemma Lift_Suc: \forall (st:seq T), (Lift st) [Suc \in] Chrel.

As a second example, if the elements of a sequence belong to a set X, then the elements of the lifted sequence belong to the product relation $X \times X$ as proved in the following lemma

Lemma Rpath_L1: \forall (st: seq T), st [\in] X \rightarrow st [L \in] (X '*' X).

• Lift bijection. The lift operation, when restricted to the subset D defined below, is bijective onto its image I

```
Definition D {T: Type}:= [set st:seq T| size(st) > 1].
Definition I {T: Type}:= [set spt:seq (T*T)| size(spt) > 0 \land spt [Suc\in] Chrel].
Lemma Lift_inj: \forall (st st': seq T), st \in D \rightarrow Lift st = Lift st' \rightarrow st = st'.
Lemma Lift_surj: \forall (spt: seq (T*T)), spt \in I \rightarrow \exists st, st\in D \land Lift st=spt.
```

Moreover, the inverse of Lift is explicitly obtained by a recursive mapping UnLift (not detailed here).

2.1.3 Graphs as binary relations

Let \mathcal{V} be a nonempty set (finite or not), whose elements are called *vertices*. Let $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ be a relation on \mathcal{V} , whose elements are ordered pairs (that is, couples) of vertices called *edges*. The first element of an edge is the *tail of the edge*, whereas the second one is the *head of the edge*. Both tail and head are called *endpoints* of the edge, and we say that the edge connects its endpoints. We define a *loop* as an element of $\Delta \cap \mathcal{E}$, that is, a loop is an edge that connects a vertex to itself.

A graph, as we use it throughout this paper, is a couple $(\mathcal{V}, \mathcal{E})$. This definition is basic, and we now stress proximities and differences with classic notions in graph theory. As we define a graph, it may hold a finite or infinite number of vertices; there is at most one edge that has a couple of ordered vertices as single endpoints, hence a graph (in our sense) is not a multigraph (in graph theory); loops are not excluded (since we do not impose $\Delta \cap \mathcal{E} = \emptyset$). Hence, what we call a graph would be called a directed simple graph permitting loops in graph theory.

To define blocked and active extended-oriented paths – an essential notion in causal inference – relative to the graph $(\mathcal{V}, \mathcal{E})$, we need to fix additional vocabulary and notation. In the graph $(\mathcal{V}, \mathcal{E})$, the *undirected edges* are the elements of $\mathcal{E} \cap \mathcal{E}^{-1}$ — that is, edges with both $(\lambda, \gamma) \in \mathcal{E}$ and $(\gamma, \lambda) \in \mathcal{E}$ (hence, including loops). Then, the graph $(\mathcal{V}, \mathcal{E})$ is said to be *undirected* if all edges are undirected edges, or, equivalently, if $\mathcal{E} = \mathcal{E} \cap \mathcal{E}^{-1}$ or if $\mathcal{E}^{-1} = \mathcal{E}$. The *undirected extension* of a graph $(\mathcal{V}, \mathcal{E})$ is the graph $(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$.

In the graph $(\mathcal{V}, \mathcal{E})$, the *directed edges* are the elements of $\mathcal{E} \cap (\mathcal{E}^{-1})^{\mathsf{c}}$ — that is, edges with $(\lambda, \gamma) \in \mathcal{E}$ such that $(\gamma, \lambda) \notin \mathcal{E}$ (recall that we do not assume that $\mathcal{E} \cap \mathcal{E}^{-1} = \emptyset$). Then, the graph $(\mathcal{V}, \mathcal{E})$ is said to be *directed* if all edges are directed edges, or, equivalently, if $\mathcal{E} \cap \mathcal{E}^{-1} = \emptyset$, that is, when no two edges have the same endpoints.

A graph $(\mathcal{V}, \mathcal{E})$ is given in Coq by an oriented pair composed of a type (T: Type) and a relation on T, that is $(\mathcal{E} : \text{relation T})$ (which is equivalent to a set declaration $(\mathcal{E} :$ set T*T)). Thus, the (classical) set definition of mathcomp analysis classical_sets.v is used to formalize a graph. We have not used the Coq package graph-theory to formalize graph as we did not want to stick to finite graphs.

2.2 Extended-oriented paths in a graph

In graph theory, one finds the notions of path, chain and walk. To avoid ambiguities, we formally define in §2.2.1 an edge path in a graph — in our sense, that is, a (directed simple) graph (permitting loops) — as the classical notion of path in a graph [Die18]. Then, in §2.2.2, we define an extended-oriented path in a graph as what corresponds to a chain path in [LDLL90]. We consider a graph (\mathcal{V}, \mathcal{E}) as defined in §2.1.3, that is, a (directed simple) graph (permitting loops).

2.2.1 Edge paths in a graph

After defining edge paths and their endpoints, we introduce deployments in edge paths (see the summary Table 1).

• Definition of edge paths. We define the set of edge paths of length $n \ (n \ge 1)$, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$P_n(\mathcal{V},\mathcal{E}) = \left\{ \left\{ (v_i^{\flat}, v_i^{\sharp}) \right\}_{i \in \llbracket 1, n \rrbracket} \in \prod_{i=1}^n \mathcal{E} \left| v_i^{\sharp} = v_{i+1}^{\flat} \text{ for } i \in \llbracket 1, n-1 \rrbracket \right\}.$$
(3a)

For $n \ge 1$, we define the set of *edge paths of length greater than n*, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$P_{>n}(\mathcal{V},\mathcal{E}) = \sqcup_{n'>n} P_{n'}(\mathcal{V},\mathcal{E}) , \qquad (3b)$$

and finally the set of *edge paths*, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$P(\mathcal{V}, \mathcal{E}) = P_{>0}(\mathcal{V}, \mathcal{E}) . \tag{3c}$$

Using the tools introduced in §2.1.2 and Equations (3) we obtain the following formalization of $P_{>n}$

```
Definition P_gt (n: nat) (E: relation T) := 
[set spt | size(spt) > n \land spt [\in] E \land spt [Suc\in] Chrel].,
```

where E is the edge relation \mathcal{E} and where Chrel was defined in §2.1.2.

We denote by $|\varrho|$ the length of an edge path $\varrho \in P(\mathcal{V}, \mathcal{E})$ (computed in Coq by the mapping size). An *edge subpath* of the edge path ϱ is an edge path obtained by a subsequence of consecutive indices.

• Definition of endpoints of edge paths. The first element v_1^{\flat} of an edge path $\rho = \{(v_i^{\flat}, v_i^{\sharp})\}_{i \in [\![1,n]\!]}$ is the *tail of the edge path*, whereas the last one v_n^{\sharp} is the *head of the edge path*. Both tail (obtained with function head in Coq) and head (obtained with function last in Coq) are called *endpoints* of the edge path.

We define the projection mapping $\varpi^n : P_n(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \times \mathcal{V}$ on the tail and head endpoints of an edge path of length n by

$$\forall \varrho = (v_i^{\flat}, v_i^{\sharp})_{i \in \llbracket 1, n \rrbracket} \in P_n(\mathcal{V}, \mathcal{E}) , \ \varpi^n(\varrho) = \varpi^n((v_i^{\flat}, v_i^{\sharp})_{i \in \llbracket 1, n \rrbracket}) = (v_1^{\flat}, v_n^{\sharp}) \in \mathcal{V} \times \mathcal{V} .$$
(4a)

We define the projection mapping $\varpi : P(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \times \mathcal{V}$ on the tail and head endpoints of an edge path by

$$\forall \varrho \in P(\mathcal{V}, \mathcal{E}) , \ \varpi(\varrho) = \varpi^{|\varrho|}(\varrho) \in \mathcal{V} \times \mathcal{V} .$$
(4b)

We also distinguish the tail and the head endpoints projection mappings of an edge path by (see Figure 1)

$$\varpi = (\varpi^{\flat}, \varpi^{\sharp}) \text{ where } \varpi^{\flat} : P(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \text{ and } \varpi^{\sharp} : P(\mathcal{V}, \mathcal{E}) \to \mathcal{V} .$$
 (4c)



Figure 1: Tail and head endpoints of an edge path projection mappings (4) for $\rho \in P(\mathcal{V}, \mathcal{E})$

The endpoints are obtained in Coq by the mapping Pe (meaning path endpoints) for a sequence of vertices, and by the mapping Epe (meaning extended path endpoints) for a sequence of edges

```
Definition Pe (st: seq T) := (head ptv.1 st, last ptv.1 st).
Definition Epe (spt: seq (T*T)) := ((head ptv spt).1, (last ptv spt).2).
```

We prove in the next two lemmata that $\tt Pe$ and $\tt Epe$ behave properly with respect to the Lift bijection between $\tt D$ and $\tt I$

Lemma Epe_Lift: \forall (st:seq T), st \in D \rightarrow Epe (Lift st) = Pe st. Lemma Pe_UnLift: \forall (spt: seq (T*T)), spt \in I \rightarrow Pe (UnLift spt ptv.1)=Epe spt. .

As a first result linking (edge) paths and relations, we prove that

Lemma TCP: E.+ = [set vp| \exists p, size(p) > 1 \land Pe ptv p = vp \land p [L \in] E].

which asserts that two nodes (v1,v2) are in relation through the transitive closure of a relation E, that is $(v1,v2) \in E.+$ if and only if there exists an edge path with endpoints (v1,v2) in the graph $(\mathcal{V},\mathcal{E})$ represented by (T: Type), (E: relation T).

• Concatenation of edge paths. Concatenation of sequences denoted by the infix operator \ltimes (and denoted by ++ in Coq) is easily defined and is associative. When considering edge paths, concatenation of $\varrho' \in P(\mathcal{V}, \mathcal{E})$ and $\varrho'' \in P(\mathcal{V}, \mathcal{E})$ gives a sequence $(\varrho' \ltimes \varrho'') \in \mathcal{S}(\mathcal{V} \times \mathcal{V})$ which belongs to $P(\mathcal{V}, \mathcal{E})$ under the additional assumption that $\varpi^{\sharp}(\varrho') = \varpi^{\flat}(\varrho'')$ (see Equation (4c)), that is,

$$\forall \varrho' \in P(\mathcal{V}, \mathcal{E}) , \ \forall \varrho'' \in P(\mathcal{V}, \mathcal{E}) , \ \varpi^{\sharp}(\varrho') = \varpi^{\flat}(\varrho'') \implies (\varrho' \ltimes \varrho'') \in P(\mathcal{V}, \mathcal{E}) .$$
(5)

• Deployment in edge paths. With any binary relation $\mathcal{R} \subset \mathcal{V} \times \mathcal{V}$, we associate the subset $D_P[\mathcal{R} \mid \mathcal{V}, \mathcal{E}]$ of $P(\mathcal{V}, \mathcal{E})$, that we call the *deployment in edge paths*, defined by

$$\forall \mathcal{R} \subset \mathcal{V} \times \mathcal{V} , \ D_P[\mathcal{R} \mid \mathcal{V}, \mathcal{E}] = \varpi^{-1}(\mathcal{R}) \subset P(\mathcal{V}, \mathcal{E}) ,$$
(6)

Name	Expression	Equation
set of (edge) paths	$P(\mathcal{V}, \mathcal{E})$	Equation (3c)
tail and head endpoints	$arpi = (arpi^{lat}, arpi^{\sharp})$	Equation (4b)
projection mappings	$\varpi^{\flat}: P(\mathcal{V}, \mathcal{E}) \to \mathcal{V}$	Equation $(4c)$
	$\varpi^{\sharp}: P(\mathcal{V}, \mathcal{E}) \to \mathcal{V}$	Equation $(4c)$
deployment in edge paths	$D_P[\cdot \mid \mathcal{V}, \mathcal{E}] = \varpi^{-1}$	Equation (6)

Table 1: Notions for edge paths in a graph $(\S2.2.1)$

where the projection ϖ has been defined in (4). The deployment in edge paths $D_P[\mathcal{R} \mid \mathcal{V}, \mathcal{E}]$ is made of the edge paths whose endpoints satisfy the binary relation \mathcal{R} .

Definition D_P (R E: relation T):= [set spt| spt \in I \land R (Epe spt) \land spt [\in] E].

It is to be noted that the deployment in edge paths may be obtained as the image by the Lift mapping of a subset of sequences of vertices as follows

Definition D_V (R E: relation T):= [set st| st \in D \land R (Pe st) \land st [Suc \in] E]. Lemma DP_DV: \forall (R E: relation T), image (D_V R E) (@Lift T) = (D_P R E).

Note that, when an edge path of length greater than zero is given as a lifted sequence of elements of T (as for example in Lift (x::(rcons p y)) = st.), the endpoints (x,y) and the intermediate nodes p of the edge path st are immediately obtained.

2.2.2 Extended-oriented paths in a graph

To define *extended-oriented paths*, we consider a set

$$\mathcal{O} = \{-1, +1\} , \tag{7}$$

with two elements, and implemented in Coq as an inductive type taking two values N (for -1) and P (for 1)

Inductive O := | P | N.,

which will serve as an orientation specification of an edge. We also introduce the set $\mathcal{E}_{\mathcal{O}} \subset \mathcal{V} \times \mathcal{V} \times \mathcal{O}$ defined by

$$(v, v', o) \in \mathcal{E}_{\mathcal{O}} \iff (v, v') \in \mathcal{E}^{(o)}$$
, (8)

where $\mathcal{E}^{(+1)} = \mathcal{E}$ and $\mathcal{E}^{(-1)} = \mathcal{E}^{-1}$.

After defining extended-oriented paths and their endpoints, we introduce deployments in extended-oriented paths (see the summary Table 2).

• Definition of extended-oriented paths. We define the set of extended-oriented paths of length $n \ (n \ge 1)$, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$U_n(\mathcal{V},\mathcal{E}) = \left\{ \left\{ (v_i^{\flat}, v_i^{\sharp}, o_i) \right\}_{i \in \llbracket 1, n \rrbracket} \in \prod_{i=1}^n \mathcal{E}_{\mathcal{O}} \left| v_i^{\sharp} = v_{i+1}^{\flat} \text{ for } i \in \llbracket 1, n-1 \rrbracket \right\},$$
(9a)

For $n \geq 1$, we define the set of extended-oriented paths⁶ of length greater than n, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$U_{>n}(\mathcal{V},\mathcal{E}) = \sqcup_{n'>n} U_{n'}(\mathcal{V},\mathcal{E}) , \qquad (9b)$$

and finally the set of *extended-oriented paths*, relative to the graph $(\mathcal{V}, \mathcal{E})$, by

$$U(\mathcal{V},\mathcal{E}) = U_{>0}(\mathcal{V},\mathcal{E}) . \tag{9c}$$

Using the tools introduced in §2.1.2 and Equations (9), we obtain the following Coq formalization of $U_{>n}(\mathcal{V}, \mathcal{E})$

```
Definition U_gt (n: nat) (E: relation T):=
    [set sto | size(sto) > n ∧ sto [∈] (Oedge E) ∧ (Lift sto) [∈] ChrelO].
Definition Oedge (E: relation T): set (T*T*0) :=
    fun (oe: T*T*0) => match oe with | (e,P) => E e | (e,N) => E.-1 e end.
Definition ChrelO := [set ppa: (T*T*0)*(T*T*0) | (ppa.1.1).2 = (ppa.2.1).1].,
```

where Oede E is used to formalize the $\mathcal{E}_{\mathcal{O}}$ subset in (8), and where ChrelO is the chain relation on $\mathcal{V} \times \mathcal{V} \times \mathcal{O}$.

An extended-oriented path can be decomposed as an oriented pair composed of an edge path and a sequence of orientations. For that purpose, we introduce the mapping

$$\pi: \mathcal{S}(\mathcal{V} \times \mathcal{V} \times \mathcal{O}) \to \mathcal{S}(\mathcal{V} \times \mathcal{V}) \times \mathcal{S}(\mathcal{O}) , \qquad (10a)$$

where $\mathcal{S}(\cdot)$ was defined in (1), given by

$$\forall \rho \in \mathcal{S}(\mathcal{V} \times \mathcal{V} \times \mathcal{O}) , \ \pi(\rho) = \left(\pi_{\mathcal{S}(\mathcal{V} \times \mathcal{V})}(\rho), \pi_{\mathcal{S}(\mathcal{O})}(\rho)\right) \in \mathcal{S}(\mathcal{V} \times \mathcal{V}) \times \mathcal{S}(\mathcal{O}) ,$$
(10b)

where
$$\pi_{\mathcal{S}(\mathcal{V}\times\mathcal{V})}(\rho) = \{\pi_{\mathcal{V}\times\mathcal{V}}(\rho_i)\}_{i\in[\![1,|\rho|]\!]} \in \mathcal{S}(\mathcal{V}\times\mathcal{V})$$
, (10c)

and
$$\pi_{\mathcal{S}(\mathcal{O})}(\rho) = \{\pi_{\mathcal{O}}(\rho_i)\}_{i \in [\![1, |\rho|]\!]} \in \mathcal{S}(\mathcal{O})$$
, (10d)

⁶It is to be noted that an extended-oriented path is not a path in the graph $(\mathcal{V}, \mathcal{E})$, neither in the undirected graph $(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$. However, considering a couple $(\varrho, o) \in U_n(\mathcal{V}, \mathcal{E})$, we obtain that $\varrho \in P_n(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$, that is, ϱ is an (edge) path in the unoriented graph $(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$. We thus obtain a natural surjection $(\varrho, o) \mapsto \varrho$ from $U(\mathcal{V}, \mathcal{E})$ to $P(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$. This canonical surjection is not necessary injective because a path in $P(\mathcal{V}, \mathcal{E} \cup \mathcal{E}^{-1})$ that has an edge in $\mathcal{E} \cap \mathcal{E}^{-1}$ is the image of two distinct extended-oriented paths. The surjection $(\varrho, o) \mapsto \varrho$ is a bijection in the special case when the graph $(\mathcal{V}, \mathcal{E})$ is directed, that is, when $\mathcal{E} \cap \mathcal{E}^{-1} = \emptyset$, that is, when no two edges have the same endpoints.

where $\pi_{\mathcal{V}\times\mathcal{V}}$ (resp. $\pi_{\mathcal{O}}$) is the projection from the set $\mathcal{V}\times\mathcal{V}\times\mathcal{O}$ onto the set $\mathcal{V}\times\mathcal{V}$ (resp. \mathcal{O}). When $\rho \in U(\mathcal{V}, \mathcal{E})$, we obtain that $\varrho = \pi_{\mathcal{S}(\mathcal{V}\times\mathcal{V})}(\rho)$ is an edge path that is $\varrho \in P(\mathcal{V}, \mathcal{E})$.

Reciprocally, given an edge path $\rho \in P(\mathcal{V}, \mathcal{E})$ and a sequence $o \in \mathcal{O}^{|\rho|}$ of orientations of the same size, we denote by $\rho = \pi^{-1}(\rho, o)$ the extended-oriented path $\rho \in U(\mathcal{V}, \mathcal{E})$, defined by

$$\pi^{-1}: (\varrho, o) \in \operatorname{Im}\pi \mapsto \rho \text{ with } \rho_i = (\varrho_i, o_i) , \ \forall i \in \llbracket 1, |\varrho| \rrbracket.$$
(11)

The mapping π^{-1} is the inverse of the mapping π , defined in Equation (10), but on the range of the mapping π (so that using π^{-1} is a slight abuse of notation).

An extended-oriented subpath of the extended-oriented path $\rho \in U(\mathcal{V}, \mathcal{E})$ is an extendedoriented path obtained by a subsequence of consecutive indices.

• Definition of endpoints of extended-oriented paths. The endpoints of an extendedoriented path ρ are defined as the endpoints of the edge path $\pi_{\mathcal{S}(\mathcal{V}\times\mathcal{V})}(\rho)$ as defined in (10c).

We define the projection mapping $\varpi_U : U(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \times \mathcal{V}$ on the tail and head endpoints of extended-oriented paths by

$$\forall \rho \in U(\mathcal{V}, \mathcal{E}) , \ \varpi_U(\rho) = \varpi \left(\pi_{\mathcal{S}(\mathcal{V} \times \mathcal{V})}(\rho) \right) \in \mathcal{V} \times \mathcal{V} ,$$
 (12a)

where the projection mapping $\varpi : P(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \times \mathcal{V}$ on the tail and head endpoints of an edge path has been introduced in (4). We also distinguish the tail and the head endpoints projection mappings on extended-oriented paths by (see Figure 2)

$$\varpi_U = (\varpi_U^\flat, \varpi_U^\sharp) \text{ where } \varpi_U^\flat : U(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \text{ and } \varpi_U^\sharp : U(\mathcal{V}, \mathcal{E}) \to \mathcal{V}.$$
(12b)



Figure 2: Projection mappings (12) on the tail and the head endpoints of an extendedoriented path $\rho \in U(\mathcal{V}, \mathcal{E})$

The Coq definition of ϖ_U follows

```
Definition Eope (stto : seq(T*T*O)) : T*T :=
  ((head (ptv,P) stto).1.1, (last (ptv,P) stto).1.2). ,
```

• Concatenation of extended-oriented paths. As already noted, concatenation of sequences denoted by the infix operator \ltimes is easily defined and is associative. When considering extended-oriented paths, concatenation of $\rho' \in U(\mathcal{V}, \mathcal{E})$ and $\rho'' \in U(\mathcal{V}, \mathcal{E})$ gives a sequence $(\rho' \ltimes \rho'') \in \mathcal{S}(\mathcal{V} \times \mathcal{V} \times \mathcal{O})$ which belongs to $U(\mathcal{V}, \mathcal{E})$ under the additional assumption that $\varpi_U^{\sharp}(\rho') = \varpi_U^{\flat}(\rho'')$ (see Equation (12b)), that is,

$$\forall \rho' \in P(\mathcal{V}, \mathcal{E}) , \ \forall \rho'' \in P(\mathcal{V}, \mathcal{E}) , \ \varpi^{\sharp}(\rho') = \varpi^{\flat}(\rho'') \implies (\rho' \ltimes \rho'') \in U(\mathcal{V}, \mathcal{E}) .$$
(13)

Moreover, for all $\rho' \in U(\mathcal{V}, \mathcal{E})$ and $\rho'' \in U(\mathcal{V}, \mathcal{E})$, we have that

$$\rho' \ltimes \rho'' = \pi^{-1} \big((\pi_{\mathcal{S}(\mathcal{V} \times \mathcal{V})}(\varrho')) \ltimes (\pi_{\mathcal{S}(\mathcal{V} \times \mathcal{V})}(\varrho'')), (\pi_{\mathcal{S}(\mathcal{O})}(o') \ltimes \pi_{\mathcal{S}(\mathcal{O})}(o'')) \big) \in U(\mathcal{V}, \mathcal{E}) .$$
(14)

• Deployment in extended-oriented paths. With any binary relation $\mathcal{R} \subset \mathcal{V} \times \mathcal{V}$, we associate the subset $D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}]$ of $U(\mathcal{V}, \mathcal{E})$ in (9) that we call the *deployment in extended*-oriented paths, defined by

$$\forall \mathcal{R} \subset \mathcal{V} \times \mathcal{V} , \ D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}] = \varpi_U^{-1}(\mathcal{R}) \subset U(\mathcal{V}, \mathcal{E}) ,$$
(15)

where the projection ϖ_U has been defined in (12).

The deployment $D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}]$ is made of the extended-oriented paths whose endpoints satisfy the binary relation \mathcal{R} .

It is formalized in Coq as follows

```
Definition D_U (R E: relation T) := [set stto : seq (T*T*O) |size(stto)>0 \land R (Eope stto) \land stto [\in] (Oedge E) \land stto [Suc\in] ChrelO].
```

Moreover, As for edge path, it is to be noted that the extended-oriented paths may be obtained as the image of a product of sequences of vertices and sequences of orientation. This is done by the Lift0 mapping combining lift and pairing

Finally, we prove that LiftO is bijective on restricted domain and image, with inverse UnLiftO, and that the bijection properly commutes with Eope

```
Lemma Eope_Lift0: ∀ (st:seq T) (so:seq 0),
    size(st) > 1 → size (so) = size st -1 → Eope (Lift0 st so) = Pe ptv st.
Lemma Pe_UnLift0: ∀ (stto: seq (T*T*0)),
    size(stto) > 0 → stto [Suc∈] Chrel0 →
    (Pe ptv (UnLift0 stto ptv.1).1) = Eope stto. .
```

Name	Expression	Equation
set of extended-oriented paths	$U(\mathcal{V}, \mathcal{E})$	Equation (9c)
tail and head endpoints	$\varpi_U: U(\mathcal{V}, \mathcal{E}) \to \mathcal{V} \times \mathcal{V}$	Equation (12a)
projection mappings	$\varpi^{\flat}_U: U(\mathcal{V}, \mathcal{E}) \to \mathcal{V}$	Equation $(12b)$
	$\varpi_U^{\sharp}: U(\mathcal{V}, \mathcal{E}) \to \mathcal{V}$	Equation $(12b)$
deployment in extended-oriented paths	$D_U[\cdot \mid \mathcal{V}, \mathcal{E}] = \varpi_U^{-1}$	Equation (15)

Table 2: Notions for extended-oriented paths in a graph $(\S 2.2.2)$

2.3 Active extended-oriented paths and d-separation

Let $(\mathcal{V}, \mathcal{E})$ be a graph — as defined in §2.1.3, that is, a (directed simple) graph (permitting loops) — and $W \subset \mathcal{V}$ be a subset of vertices.

In §2.3.1 we formally adapt Pearl's definition of active (and blocked) extended-oriented paths in a graph, from which we deduce the (conditional) d-separation binary relation in §2.3.2.

2.3.1 Definition of active extended-oriented paths

We take inspiration from [Pea86] to define the notion of blocked paths on a graph, not necessarily finite nor acyclic. For this purpose, we first define active extended-oriented paths relative to the graph $(\mathcal{V}, \mathcal{E})$ in Definition 2. Then, we obtain the definition of blocked extended-oriented paths relative to the graph $(\mathcal{V}, \mathcal{E})$, as defined by [Pea86], by switching to the complementary set.

We start by introducing a binary relation, A^W_{TR} (active triplet), on the set $\mathcal{V} \times \mathcal{V} \times \mathcal{O}$, which is parameterized by the set of edges \mathcal{E} of a graph $(\mathcal{V}, \mathcal{E})$ and by a subset $W \subset \mathcal{V}$.

Definition 1 The active triplet binary relation A_{TR}^W on the set $\mathcal{V} \times \mathcal{V} \times \mathcal{O}$ is defined as follows

$$\int o_1 = +1$$
, $o_2 = +1$ and $v_1^{\sharp} = v_2^{\flat} \in W^{\mathsf{c}}$, (16a)

$$(v_1^{\flat}, v_1^{\ddagger}, o_1) A_{TR}^W (v_2^{\flat}, v_2^{\ddagger}, o_2) \iff \begin{cases} o_1 = -1 , & o_2 = -1 \text{ and } v_1^{\ddagger} = v_2^{\flat} \in W^{\mathsf{c}} , \\ 0 = -1 & 0 \\ 0 = -1$$

$$\iff \begin{cases} o_1 = -1 , \ o_2 = +1 \ and \ v_1^{\sharp} = v_2^{\flat} \in W^{\mathsf{c}} , \qquad (16c) \end{cases}$$

$$o_1 = +1 , \ o_2 = -1 \ and \ v_1^{\sharp} = v_2^{\flat} \in \mathcal{E}^* W ,$$
 (16d)

where
$$\mathcal{E}^* = \mathcal{E}^+ \cup \Delta$$
 is the reflexive and transitive closure of the relation \mathcal{E} .

Definition 2 (active extended-oriented paths $U_a^W(\mathcal{V}, \mathcal{E})$) We say that an extended-oriented path $\rho \in U(\mathcal{V}, \mathcal{E})$ in (9) relative to the graph $(\mathcal{V}, \mathcal{E})$, is an active extended-oriented path (w.r.t.⁷ the subset W) if the successive elements (triplets) of ρ satisfy the binary relation A_{TR}^W defined in Equation (16), that is, $\rho_i A_{\text{TR}}^W \rho_{i+1}$, for all $i \in [[1, |\rho|-1]]$. Notice that any extended-oriented path of length 1 is active by definition.

⁷w.r.t. stands for "with respect to".

We denote by $U_a^W(\mathcal{V}, \mathcal{E}) \subset U(\mathcal{V}, \mathcal{E})$ the subset of all active extended-oriented paths (w.r.t. the subset W). We say that an extended-oriented path is blocked if it is not active and we denote by $U_b^W(\mathcal{V}, \mathcal{E}) = (U_a^W(\mathcal{V}, \mathcal{E}))^c$ the subset of all blocked extended-oriented paths (w.r.t. the subset W).

The Coq formalization of the binary relation $A^W_{\mbox{\tiny TR}}$ easily follows

The binary relation A_{TR}^W contains the (oriented chain) relation – denoted by ChrelO in Coq – and defined by avec $((v_1^{\flat}, v_1^{\sharp}, o_1) C_{\text{H}}^{\mathcal{O}}(v_2^{\flat}, v_2^{\sharp}, o_2) \iff v_1^{\sharp} = v_2^{\flat})$. The forward set \mathcal{E}^*W is implemented by Fset in Coq.

Now, the Coq formalization of $D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ is obtained as an intersection of two sets

Definition D_U_a (R E: relation T) (W: set T) (x y:T):= $(D_U R E) \cap [set stto | stto [Suc \in] (A_tr W E)]$.

When the relation \mathcal{R} is a singleton $\mathcal{R} = \{(x, y)\}$, the set $D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ boils down to the following equivalent definition

Definition D_U_a1 (E: relation T) (W: set T) (x y:T):= [set stto |size(stto)>0 \land (Eope stto)=(x,y) \land stto [\in] (Oedge E) \land stto [Suc \in] ChrelO \land stto [Suc \in] (A_tr W E)].

2.3.2 Definition of conditional directional separation (d-separation)

We introduce in Definition 3 a new binary relation between vertices: we say that two vertices are (conditionally) directionally separated if and only if the two vertices are different and all the extended-oriented paths, having them as endpoints, are blocked (equivalently they are different and there does not exist an active extended-oriented paths having them as endpoints). This definition mimics Pearl's d-separation [Pea86], but with two differences: the graph is not supposed to be acyclic, and the separation is between vertices and not between disjoint subsets.

Definition 3 Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. We denote

$$\gamma \perp_{d} \lambda \mid W \iff (\gamma \neq \lambda) \land \left(D_{U}[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \subset U_{b}^{W}(\mathcal{V}, \mathcal{E}) \right) \qquad \left(\forall \gamma, \lambda \in \mathcal{V} \right),$$
(17)

and we say that the vertices γ and λ are (conditionally) directionally separated (w.r.t. the subset W).

The Coq implementation of d-separation is given by

```
Notation "( x [\perp d] y \mid W)" := (D_separated W E x y).
Definition D_separated (W: set T) (E: relation T) (x y: T) :=
  ~(\exists (p: seq (T*T*O)), Active_path W E p x y).
Definition Active_path
  (W: set T) (E: relation T) (p: seq (T*T*O)) (x y: T) :=
  match p with
  | [::] => x = y
  | [::eo1] => eo1.1.1 = x \land eo1.1.2 = y \land Oedge E eo1
  | eo1 :: [:: eo2 & p]
    \Rightarrow eo1.1.1 = x \land (last eo2 p).1.2 = y
       ∧ allL (ActiveOe W E) (belast eo2 p) eo1 (last eo2 p)
  end.
          Definition ActiveOe (W: set T) (E: relation T) :=
  [set oe : (T*T*O) * (T*T*O) |
    Oedge E oe.1 \land Oedge E oe.2 \land (ChrelO oe)
     ∧ match (oe.1.2, oe.2.2, oe.1.1.2) with
       | (P,P,v) => W.^c v
       | (N, N, v) => W.^{c} v
       | (N,P,v) => W.^c v
       | (P,N,v) => (Fset E.* W) v
       end].
Definition allL (R: relation T) st x y := (x::(rcons st y)) [L\in] R.
```

The retained formulation is indeed equivalent to Definition 3, as proved in Coq lemma Active_eq given below

Lemma Active_eq: \forall (E: relation T) (W: set T) (x y:T) stto, ((x=y \land stto = [::]) \lor stto \in (D_U_a1 E W x y)) \leftrightarrow Active_path W E stto x y. .

3 Characterization of *d*-separation by means of binary relations

Our main result is the characterization of the conditional directional separation relation — the extension $(\coprod_d | W)$, or shortly \coprod_d , of the d-separation introduced in Definition 3 — as the complementary of the conditional active relation — Equation (18g) in Definition 4 below.

For this purpose, we introduce the following binary relations on the vertices of a graph — as defined in $\S2.1.3$, that is, a (directed simple) graph (permitting loops).

Definition 4 Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. We define the conditional parental relation \mathcal{E}^{W} as

$$\mathcal{E}^{W} = \Delta_{W^{\mathsf{c}}} \mathcal{E} \qquad that \ is, \ \gamma \mathcal{E}^{W} \lambda \iff \gamma \in W^{\mathsf{c}} \ and \ \gamma \mathcal{E} \lambda \qquad (\forall \gamma, \lambda \in \mathcal{V}) \ , \tag{18a}$$

the conditional ascendent relation $\mathcal{B}^{\scriptscriptstyle W}$ as

$$\mathcal{B}^{W} = \mathcal{E}(\Delta_{W^{c}}\mathcal{E})^{*} = \mathcal{E}\mathcal{E}^{W^{*}}, \qquad (18b)$$

which relates a descendent with an ascendent by means of elements in W^c. We define their converses \mathcal{E}^{-W} and \mathcal{B}^{-W} as

$$\mathcal{E}^{-W} = (\mathcal{E}^{W})^{-1} = \mathcal{E}^{-1} \Delta_{W^{c}} , \qquad (18c)$$

$$\mathcal{B}^{-W} = \left(\mathcal{B}^{W}\right)^{-1} = \left(\mathcal{E}^{-1}\Delta_{W^{c}}\right)^{*}\mathcal{E}^{-1} = \mathcal{E}^{-W*}\mathcal{E}^{-1} .$$
(18d)

With these elementary binary relations, we define the conditional common cause relation \mathcal{K}^w as the symmetric relation

$$\mathcal{K}^{W} = \mathcal{B}^{-W} \Delta_{W^{c}} \mathcal{B}^{W} = \mathcal{E}^{-W+} \mathcal{E}^{W+} , \qquad (18e)$$

the conditional cousinhood relation \mathcal{C}^{W} as the partial equivalence relation

$$\mathcal{C}^{W} = \left(\Delta_{W}\mathcal{K}^{W}\Delta_{W}\right)^{+} \cup \Delta_{W} , \qquad (18f)$$

and the conditional active relation \mathcal{A}^{W} as the symmetric relation

$$\mathcal{A}^{W} = \Delta \cup \mathcal{B}^{W} \cup \mathcal{B}^{-W} \cup \mathcal{K}^{W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W}\right) \mathcal{C}^{W} \left(\mathcal{B}^{-W} \cup \mathcal{K}^{W}\right) \,. \tag{18g}$$

The Coq implementation is straightforward using the binary relation library rel.v that we have developed.

```
Definition Em := E.-1.

Definition Ew := \Delta_{-}(W.\cap{c});E.

Definition Bw := E;Ew.*.

Definition Emw := Ew.-1.

Definition Bmw := Bw.-1.

Definition Kw := (Bmw;\Delta_{-}(W.\cap{c});Bw).

Definition DKD := (\Delta_{-}(W);Kw; \Delta_{-}(W)).

Definition Cw := ((DKD).+) \cup \Delta_{-}(W).

Definition Dw := (Bw \cup Kw);(Cw;(Bmw \cup Kw)).

Definition Aw := '\Delta_{-} \cup Bw \cup Bmw \cup Kw \cup Dw.
```

We now state the main result of this paper.

Theorem 5 (Coq **Theorem Th5**) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. The conditional directional separation relation \coprod_d (Definition 3) is the complementary $(\mathcal{A}^W)^{\mathsf{c}}$ of the conditional active relation \mathcal{A}^W (Equation (18g) in Definition 4):

$$\left(\perp d \mid W \right) = \left(\mathcal{A}^{W} \right)^{\mathsf{c}} \text{ or, equivalently, } \gamma \perp d \lambda \mid W \iff \neg(\gamma \mathcal{A}^{W} \lambda) \qquad \left(\forall \gamma, \lambda \in \mathcal{V} \right).$$
(19)

In other words, we have that

$$\{(\gamma,\lambda)\in\mathcal{V}\times\mathcal{V}\mid (\gamma\neq\lambda)\wedge D_U[\{(\gamma,\lambda)\}\mid\mathcal{V},\mathcal{E}]\subset U_b^W(\mathcal{V},\mathcal{E})\}=(\mathcal{A}^W)^{\mathsf{c}}.$$
 (20)



Figure 3: Sketch of proof of Theorem 5, mentioning the corresponding Appendices and lemmata

Proof. The proof of Theorem 5 is broken in three steps and summarized in Figure 3.

First, we will prove in postponed Lemma 7 (in §B.1) that $\mathcal{A}^W = \mathcal{A}^W_*$, where the binary relation \mathcal{A}^W_* is defined by Equation (41a).

Second, we will prove in postponed Proposition 8 (in Appendix C) that, for any vertices $\gamma, \lambda \in \mathcal{V}$, we have the implication $\gamma \mathcal{A}^W_* \lambda \implies \neg \left(\gamma \coprod_d \lambda \mid W \right)$ or, equivalently (see (17) in Definition 3), the implication

$$\gamma \mathcal{A}^{W}_{*} \lambda \implies (\gamma = \lambda) \lor \left(D_{U}[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \cap U^{W}_{a}(\mathcal{V}, \mathcal{E}) \neq \emptyset \right).$$

We simply give a sketch of proof here as details are to be found in Proposition 8 accompanied by postponed lemmata given in Appendix C. The binary relation \mathcal{A}^W_* defined in (23) is given by the union of five relations. Then, the proof of Proposition 8 examines the five cases and exhibits an active path (one in $U^W_a(\mathcal{V}, \mathcal{E})$, see Definition 2) that joins the vertices γ and λ in the five cases when $\gamma \mathcal{A}^W_* \lambda$.

Third, we will prove in Proposition 15 (in Appendix D) that, for any vertices $\gamma, \lambda \in \mathcal{V}$, we have the implication $\neg(\gamma \perp \lambda \mid W) \implies \gamma \mathcal{A}^{W}_{*} \lambda$ or, equivalently (see (17) in Definition 3), that

$$(\gamma = \lambda) \lor \left(D_U[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) \neq \emptyset \right) \implies \gamma \mathcal{A}_*^W \lambda$$

We give again a sketch of proof. The case $\gamma = \lambda$ is immediate. Thus, we assume that there exists an extended-oriented path $\rho \in U(\mathcal{V}, \mathcal{E})$ joining the vertices γ and λ and such that ρ is active. If the path length of ρ is equal to one, the proof easily follows. If the path length of ρ is ≥ 2 a proof by induction on the path length is obtained using Lemma 18. During the induction step, four cases are to be discussed, following the fact that the active triplet binary relation A_{TR}^W is governed by four cases. The scheme of the induction step is summarized in Figure 6.

This ends the proof.

We end this section by giving the Coq statement of Theorem 5 together with the corresponding Coq proof dependency graph in Figure 4.

Theorem Th5: \forall (x y: T), (x [\perp d] y | W) \leftrightarrow ~ Aw (x,y).



Figure 4: Coq-produced dependency graph for Coq Theorem 5 (B_L7 is Lemma 7, D_P15 is Proposition 15 and C_P8 is Proposition 8)

4 Conclusion

Together with its two companion papers [DCH21, HDC21], this paper is a contribution to providing another perspective on conditional independence and do-calculus. In this paper, we have considered directed graphs (DGs) not necessarily acyclic, and we have shown how the d-separation can be extended beyond acyclic graphs and can be expressed and characterized as a binary relation between vertices. The results in this paper are instrumental in proving those in [DCH21] on topological conditional separation (t-separation), hence in the use of t-separation to establish conditional independence in [HDC21].

Moreover, there are other perspectives. First, such developpement of a theory based on binary relations is interesting in itself as it makes it amenable to computer aided proof. Second, there are other notions of separation (between subsets) in graph theory that can also be expressed by means of binary relations (between vertices). We illustrate this with an example. Let $(\mathcal{V}, \mathcal{E})$ be a graph, $W \subset \mathcal{V}$ be a subset of vertices, and $\gamma, \lambda \in \mathcal{V}$ be vertices. Then, the three following statements are equivalent: any path from γ to λ passes through W; there does not exist a path from γ to λ which passes through W^{c} ; $\neg(\gamma(\mathcal{E}\Delta_{W^{c}}\mathcal{E})^{+}\lambda)$.

A Comments on Coq in the appendices proofs

The Coq proof of Theorem 5 closely follows the mathematical proof detailed in the three following Appendices (see also Figures 3 and 4) and, for each (mathematical) lemma, we will give its Coq name.

The Coq proof is obtained with the help of a novel library, developed by J.P. Chancelier and which provides tools for reasoning on binary relations and on active extended-oriented paths. This library is publicly available on GitHub at URL

https://github.com/jpc-cermics/relations.git

A.1 Binary relations

All the mathematical objects described in §2.1.1, together with associated lemmata for manipulating them, are implemented in a Coq library. As relations are coded as sets, the library we have developed (mainly contained in file rel.v) is based on the *mathcomp* implementation of sets $classical_sets.v$. It also contains a SSReflect reimplementation of transitive (reflexive) closures of relation (ssrel.v) that are found in the Coq standard library. Moreover — as proofs on relations proceed by rewriting rules using intensively associative and commutative properties of union and intersection of relations — we use the AAC_tactics to ease equality proofs between long expressions with relations containing unions, intersections, compositions and diagonal relations. For this to be possible, some specific properties of relations with respect to AAC are to be listed and proved in Coq. This is done in aacset.v.

A.2 Extended-oriented paths in a graph

We have also developed a library for manipulating paths in a graph (seq1.v), which contains the objects described in §2.2. Even if the the concepts of extended-oriented paths and active extended-oriented paths are quite specific to d-separation, the library we have developed contains many tools for manipulating node or edge paths which are of more general interest.

A.3 Coq proofs of Theorem 5

Two files are specifically devoted to the proof of Theorem 5. The file paper_relations.v contains the definition of the binary relations contained in Definition 4 and 6 and in Lemma 16, together with some lemmata on their respective properties. The file paper_csbr.v contains the proofs of the propositions and lemmata which are mathematically proved in the following appendices.

B The star conditional active relation $\mathcal{A}^{\scriptscriptstyle W}_*$

In §B.1, we introduce new binary relations to define the star conditional active relation \mathcal{A}_*^W . In §B.2, we prove that $\mathcal{A}^W = \mathcal{A}^W_*$, where the conditional active relation \mathcal{A}^W has been introduced in Equation (18g) of Definition 4.

B.1 Definition and properties of the star conditional active relation $\mathcal{A}^{\scriptscriptstyle W}_*$

We refer the reader to Definition 4 for the definitions of basic binary relations. We add two new ones.

Definition 6 Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. We introduce the notation

$$\overline{W}^{\mathcal{E}} = \mathcal{E}^* W , \qquad (21)$$

and we define the star conditional cousinhood relation

$$\mathcal{C}^{W}_{*} = \left(\Delta_{\overline{W}} \varepsilon \mathcal{K}^{W} \Delta_{\overline{W}} \varepsilon\right)^{+} \cup \Delta_{\overline{W}} \varepsilon , \qquad (22)$$

and the star conditional active relation

$$\mathcal{A}^{W}_{*} = \Delta \cup \mathcal{B}^{W} \cup \mathcal{B}^{-W} \cup \mathcal{K}^{W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W}\right) \mathcal{C}^{W}_{*} \left(\mathcal{B}^{-W} \cup \mathcal{K}^{W}\right) \,. \tag{23}$$

Notice that the star conditional cousinhood relation C^w_* in (22) is the relation C^w in (18f) with W replaced by $\overline{W}^{\varepsilon}$, and the star conditional active relation \mathcal{A}^w_* in (23) is the relation \mathcal{A}^w in (18g) with \mathcal{C}^w replaced by \mathcal{C}^w_* .

B.2 Proof that $\mathcal{A}^{\scriptscriptstyle W} = \mathcal{A}^{\scriptscriptstyle W}_*$

Recall that the conditional active relation \mathcal{A}^{W} has been introduced in Equation (18g) of Definition 4.

Lemma 7 (Coq **Lemma 7**) We have that

$$\mathcal{A}^W = \mathcal{A}^W_* \ . \tag{24}$$

Proof. The proofs is in three steps.

• (Lemma L7 E25) We prove that

$$\forall \mathcal{R} \subset \mathcal{V} \times \mathcal{V} , \ \forall \Gamma \subset \mathcal{V} , \ \mathcal{R}^* \Gamma = (\Delta_{\Gamma^c} \mathcal{R})^* \Gamma .$$
⁽²⁵⁾

For this purpose, we prove the following induction assumption \mathcal{H}_n : for any $n \geq 1$, we have that $(\bigcup_{k=0}^n \mathcal{R}^k)\Gamma = (\bigcup_{k=0}^n (\Delta_{\Gamma^c} \mathcal{R})^k)\Gamma$, where we recall the convention $\mathcal{R}^0 = \Delta$.

As a preliminary result, for any $\Gamma, \Lambda \subset \mathcal{V}$, from the sequence of equalities $(\Delta\Gamma) \cup (\mathcal{R}\Lambda) = \Gamma \cup ((\mathcal{R}\Lambda) \setminus \Gamma) = \Gamma \cup (\Delta_{\Gamma^c} \mathcal{R}\Lambda) = (\Delta\Gamma) \cup (\Delta_{\Gamma^c} \mathcal{R}\Lambda)$, we deduce that

$$(\Delta\Gamma) \cup (\mathcal{R}\Lambda) = (\Delta\Gamma) \cup (\Delta_{\Gamma^{c}}\mathcal{R}\Lambda) .$$
⁽²⁶⁾

Thus, with $\Lambda = \Gamma$, we obtain that $(\bigcup_{k=0}^{1} \mathcal{R}^{k})\Gamma = (\bigcup_{k=0}^{1} (\Delta_{\Gamma^{c}} \mathcal{R})^{k})\Gamma$, that is, assumption \mathcal{H}_{1} holds true.

Now, we suppose that, for a given $n \ge 1$, the induction assumption \mathcal{H}_n holds true. Then, we have that

$$(\cup_{k=0}^{n+1}\mathcal{R}^k)\Gamma = (\Delta\Gamma) \cup \left(\mathcal{R}\left((\cup_{k=0}^n\mathcal{R}^k)\right)\Gamma\right) \qquad (\text{using the convention } \mathcal{R}^0 = \Delta)$$
$$= (\Delta\Gamma) \cup \left(\Delta_{\Gamma^c}\mathcal{R}\left((\cup_{k=0}^n\mathcal{R}^k)\right)\Gamma\right)$$

using the preliminary result (26) but with the binary relation $\mathcal{R}((\cup_{k=0}^{n} \mathcal{R}^{k}))$

$$= (\Delta\Gamma) \cup \left(\Delta_{\Gamma^{c}} \mathcal{R} \left(\cup_{k=0}^{n} (\Delta_{\Gamma^{c}} \mathcal{R})^{k} \right) \Gamma \right) \qquad \text{(using the induction assumption } \mathcal{H}_{n})$$
$$= (\Delta\Gamma) \cup \left(\left(\cup_{k=1}^{n+1} (\Delta_{\Gamma^{c}} \mathcal{R})^{k} \right) \Gamma \right)$$
$$= \left(\cup_{k=0}^{n+1} (\Delta_{\Gamma^{c}} \mathcal{R})^{k} \right) \Gamma . \qquad \text{(as } (\Delta_{\Gamma^{c}} \mathcal{R})^{0} = \Delta)$$

Thus, we have proven the induction assumption \mathcal{H}_{n+1} .

Now, let us suppose that $\gamma \in \mathcal{R}^*\Gamma$. Then, there exists a positive integer $n \geq 1$ such that $\gamma \in (\bigcup_{k=0}^n \mathcal{R}^k)\Gamma$; using the just proven property \mathcal{H}_n , we get that $\gamma \in (\bigcup_{k=0}^n (\Delta_{\Gamma^c} \mathcal{R})^k)\Gamma$ and, therefore, $\gamma \in (\Delta_{\Gamma^c} \mathcal{R})^*\Gamma$. Thus, we have shown that $\mathcal{R}^*\Gamma \subset (\Delta_{\Gamma^c} \mathcal{R})^*\Gamma$. The converse inclusion is easier to prove as $\Delta_{\Gamma^c} \mathcal{R} \subset \mathcal{R}$. Finally, we have shown the equality $\mathcal{R}^*\Gamma = (\Delta_{\Gamma^c} \mathcal{R})^*\Gamma$, which is (25).

• (Lemma L7_E27) The following inclusion is easy to prove:

$$\forall \mathcal{R} \subset \mathcal{V} \times \mathcal{V} , \ \forall \Gamma \subset \mathcal{V} , \ \Delta_{\mathcal{R}\Gamma} \subset \mathcal{R} \Delta_{\Gamma} \mathcal{R}^{-1} .$$
(27)

• (Lemma L7_E28) We prove that

$$\mathcal{E}^{W*}\Delta_W \mathcal{E}^{-W*} = \mathcal{E}^{W*}\Delta_{(\mathcal{E}^*W)} \mathcal{E}^{-W*} .$$
⁽²⁸⁾

Using Equation (25) with $\mathcal{R}=\mathcal{E}$ and $\Gamma=W$ gives $\mathcal{E}^*W = (\Delta_W c \mathcal{E})^*W = \mathcal{E}^{W*}W$. Combined with the Inclusion (27), we get $\Delta_{\mathcal{E}^*W} = \Delta_{\mathcal{E}^{W*}W} \subset \mathcal{E}^{W*}\Delta_W \mathcal{E}^{-W*}$. Thus, we obtain that

$$\mathcal{E}^{W*}\Delta_{(\mathcal{E}^*W)}\mathcal{E}^{-W*}\subset \mathcal{E}^{W*}(\mathcal{E}^{W*}\Delta_W\mathcal{E}^{-W*})\mathcal{E}^{-W*}=\mathcal{E}^{W*}\Delta_W\mathcal{E}^{-W*}.$$

Thus, we have obtained the inclusion $\mathcal{E}^{W*}\Delta_W \mathcal{E}^{-W*} \supset \mathcal{E}^{W*}\Delta_{(\mathcal{E}^*W)} \mathcal{E}^{-W*}$. The reverse inclusion follows from the fact that $W \subset \overline{W}^{\mathcal{E}} = \mathcal{E}^*W$ by (21), which gives $\mathcal{E}^{W*}\Delta_W \mathcal{E}^{-W*} \subset \mathcal{E}^{W*}\Delta_{(\mathcal{E}^*W)} \mathcal{E}^{-W*}$.

• (Lemma L7) Finally, we prove that $\mathcal{A}^W = \mathcal{A}^W_*$. For that purpose, it suffices to show that replacing the subexpressions Δ_W by $\Delta_{(\mathcal{E}^*W)}$ in the expression (18g) of \mathcal{A}^W does not change the relation. Using the definition of \mathcal{A}^W in Equation (18g), we obtain that Δ_W appears only in subexpressions of the form $\mathcal{B}^W \Delta_W \mathcal{B}^{-W}$ or $\mathcal{K}^W \Delta_W \mathcal{B}^{-W}$ or $\mathcal{B}^W \Delta_W \mathcal{K}^W$ or $\mathcal{K}^W \Delta_W \mathcal{K}^W$. Now, using the fact that the two relations \mathcal{B}^W and \mathcal{K}^W always end with \mathcal{E}^{W*} and the two relation \mathcal{B}^{-W} and \mathcal{K}^W always start with \mathcal{E}^{-W*} we obtain that Δ_W appears only in subexpressions of the form $\mathcal{E}^{W*} \Delta_W \mathcal{E}^{-W*}$. We conclude, using Equation (28), that Δ_W can be replaced by $\Delta_{(\mathcal{E}^*W)}$ in \mathcal{A}^W without changing the relation.

This ends the proof.

C Proof of
$$\gamma \mathcal{A}^{\scriptscriptstyle W}_* \lambda \implies \neg(\gamma \parallel \lambda \mid W)$$

The following Proposition 8, that we are going to prove, is half of the proof of Theorem 5. It relies on six postponed lemmata given in this Appendix C.

C.1 Proposition 8

Proposition 8 (Coq **Proposition** P8) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. Let $\gamma, \lambda \in \mathcal{V}$ be vertices.

We have the implication

$$\gamma \mathcal{A}^{W}_{*} \lambda \implies \neg \left(\gamma \perp \lambda \mid W \right)$$
(29)

where \mathcal{A}^{W}_{*} is the star conditional active relation (23) and \coprod_{d} is the conditional directional separation relation (17).

Proof. Let $\gamma, \lambda \in \mathcal{V}$ be vertices, and assume that $\gamma \mathcal{A}^{W}_{*} \lambda$ where \mathcal{A}^{W}_{*} is the conditional active relation (23). We start by proving that either $\gamma = \lambda$ or there exists an active extended-oriented path ρ , joining the vertices γ and λ .

Now, by (23), giving \mathcal{A}^{W}_{*} , we have that

$$\gamma \bigg(\Delta \cup \mathcal{B}^{W} \cup \mathcal{B}^{-W} \cup \mathcal{K}^{W} \cup \big((\mathcal{B}^{W} \cup \mathcal{K}^{W}) \mathcal{C}^{W}_{*} (\mathcal{B}^{-W} \cup \mathcal{K}^{W}) \big) \bigg) \lambda .$$

We consider the five cases, one by one. The first case is $\gamma \Delta \lambda$, that is, $\gamma = \lambda$ and the conclusion is immediate. Now, for each of the remaining case, we are going to show that there exists $\rho \in$ $D_U[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ that joins γ and λ , recalling that the deployment $D_U[\mathcal{R} \mid \mathcal{V}, \mathcal{E}]$ in extended-oriented paths of a binary relation \mathcal{R} has been defined in (15).

The second case is $\gamma \mathcal{B}^W \lambda$. We conclude that there exists $\rho \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ thanks to (32) in Lemma 10.

The third case is $\gamma \mathcal{B}^{-W} \lambda$. We conclude that there exists $\rho \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ thanks to (33) in Lemma 11.

The fourth case is $\gamma \mathcal{K}^W \lambda$. We conclude that there exists $\rho \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ thanks to (34) in Lemma 12.

The fifth case is $\gamma \left(\left(\mathcal{B}^W \cup \mathcal{K}^W \right) \mathcal{C}^W_* \left(\mathcal{B}^{-W} \cup \mathcal{K}^W \right) \right) \lambda$. We conclude that there exists $\rho \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ thanks to (37) in Lemma 14.

Finally, we successively have that

$$\gamma \mathcal{A}^{W}_{*} \lambda \implies (\gamma = \lambda) \lor \exists \rho \in D_{U}[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \cap U^{W}_{a}(\mathcal{V}, \mathcal{E}) \qquad (\text{as just proved above}) \\ \implies \neg \Big((\gamma = \lambda) \lor D_{U}[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \subset U^{W}_{b}(\mathcal{V}, \mathcal{E}) \Big)$$

by definition of the subset $U_b^W(\mathcal{V}, \mathcal{E}) = (U_a^W(\mathcal{V}, \mathcal{E}))^{\mathsf{c}}$ of all blocked extended-oriented paths (see Definition 2)

$$\implies \neg \left(\gamma \perp \lambda \mid W \right) \,. \tag{by (17) in Definition 3)}$$

This ends the proof.

C.2 Proof of Proposition 8 broken in six lemmata

The first Lemma 9 is instrumental for the following five lemmata. It is used to obtain active extended-oriented path by concatenation. Then, the following lemmata display elementary relational patterns (composition of relations) whose deployment in edge paths contain active extended-oriented paths. For each relation, an explicit active extended-oriented path is built.

The binary relations used below have been introduced in Definition 4, except for the two additional ones defined in (22) and in (23). For any positive integer $n \ge 1$, we denote by $\mathbf{1}_n = (+1, \ldots, +1)$ (resp. $-\mathbf{1}_n = (-1, \ldots, -1)$) the vector of length n made of +1 (resp. of -1).

C.2.1 Concatenation of extended-oriented paths in a graph

We recall that $U(\mathcal{V}, \mathcal{E})$ in (9c) is the set of extended-oriented paths of positive length relative to the graph $(\mathcal{V}, \mathcal{E})$. Now, we develop the machinery to analyze active extended-oriented paths by considering decomposition into subpaths and junctions when reconcatenating. For this purpose, we need notation.

We denote by $\Omega^{\flat} : U(\mathcal{V}, \mathcal{E}) \to U_1(\mathcal{V}, \mathcal{E})$ (resp. $\Omega^{\sharp} : U(\mathcal{V}, \mathcal{E}) \to U_1(\mathcal{V}, \mathcal{E})$ the projection on the tail (resp. head) subpath of an extended-oriented path, defined, for $\rho \in U_n(\mathcal{V}, \mathcal{E})$ and $n \ge 1$, by

$$\Omega^{\flat}(\rho) = \Omega^{\flat}\left(\left\{\left(v_{i}^{\flat}, v_{i}^{\sharp}, o_{i}\right)\right\}_{i \in \llbracket 1, n \rrbracket}\right) = \left\{\left(v_{1}^{\flat}, v_{1}^{\sharp}, o_{1}\right)\right\},\tag{30a}$$

$$\Omega^{\sharp}(\rho) = \Omega^{\sharp}\left(\left\{\left(v_{i}^{\flat}, v_{i}^{\sharp}, o_{i}\right)\right\}_{i \in [\![1,n]\!]}\right) = \left\{\left(v_{n}^{\flat}, v_{n}^{\sharp}, o_{n}\right)\right\}.$$
(30b)

The extended-oriented path $\Omega^{\flat}(\rho)$ (resp. $\Omega^{\sharp}(\rho)$), depicted in Figure 5, is an extended-



Figure 5: Projection on the tail (resp. head) subpath of an extended-oriented path

oriented path of length one built with the first (resp. last) extended-oriented edge of the extended-oriented path (ρ).

The following Lemma 9 is a straightforward consequence of the definitions of active extended-oriented paths in $U_a^W(\mathcal{V}, \mathcal{E})$ (see Definition 2), of concatenation \ltimes in (14) and of the projection mappings Ω^{\flat} and Ω^{\sharp} in (30). The proof is left to the reader.

Lemma 9 (Coq Lemma Active_path_cat) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. Let $\rho \in U(\mathcal{V}, \mathcal{E})$ be an extended-oriented path of length $n \geq 2$. We have that

$$\rho \in U_a^W(\mathcal{V}, \mathcal{E}) \iff \exists \rho', \rho'' \in U_a^W(\mathcal{V}, \mathcal{E}) , \ \rho = \rho' \ltimes \rho'' , \ \Omega^{\sharp}(\rho') \ltimes \Omega^{\flat}(\rho'') \in U_a^W(\mathcal{V}, \mathcal{E}) .$$
(31)

This Lemma 9 is mathematically simple, but more involved in Coq where manipulation of active extended-oriented paths is more tedious, as it frequently requires proofs by induction on path lengths.

C.2.2 Case $\gamma \mathcal{B}^W \lambda$

Lemma 10 (Coq Lemma L10) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any vertices $\gamma, \lambda \in \mathcal{V}$, we have that

$$\gamma \mathcal{B}^{W} \lambda \implies \text{there exists } \rho \in U(\mathcal{V}, \mathcal{E}) \text{ such that } \rho = \pi^{-1}(\varrho, \mathbf{1}_{|\varrho|}) \text{ and} \\ \rho \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) .$$
(32)

Proof. We prove the implication (32). Let γ , $\lambda \in \mathcal{V}$ be such that $\gamma \mathcal{B}^W \lambda$. By (18b), we have that $\mathcal{B}^W \lambda = \mathcal{E}(\Delta_{W^c} \mathcal{E})^*$, hence that $\gamma \mathcal{E}(\Delta_{W^c} \mathcal{E})^* \lambda$. As $(\Delta_{W^c} \mathcal{E})^* = \Delta \cup \bigcup_{n=1}^{\infty} (\Delta_{W^c} \mathcal{E})^n$ by definition, if $\gamma \mathcal{E}(\Delta_{W^c} \mathcal{E})^* \lambda$, then either $\gamma \mathcal{E} \lambda$ or there exists $n \geq 1$ such that $\gamma \mathcal{E}(\Delta_{W^c} \mathcal{E})^n \lambda$. Thus, we consider two cases.

If $\gamma \mathcal{E}\lambda$, the extended-oriented path $\{(\gamma, \lambda, +1)\}$ is both in $D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}]$, by definition (15), and belongs to $U_a^W(\mathcal{V}, \mathcal{E})$, as it is of length 1 hence is active (see Definition 2).

If $\gamma \mathcal{E}(\Delta_{W^c} \mathcal{E})^n \lambda$, with $n \geq 1$, then there exists a sequence $\{v_i\}_{i \in [0,n+1]}$ in \mathcal{V} such that $v_0 = \gamma$, $v_{n+1} = \lambda$, and $v_{i-1} \mathcal{E}v_i$, $v_i \in W^c$, $v_i \mathcal{E}v_{i+1}$, for $i \in [1, n]$. The following $\rho = \pi^{-1}(\{(v_i, v_{i+1})\}_{i \in [0,n]}, \mathbf{1}_{n+1})$ is an extended-oriented path that belongs to $D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}]$, as $\varpi(\rho) = (\gamma, \lambda)$, and also to $U_a^W(\mathcal{V}, \mathcal{E})$. Indeed, all the extended-oriented subpaths $\{(v_{i-1}, v_i, +1), (v_i, v_{i+1}, +1)\}$ for $i \in [[1, n]]$, satisfy Item 16a in Definition 2 because $v_i \in W^c$.

This ends the proof.

C.2.3 Case $\gamma \mathcal{B}^{-W} \lambda$

Lemma 11 (Coq Lemma L11) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any vertices $\gamma, \lambda \in \mathcal{V}$, we have that

$$\gamma \mathcal{B}^{-W} \lambda \implies \text{there exists } \rho \in U(\mathcal{V}, \mathcal{E}) \text{ such that } \rho = \pi^{-1}(\varrho, -\mathbf{1}_{|\varrho|}) \text{ and} \\ \rho \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) .$$
(33)

Proof. We prove the implication (33) in the same way as for implication (32) in Lemma 10 (here, all the extended-oriented subpaths satisfy Item 16b in Definition 2). \Box

C.2.4 Case $\gamma \mathcal{K}^W \lambda$

Lemma 12 (Coq Lemma L12) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any vertices $\gamma, \lambda \in \mathcal{V}$, we have that

$$\gamma \mathcal{K}^{W} \lambda \implies \text{there exists } \rho = \pi^{-1}(\varrho, o) \in U(\mathcal{V}, \mathcal{E}), \text{ with } |\rho| \ge 2$$

and $o = (-1, \dots, +1) \in \{-1\} \times \{-1, +1\}^{|\rho|-2} \times \{+1\}, \text{ such that}$
$$\rho = \pi^{-1}(\varrho, o) = \pi^{-1}(\varrho, (-1, \dots, +1)) \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}).$$
(34)

Proof. We prove the implication (34). Let $\gamma, \lambda \in \mathcal{V}$ be such that $\gamma \mathcal{K}^W \lambda$. By definition (18e) of \mathcal{K}^W , we obtain that $\gamma \mathcal{B}^{-W} \Delta_{W^c} \mathcal{B}^W \lambda$. As a consequence of the definition of the composition of relations, there exists $\delta \in W^c$ such that $\gamma \mathcal{B}^{-W} \delta$ and $\delta \mathcal{B}^W \lambda$. Thus, by (33), there exists $\rho' = \pi^{-1}(\varrho', -\mathbf{1}_{|\varrho'|}) \in D_U[(\gamma, \delta) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$ and by (32), there exists $\rho'' = \pi^{-1}(\varrho'', \mathbf{1}_{|\varrho''|}) \in D_U[(\delta, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$. We consider the extended-oriented path $\rho = \rho' \ltimes \rho'' \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}]$ obtained by concatenation as in (14), and which is such that $|\rho| \geq 2$. We claim that $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$. Indeed, $\rho' \in U_a^W(\mathcal{V}, \mathcal{E})$ and $\rho'' \in U_a^W(\mathcal{V}, \mathcal{E})$ by assumption, so that, by Equation (31) in Lemma 9, it only remains to show that

$$\left\{(v',\delta,-1),(\delta,v'',+1)\right\} = \Omega^{\sharp}(\rho') \ltimes \Omega^{\flat}(\rho'') \in U_{a}^{W}(\mathcal{V},\mathcal{E}) ,$$

where (v', δ) is the first edge of the extended-oriented path $\rho' = \pi^{-1}(\varrho', -\mathbf{1}_{|\varrho'|})$ and (δ, v'') is the last edge of the extended-oriented path $\rho'' = \pi^{-1}(\varrho'', \mathbf{1}_{|\varrho''|})$. Now, the above subpath satisfies Item 16c in Definition 2 because $v_i \in W^{\mathsf{c}}$. We deduce that $\rho = \rho' \ltimes \rho'' = \pi^{-1}((\varrho', \varrho''), (-\mathbf{1}_{|\varrho'|}, \mathbf{1}_{|\varrho''|})) \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}).$

This ends the proof.

C.2.5 Case $\gamma C^{W}_{*} \lambda$

Lemma 13 (Coq lemmata L13_1 and L13_2) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any vertices $\gamma, \lambda \in \mathcal{V}$, we have that

$$\gamma \mathcal{C}^{W}_{*} \lambda \implies \gamma \in \overline{W}^{\mathcal{E}}, \ \lambda \in \overline{W}^{\mathcal{E}} \quad and \ \gamma = \lambda \quad or$$

$$there \ exists \ \rho = \pi^{-1}(\varrho, o) \in U(\mathcal{V}, \mathcal{E}), \ with \ |\rho| \ge 2$$

$$and \ o = (-1, \dots, +1) \in \{-1\} \times \{-1, +1\}^{|\rho|-2} \times \{+1\}, \ such \ that$$

$$\rho = \pi^{-1}(\varrho, o) = \pi^{-1}(\varrho, (-1, \dots, +1)) \in D_{U}[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U^{W}_{a}(\mathcal{V}, \mathcal{E}) .$$
(35)

Proof. We prove the implication (35). We suppose that $\gamma C^w_* \lambda$. As $\mathcal{C}^W_* = \Delta_{\overline{W}} \varepsilon \cup \left(\Delta_{\overline{W}} \varepsilon \mathcal{K}^W \Delta_{\overline{W}} \varepsilon \right)^+$ by (22), we consider three cases: either $\gamma \Delta_{\overline{W}} \varepsilon \lambda$, or $\gamma \Delta_{\overline{W}} \varepsilon \mathcal{K}^W \Delta_{\overline{W}} \varepsilon \lambda$ or there exists $n \ge 1$ such that $\gamma \left(\Delta_{\overline{W}} \varepsilon \mathcal{K}^{W} \Delta_{\overline{W}} \varepsilon \right)^{n+1} \lambda.$ Suppose that $\gamma \Delta_{\overline{W}} \varepsilon \lambda$. Then $\gamma = \lambda$, and thus we have obtain the implication (35).

Suppose that $\gamma \Delta_{\overline{W}}^{\mathcal{L}} \mathcal{K}^W \Delta_{\overline{W}} \mathcal{E} \lambda$. Then, $\gamma \in \overline{W}^{\mathcal{E}}$, $\lambda \in \overline{W}^{\mathcal{E}}$ and $\gamma \mathcal{K}^W \lambda$. Therefore, by (34) there exists $\rho \in U(\mathcal{V}, \mathcal{E})$, with $|\rho| \geq 2$, and $o \in \{-1\} \times \{-1, +1\}^{|\rho|-2} \times \{+1\}$ such that $\pi^{-1}(\varrho, o) \in \mathbb{C}$ $D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}).$

Suppose that $\gamma(\Delta_{\overline{W}} \mathcal{E} \mathcal{K}^W \Delta_{\overline{W}} \mathcal{E})^{n+1} \lambda$. Then, there exists a sequence $\{\delta_i\}_{i \in [\![0,n+1]\!]}$ in $\overline{W}^{\mathcal{E}}$ such that $\delta_0 = \gamma$, $\delta_{n+1} = \lambda$ and $\delta_i \mathcal{K}^W \delta_{i+1}$ for $i \in [\![0,n]\!]$. Therefore, by (34), there exists a sequence $\{\rho^{(i)}\}_{i \in [\![0,n]\!]}$ in $U(\mathcal{V}, \mathcal{E})$ of extended-oriented paths such that $|\rho^{(i)}| \geq 2$ for $i \in [\![0,n]\!]$, and that $\rho^{(i)} = 0$. $\pi^{-1}(\varrho^{(i)}, o^{(i)}) \in D_U[(\delta_i, \delta_{i+1}) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) \text{ for } i \in [0, n], \text{ where } o^{(i)} \text{ is of the form } (-1, \ldots, +1).$ We define the extended-oriented path $\rho = \rho^{(0)} \ltimes \cdots \ltimes \rho^{(n)} \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}]$, by iterated (associative) concatenation as in (14), which is such that $|\rho| \geq 2$ and that

$$\rho = \pi^{-1}(\varrho^{(0)} \ltimes \cdots \ltimes \varrho^{(n)}, (o^{(0)}, \dots, o^{(n)})) \text{ where } o^{(i)} \in \{-1\} \times \{-1, +1\}^{|\varrho_i|-2} \times \{+1\}, \ \forall i \in [\![0, n]\!].$$

We claim that $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$. Indeed, $\rho^{(i)} \in U_a^W(\mathcal{V}, \mathcal{E})$ for $i \in [0, n]$, so that, by Equation (31) in Lemma 9, it only remains to show that, for $i \in [0, n-1]$,

$$\left\{ (v_i^{\flat}, \delta_{i+1}, +1), (\delta_{i+1}, v_{i+1}^{\sharp}, -1) \right\} = \Omega^{\sharp}(\rho_i) \ltimes \Omega^{\flat}(\rho_{i+1}) \in U_a^W(\mathcal{V}, \mathcal{E}) , \qquad (36)$$

where $(v_i^{\flat}, \delta_{i+1})$ is the last edge of the extended-oriented path $\rho^{(i)} = \pi^{-1}(\varrho^{(i)}, o^{(i)})$ and $(\delta_{i+1}, v_{i+1}^{\sharp})$ is the first edge of the extended-oriented path $\rho^{(i+1)} = \pi^{-1}(\rho^{(i+1)}, o^{(i+1)})$. As $\delta_{i+1} \in \overline{W}^{\varepsilon}$, for $i \in [0, n-1]$, and because of the orientation (-1, +1), all the above subpaths satisfy Item 16d in Definition 2. We conclude that $\rho = \rho^{(0)} \ltimes \cdots \ltimes \rho^{(n)} \in D_U[(\gamma, \lambda) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}).$

This ends the proof.

C.2.6 Case
$$\gamma \Big((\mathcal{B}^{W} \cup \mathcal{K}^{W}) \mathcal{C}^{W}_{*} (\mathcal{B}^{-W} \cup \mathcal{K}^{W}) \Big) \lambda$$

Lemma 14 (Coq Lemma L14) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any vertices γ , $\lambda \in \mathcal{V}$, we have that

$$\gamma\Big(\big(\mathcal{B}^{W}\cup\mathcal{K}^{W}\big)\mathcal{C}^{W}_{*}\big(\mathcal{B}^{-W}\cup\mathcal{K}^{W}\big)\Big)\lambda \implies \text{there exists } \rho\in U(\mathcal{V},\mathcal{E}), \text{ with } |\rho|\geq 2, \text{ such that} \\ \rho\in D_{U}[(\gamma,\lambda)\mid\mathcal{V},\mathcal{E}]\cap U_{a}^{W}(\mathcal{V},\mathcal{E}).$$
(37)

Proof. Suppose that $\gamma ((\mathcal{B}^W \cup \mathcal{K}^W)\mathcal{C}^W_*(\mathcal{B}^{-W} \cup \mathcal{K}^W))\lambda$. Therefore, there exist δ_1 and δ_2 in \mathcal{V} such that

 $\gamma(\mathcal{B}^W \cup \mathcal{K}^W) \delta_1$ and $\delta_1 \mathcal{C}^W_* \delta_2$ and $\delta_2(\mathcal{B}^{-W} \cup \mathcal{K}^W) \lambda$.

We are going to display an extended-oriented path $\rho \in D_U[(\delta, \gamma) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}).$

• Considering the left hand side $\gamma(\mathcal{B}^W \cup \mathcal{K}^W) \delta_1$ and using Lemma 10 and 12, we obtain either by (32) applied to $\gamma \mathcal{B}^W \delta_1$, or by (34) applied to $\gamma \mathcal{K}^W \delta_1$ — that there exists

$$\rho^{(1)} = \pi^{-1}(\varrho^{(1)}, o^{(1)}) = \pi^{-1}(\varrho^{(1)}, (\dots, +1)) \in D_U[(\gamma, \delta_1) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) .$$

• In the same way, considering the right hand side $\delta_2(\mathcal{B}^{-W} \cup \mathcal{K}^W)\lambda$ and using Lemma 11 and 12, we obtain — either by (33) applied to $\delta_2 \mathcal{B}^{-W}\lambda$, or by (34) applied to $\delta_2 \mathcal{K}^W \lambda$ — that there exists

$$\rho^{(2)} = \pi^{-1}(\varrho_2, o_2) = \pi^{-1}(\varrho^{(2)}, (-1, \ldots)) \in D_U[(\delta_2, \gamma) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$$

• Considering the middle expression $\delta_1 \mathcal{C}^W_* \delta_2$ and using Lemma 13, we obtain by (35) that $\delta_1 \in \overline{W}^{\mathcal{E}}, \, \delta_2 \in \overline{W}^{\mathcal{E}}$, and that there exists

$$\rho' = \pi^{-1}(\varrho', o') = \pi^{-1}(\varrho', (-1, \dots, +1)) \in D_U[(\delta_1, \delta_2) \mid \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E}) .$$

We consider the extended-oriented path $\rho = \rho^{(1)} \ltimes \rho' \ltimes \rho^{(2)}$ obtained by concatenation as in (14). By construction, we have that $\rho \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}]$. We claim that $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$. Indeed, $\rho^{(1)}, \rho', \rho^{(2)} \in U_a^W(\mathcal{V}, \mathcal{E})$ by assumption, so that, by Equation (31) in Lemma 9, it only remains to show that

$$\left\{(v_1^{\flat}, \delta_1, +1), (\delta_1, v_1^{\sharp}, -1)\right\} = \Omega^{\sharp}(\rho^{(1)}) \ltimes \Omega^{\flat}(\rho') \in U_a^W(\mathcal{V}, \mathcal{E}) , \qquad (38)$$

where (v_1^{\flat}, δ_1) is the last edge of the extended-oriented path $\rho^{(1)}$ and (δ_1, v_1^{\sharp}) is the first edge of the extended-oriented path ρ' , and that

$$\left\{ (v_2^{\flat}, \delta_2, +1), (\delta_2, v_2^{\sharp}, -1) \right\} = \Omega^{\sharp}(\rho') \ltimes \Omega^{\flat}(\rho^{(2)}) \in U_a^W(\mathcal{V}, \mathcal{E}) , \qquad (39)$$

where (v_2^{\flat}, δ_2) is the last edge of the extended-oriented path ρ' and (δ_2, v_2^{\sharp}) is the first edge of the extended-oriented path $\rho^{(2)}$. As $\delta_1, \delta_2 \in \overline{W}^{\mathcal{E}}$ and because of the orientation (-1, +1), the two subpaths hereabove satisfy Item 16d in Definition 2. We conclude that $\rho \in D_U[(\gamma, \lambda) | \mathcal{V}, \mathcal{E}] \cap U_a^W(\mathcal{V}, \mathcal{E})$.

This ends the proof.

The following Proposition 15, that we are going to prove, is the second half of the proof of Theorem 5. It relies on the three Lemmata 16, 17 and 18, postponed at the end of this Appendix D.

D.1 Proposition 15

Proposition 15 (Coq Proposition P15) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. Let $\gamma, \lambda \in \mathcal{V}$ be vertices. We have the implication

$$\neg \left(\gamma \perp_{d} \lambda \mid W \right) \implies \gamma \mathcal{A}_{*}^{W} \lambda \tag{40}$$

where \mathcal{A}^{W}_{*} is the star conditional active relation (23) and $\perp d$ is the conditional directional separation relation (17).

Proof. Let $\gamma, \lambda \in \mathcal{V}$ be vertices. We show that $\neg(\gamma \coprod_d \lambda \mid W) \implies \gamma \mathcal{A}^W_* \lambda$ or, equivalently (see (17) in Definition 3), that $(\gamma = \lambda) \lor (D_U[\{(\gamma, \lambda)\} \mid \mathcal{V}, \mathcal{E}] \cap U^W_a(\mathcal{V}, \mathcal{E}) \neq \emptyset) \implies \gamma \mathcal{A}^W_* \lambda$. First, when $\gamma = \lambda$ it is clear that $\gamma \mathcal{A}^W_* \lambda$ as $\Delta \subset \mathcal{A}^W_*$ by (23). Second, we assume that there exists an extended-oriented path $\rho \in U(\mathcal{V}, \mathcal{E})$ joining the two vertices γ and λ and such that ρ is active. We are going to prove that $\gamma \mathcal{A}^W_* \lambda$.

- If the path length of ρ is equal to 1, then, by definition (9c) of $U_1(\mathcal{V}, \mathcal{E})$, we necessarily have that either $\gamma \mathcal{E}\lambda$, or $\gamma \mathcal{E}^{-1}\lambda$. Now, as $\mathcal{E} \subset \mathcal{B}^W \subset \mathcal{A}^W_*$ by (23), as $\mathcal{E}^{-1} \subset \mathcal{B}^{-W} \subset \mathcal{A}^W_*$ by (23), we conclude that $\gamma \mathcal{A}^W_* \lambda$.
- If the path length of ρ is ≥ 2 , we prove by induction that we have either $\gamma \mathcal{A}_{*+}^W \lambda$ or $\gamma \mathcal{A}_{*-}^W \lambda$, where the two relations \mathcal{A}_{*+}^W and \mathcal{A}_{*-}^W are defined in Equations (41a) and (41b).
 - The case where the path length of ρ is equal to 2 is treated in Lemma 17.
 - The proof by induction on the path length is done in Lemma 18.
 - We therefore conclude that $\gamma \mathcal{A}^{W}_{*} \lambda$ since $\mathcal{A}^{W}_{*} = \Delta \cup \mathcal{A}^{W}_{*+} \cup \mathcal{A}^{W}_{*-}$ by (42a), obtained in Lemma 16.

This ends the proof.

D.2 Proof of Proposition 15 broken in three lemmata

D.2.1 Definition and properties of $\mathcal{A}^{\scriptscriptstyle W}_{*+}$ and $\mathcal{A}^{\scriptscriptstyle W}_{*-}$

We introduce two binary relation \mathcal{A}_{*+}^{W} and \mathcal{A}_{*-}^{W} and establish three properties which are instrumental in the next lemmata 17 and 18.

Lemma 16 (Coq Lemma L16_E42a, L16_E42b and L16_E42c) The two following relations

$$\mathcal{A}_{*+}^{W} = \mathcal{B}^{W} \cup \mathcal{K}^{W} \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{K}^{W} \right),$$
(41a)

$$\mathcal{A}_{*-}^{W} = \mathcal{B}^{-W} \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{B}^{-W} \right),$$
(41b)

satisfy the following properties

$$\mathcal{A}^{W}_{*} = \Delta \cup \mathcal{A}^{W}_{*+} \cup \mathcal{A}^{W}_{*-} , \qquad (42a)$$

$$\mathcal{A}_{*+}^{W} \supset \mathcal{A}_{*-}^{W} \Delta_{W^{c}} \mathcal{E} , \qquad (42b)$$

$$\mathcal{A}_{*-}^{W} \supset \mathcal{A}_{*+}^{W} \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} .$$
(42c)

Proof. • (Lemma L16_E42a) We prove (42a) as follows:

$$\mathcal{A}^{W}_{*} = \Delta \cup \mathcal{B}^{W} \cup \mathcal{B}^{-W} \cup \mathcal{K}^{W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W}\right) \mathcal{C}^{W}_{*} \left(\mathcal{B}^{-W} \cup \mathcal{K}^{W}\right) \qquad \text{(by definition (23) of } \mathcal{A}^{W}_{*})$$
$$= \Delta \cup \underbrace{\mathcal{B}^{W} \cup \mathcal{K}^{W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W}\right) \mathcal{C}^{W}_{*} \mathcal{K}^{W}}_{=\mathcal{A}^{W}_{*+} \text{by (41a)}} \cup \underbrace{\mathcal{B}^{-W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W}\right) \mathcal{C}^{W}_{*} \mathcal{B}^{-W}}_{=\mathcal{A}^{W}_{*-} \text{by (41b)}}.$$

• (Lemma L16_E42b) We prove (42b) as follows:

$$\begin{aligned} \mathcal{A}_{*-}^{W} \Delta_{W^{c}} \mathcal{E} &= \left(\mathcal{B}^{-W} \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{B}^{-W} \right) \right) \Delta_{W^{c}} \mathcal{E} & \text{(by definition (41b) of } \mathcal{A}_{*-}^{W}) \\ &= \left(\Delta \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \right) \right) \mathcal{B}^{-W} \Delta_{W^{c}} \mathcal{E} & \text{(by factorizing } \mathcal{B}^{-W}) \\ &\subset \left(\Delta \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \right) \right) \mathcal{B}^{-W} \Delta_{W^{c}} \mathcal{B}^{W} & \text{(as } \mathcal{E} \subset \mathcal{B}^{W} \text{ by (18b)}) \\ &= \left(\Delta \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \right) \right) \mathcal{K}^{W} & \text{(by definition (18e) of } \mathcal{K}^{W}) \\ &= \mathcal{K}^{W} \cup \left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{K}^{W} & \text{(by definition (14e) of } \mathcal{A}_{*+}^{W}) \\ &\subset \mathcal{A}_{*+}^{W} & \text{(by definition (41a) of } \mathcal{A}_{*+}^{W}) \end{aligned}$$

• (Lemma L16_E42c) We prove (42c) as follows:

$$\mathcal{A}_{*+}^{W} \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} = \left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{K}^{W} \right) \right) \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} \qquad \text{(by definition (41a) of } \mathcal{A}_{*+}^{W})$$
$$= \left((\mathcal{B}^{W} \cup \mathcal{K}^{W}) \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} \right) \cup \left(\left(\mathcal{B}^{W} \cup \mathcal{K}^{W} \right) \mathcal{C}_{*}^{W} \mathcal{K}^{W} \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} \right). \qquad \text{(by developing)}$$

We treat each of the two terms in the union separately. We are going to show that each term is included in \mathcal{A}^W_{*-} .

For the first term, we have that

$$(\mathcal{B}^{W}\cup\mathcal{K}^{W})\Delta_{\overline{W}^{\mathcal{E}}}\mathcal{E}^{-1}\subset (\mathcal{B}^{W}\cup\mathcal{K}^{W})\mathcal{C}_{*}^{W}\mathcal{B}^{-W}$$

as $\Delta_{\overline{W}} \varepsilon \subset \mathcal{C}^W_*$ by (22), and as $\mathcal{E}^{-1} \subset \mathcal{B}^{-W}$ by (18d)

$$\subset \mathcal{A}_{*-}^{W}$$
. (as $\mathcal{A}_{*-}^{W} = \mathcal{B}^{-W} \cup ((\mathcal{B}^{W} \cup \mathcal{K}^{W})\mathcal{C}_{*}^{W}\mathcal{B}^{-W})$ by definition (41b))

For the second term, we have that

$$\begin{aligned} \left(\mathcal{B}^{W}\cup\mathcal{K}^{W}\right)\mathcal{C}_{*}^{W}\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\mathcal{E}^{-1} \\ &= \left(\mathcal{B}^{W}\cup\mathcal{K}^{W}\right)\left(\left(\Delta_{\overline{W}}\varepsilon\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\right)^{+}\cup\Delta_{\overline{W}}\varepsilon\right)\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\mathcal{E}^{-1} \qquad \text{(by definition (22) of } \mathcal{C}_{*}^{W}) \\ &= \left(\mathcal{B}^{W}\cup\mathcal{K}^{W}\right)\left(\left(\Delta_{\overline{W}}\varepsilon\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\right)^{+}\cup\Delta_{\overline{W}}\varepsilon\right)\left(\Delta_{\overline{W}}\varepsilon\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\right)\mathcal{E}^{-1} \qquad \text{(by inserting } \Delta_{\overline{W}}\varepsilon) \\ &\subset \left(\mathcal{B}^{W}\cup\mathcal{K}^{W}\right)\left(\left(\Delta_{\overline{W}}\varepsilon\mathcal{K}^{W}\Delta_{\overline{W}}\varepsilon\right)^{+}\cup\Delta_{\overline{W}}\varepsilon\right)\mathcal{E}^{-1} \end{aligned}$$

as $(\mathcal{R}^+ \cup \Delta_{\overline{W}} \varepsilon)\mathcal{R} \subset \mathcal{R}^+$ for any relation \mathcal{R} such that $\mathcal{R}\Delta_{\overline{W}} \varepsilon = \Delta_{\overline{W}} \varepsilon \mathcal{R} = \mathcal{R}$, which is the case for $\mathcal{R} = \Delta_{\overline{W}} \varepsilon \mathcal{K}^W \Delta_{\overline{W}} \varepsilon$

$$= (\mathcal{B}^{W} \cup \mathcal{K}^{W})\mathcal{C}_{*}^{W}\mathcal{E}^{-1}$$
 (by definition (22) of \mathcal{C}_{*}^{W})

$$\subset (\mathcal{B}^{W} \cup \mathcal{K}^{W})\mathcal{C}_{*}^{W}\mathcal{B}^{-W}$$
 (as $\mathcal{E}^{-1} \subset \mathcal{B}^{-W}$ by (18d))

$$\subset \mathcal{A}_{*-}^{W}.$$
 (as $\mathcal{A}_{*-}^{W} = \mathcal{B}^{-W} \cup ((\mathcal{B}^{W} \cup \mathcal{K}^{W})\mathcal{C}_{*}^{W}\mathcal{B}^{-W})$ by definition (41b))

We conclude that $\mathcal{A}_{*+}^{W}\Delta_{\overline{W}} \mathcal{E}^{-1} \subset \mathcal{A}_{*-}^{W}$.

This ends the proof.

D.2.2 Case of active extended-oriented path of length 2

The following Lemma 17 is instrumental in the proof of Proposition 15. It covers the easy case of active extended-oriented paths of length 2.

Lemma 17 (Coq Lemma L17) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. Let $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$ be a given active extended-oriented path of length 2 (see Definition 2) with γ as head endpoint and λ as tail endpoint, that is, there exists a vertex $\delta \in \mathcal{V}$ such that

$$\rho = \left\{ (\gamma, \delta, o_1), (\delta, \lambda, o_2) \right\} \text{ with } (o_1, o_2) \in \mathcal{O}^2 .$$

$$(43)$$

Then, one of the following two possibilities holds true:

- 1. the extended-oriented path ρ ends with $o_2 = +1$ orientation, and then $\gamma \mathcal{A}_{*+}^W \lambda$.
- 2. the extended-oriented path ρ ends with $o_2 = -1$ orientation, and then $\gamma \mathcal{A}^{W}_{*-} \lambda$.

Proof. As ρ in (43) belongs to $U_a^W(\mathcal{V}, \mathcal{E})$ — hence to $U(\mathcal{V}, \mathcal{E})$, the set of extended-oriented paths of positive length in (9c) — we have that $(\gamma, \delta) \in \mathcal{E}$ if $o_1 = +1$, $(\gamma, \delta) \in \mathcal{E}^{-1}$ if $o_1 = -1$, $(\delta, \lambda) \in \mathcal{E}$ if $o_2 = +1$, and $(\delta, \lambda) \in \mathcal{E}^{-1}$ if $o_2 = -1$. Now, we consider the four conditions enumerated in Definition 2 which must be satisfied for the extended-oriented path ρ to be active and which impose constraints on the vertex δ according to the possible orientations.

- 1. First, we consider the case when the extended-oriented path ρ ends with +1 orientation, that is, when $o_2 = +1$.
 - Item 16a in Definition 2 corresponds to $o_1 = +1$, $o_2 = +1$ and $\delta \in W^{\mathsf{c}}$, which gives that $\gamma \mathcal{E}^{(+1)} \Delta_{W^{\mathsf{c}}} \delta$ and $\delta \Delta_{W^{\mathsf{c}}} \mathcal{E}^{(+1)} \lambda$. Hence, by composition of binary relations, we get that $\gamma \mathcal{E} \Delta_{W^{\mathsf{c}}} \mathcal{E} \lambda$, using the property $\Delta_{W^{\mathsf{c}}} \Delta_{W^{\mathsf{c}}} = \Delta_{W^{\mathsf{c}}}$.
 - Item 16c in Definition 2 corresponds to $o_1 = -1$, $o_2 = +1$ and $\delta \in W^c$, which gives that $\gamma \mathcal{E}^{(-1)} \Delta_{W^c} \delta$ and $\delta \Delta_{W^c} \mathcal{E}^{(+1)} \lambda$. Hence, we get that $\gamma \mathcal{E}^{-1} \Delta_{W^c} \mathcal{E} \lambda$.

We have obtained that the extended-oriented path ρ ends with orientation +1 and is such that either $\gamma \mathcal{E}\Delta_{W^c}\mathcal{E}\lambda$ or $\gamma \mathcal{E}^{-1}\Delta_{W^c}\mathcal{E}\lambda$. Using the properties that $\mathcal{E}\Delta_{W^c}\mathcal{E} \subset \mathcal{B}^W \subset \mathcal{A}^W_{*+}$ (by (18b) and (41a)) and that $\mathcal{E}^{-1}\Delta_{W^c}\mathcal{E} \subset \mathcal{K}^W \subset \mathcal{A}^W_{*+}$ (by (18e) and (41a)), we obtain that $\gamma \mathcal{A}^W_{*+}\lambda$.

- 2. Second, we consider the case when the extended-oriented path ρ ends with -1 orientation, that is, when $o_2 = -1$:
 - Item 16b in Definition 2 corresponds to $o_1 = -1$, $o_2 = -1$ and $\delta \in W^c$, which gives that $\gamma \mathcal{E}^{(-1)} \Delta_{W^c} \delta$ and $\delta \Delta_{W^c} \mathcal{E}^{(-1)} \lambda$. Hence, we get that $\gamma \mathcal{E}^{-1} \Delta_{W^c} \mathcal{E}^{-1} \lambda$,
 - Item 16d in Definition 2 corresponds to $o_1 = +1$, $o_2 = -1$ and $\delta \in \overline{W}^{\varepsilon}$, which gives that $\gamma \mathcal{E}^{(+1)} \Delta_{\overline{W}} \varepsilon \delta$ and $\delta \Delta_{\overline{W}} \varepsilon \mathcal{E}^{(-1)} \lambda$. Hence, we get that $\gamma \mathcal{E} \Delta_{\overline{W}} \varepsilon \mathcal{E}^{-1} \lambda$, using the property $\Delta_{\overline{W}} \varepsilon \Delta_{\overline{W}} \varepsilon = \Delta_{\overline{W}} \varepsilon$.

We have obtained that the extended-oriented path ρ ends with orientation -1 and is such that either $\gamma \mathcal{E}\Delta_{\overline{W}} \mathcal{E} \mathcal{E}^{-1} \lambda$ or $\gamma \mathcal{E}^{-1} \Delta_{W^{c}} \mathcal{E}^{-1} \lambda$. Using the properties that $\mathcal{E}\Delta_{\overline{W}} \mathcal{E} \mathcal{E}^{-1} \subset \mathcal{B}^{W} \Delta_{\overline{W}} \mathcal{E} \mathcal{B}^{-W} \subset \mathcal{A}_{*-}^{W}$ (by (18b) and (41b)) and that $\mathcal{E}^{-1} \Delta_{W^{c}} \mathcal{E}^{-1} \subset \mathcal{B}^{-W} \subset \mathcal{A}_{*-}^{W}$ (by (18d) and (41b)), we obtain that $\gamma \mathcal{A}_{*-}^{W} \lambda$.

This ends the proof.

D.2.3 Case of active extended-oriented path of length greater than 2

The following Lemma 18 is instrumental in the proof of Proposition 15. It covers by induction the case of active extended-oriented paths of length greater than 2.



Figure 6: Sketch of proof of induction Lemma 18 used in Proposition 15 in Appendix D

Lemma 18 (Coq Lemma L18) Let $(\mathcal{V}, \mathcal{E})$ be a graph, and $W \subset \mathcal{V}$ be a subset of vertices. For any $n \geq 2$ and $\gamma, \lambda \in \mathcal{V}$, the following statement holds true. For any extended-oriented path $\rho \in U_n(\mathcal{V}, \mathcal{E})$ of length n joining vertices γ and λ (that is, $\varpi_U(\rho) = (\gamma, \lambda)$ as in (12)), and such that ρ is active (that is, $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$ as in Definition 2), one of the two following properties is fullfiled:

- 1. Either $\gamma \mathcal{A}_{*+}^{W} \lambda$ and the last orientation of ρ is $o_n = +1$,
- 2. Or $\gamma \mathcal{A}_{*-}^{W} \lambda$ and the last orientation of ρ is $o_n = -1$.

Proof. We call \mathcal{H}_n the statement in Lemma 18 and we prove by induction that it is satisfied for all $n \geq 2$.

The proof of \mathcal{H}_2 is given by Lemma 17.

We suppose that the induction assumption \mathcal{H}_{n-1} holds true, where $n-1 \geq 2$, and we are going to show that \mathcal{H}_n holds true. For this purpose, we consider an extended-oriented path ρ of length n $(n \geq 2)$, joining vertices γ and λ in the graph $(\mathcal{V}, \mathcal{E})$, and which is active, that is,

$$\rho \in U_n(\mathcal{V}, \mathcal{E})$$
 and $\varpi_U(\rho) = (\gamma, \lambda)$ and $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$.

We decompose the extended-oriented path ρ as

$$\rho = \{ (v_i^{\flat}, v_i^{\sharp}, o_i) \}_{i \in \llbracket 1, n \rrbracket} = \rho' \times \rho'' ,$$

where $\rho' = \{(v_i^{\flat}, v_i^{\sharp}, o_i)\}_{i \in [\![1, n-1]\!]} \in U_{n-1}(\mathcal{V}, \mathcal{E})$ is an extended-oriented path of length n-1, and where $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, o_n)\} \in U_1(\mathcal{V}, \mathcal{E})$ is an extended-oriented path of length 1. We have that $v_1^{\flat} = \gamma$ and $v_n^{\sharp} = \lambda$. It is clear that the extended-oriented path ρ' is active, that is, $\rho' \in U_a^W(\mathcal{V}, \mathcal{E})$. Indeed, otherwise, the extended-oriented path ρ' would be in one of the four cases listed in Definition 3, hence so would be the extended-oriented path ρ . But this would contradict the assumption that $\rho \in U_a^W(\mathcal{V}, \mathcal{E})$. As the extended-oriented path ρ' is active and of length n-1, it satisfies the induction assumption \mathcal{H}_{n-1} . We deduce that either $\gamma \mathcal{A}_{**}^W v_{n-1}^{\sharp}$ and the last orientation of ρ' is $o_{n-1} = +1$, or $\gamma \mathcal{A}_{*-}^W v_{n-1}^{\sharp}$ and the last orientation of ρ' is $o_{n-1} = -1$. We analyze the two cases separately. Each case being subdivided in two cases, we will analyse four different cases as summarized in Figure 6.

• Assume that we have $\gamma \mathcal{A}_{*+}^{W} v_{n-1}^{\sharp}$ and that the last orientation of ρ' is $o_{n-1} = +1$, that is, ρ' ends with $(v_{n-1}^{\flat}, v_{n-1}^{\sharp}, +1)$. There are two possibilities for the extended-oriented path $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, o_n)\}$.

- Suppose that $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, +1)\} = \{(v_n^{\flat}, \lambda, +1)\}$, that is, $(v_n^{\flat}, \lambda) \in \mathcal{E}$ by (9). As the path ρ is active by assumption, the pattern $\{(v_{n-1}^{\flat}, v_{n-1}^{\sharp}, +1), (v_n^{\flat}, v_n^{\sharp}, +1)\}$ must satisfy Item 16a in Definition 2. We deduce that $v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$. Now, we wrap up the results obtained so far. On the one hand, from $\gamma \mathcal{A}_{*+}^W v_{n-1}^{\sharp}$, $v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$ and $(v_n^{\flat}, \lambda) \in \mathcal{E}$, we get that $\gamma \mathcal{A}_{*+}^W \Delta_{W^{\mathsf{c}}} \mathcal{E} \lambda$, hence that $\gamma \mathcal{A}_{*+}^W \lambda$ because the relation \mathcal{A}_{*+}^W in (41a) ends with the relation \mathcal{B}^W and as $\mathcal{B}^W \Delta_{W^{\mathsf{c}}} \mathcal{E} = \mathcal{E}(\Delta_{W^{\mathsf{c}}} \mathcal{E})^* (\Delta_{W^{\mathsf{c}}} \mathcal{E}) \subset \mathcal{B}^W$ by (18b). On the other hand, the extended-oriented path ρ of length n satisfies the case 1 of \mathcal{H}_n , since it ends with +1 and its endpoints are such that $\gamma \mathcal{A}_{*+}^W \lambda$. Therefore, we have proven the case 1 of the induction assumption \mathcal{H}_n for the extended-oriented paths of length n.
- Suppose that $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, -1)\} = \{(v_n^{\flat}, \lambda, -1)\}$, that is, $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$ by (9). As the path ρ is active, the pattern $\{(v_{n-1}^{\flat}, v_{n-1}^{\sharp}, +1), (v_n^{\flat}, v_n^{\sharp}, -1)\}$ must satisfy Item 16d in Definition 2. We deduce that $v_{n-1}^{\sharp} = v_n^{\flat} \in \overline{W}^{\mathcal{E}}$. Now, we wrap up the results obtained so far. On the one hand, from $\gamma \mathcal{A}_{*+}^W v_{n-1}^{\sharp}, v_{n-1}^{\sharp} = v_n^{\flat} \in \overline{W}^{\mathcal{E}}$ and $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$, we get that $\gamma \mathcal{A}_{*+}^W \Delta_{\overline{W}} \mathcal{E} \mathcal{E}^{-1} \lambda$, hence that $\gamma \mathcal{A}_{*-}^W \lambda$ by (42c). On the other hand, the extended-oriented path ρ of length n satisfies the case 2 of \mathcal{H}_n , since it ends with -1 and its endpoints are such that $\gamma \mathcal{A}_{*-}^W \lambda$. Therefore, we have proven the case 2 of the induction assumption \mathcal{H}_n for the extended-oriented paths of length n.

• Assume that we have $\gamma \mathcal{A}_{*-}^{W} v_{n-1}^{\sharp}$ and that the last orientation of ρ' is $o_{n-1} = -1$, that is, $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$. There are two possibilities for the extended-oriented path $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, o_n)\}$.

• Suppose that $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, +1)\} = \{(v_n^{\flat}, \lambda, +1)\}$, that is, $(v_n^{\flat}, \lambda) \in \mathcal{E}$ by (9). As the path ρ is active, the pattern $\{(v_{n-1}^{\flat}, v_{n-1}^{\sharp}, -1), (v_n^{\flat}, v_n^{\sharp}, +1)\}$ must satisfy Item 16c in Definition 2. We deduce that $v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$. Now, we wrap up the results obtained so far. On the one hand, from $\gamma \mathcal{A}_{*-}^W v_{n-1}^{\sharp}, v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$ and $(v_n^{\flat}, \lambda) \in \mathcal{E}$, we get that $\gamma \mathcal{A}_{*-}^W \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} \lambda$, hence that $\gamma \mathcal{A}_{*+}^W \lambda$ by (42c). On the other hand, the extended-oriented path ρ ends with +1, as it is the case for ρ'' . We conclude that the extended-oriented path ρ of length n satisfies the case 1 of \mathcal{H}_n , since it ends with +1 and its endpoints are such that $\gamma \mathcal{A}_{*+}^W \lambda$. Therefore, we

have proven the case 1 of the induction assumption \mathcal{H}_n for the extended-oriented paths of length n.

• Suppose that $\rho'' = \{(v_n^{\flat}, v_n^{\sharp}, -1)\} = \{(v_n^{\flat}, \lambda, -1)\}$, that is, $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$ by (9). As the path ρ is active, the pattern $\{(v_{n-1}^{\flat}, v_{n-1}^{\sharp}, -1), (v_n^{\flat}, v_n^{\sharp}, -1)\}$ must satisfy Item 16b in Definition 2. We deduce that $v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$. Now, we wrap up the results obtained so far. On the one hand, from $\gamma \mathcal{A}_{*-}^W v_{n-1}^{\sharp}, v_{n-1}^{\sharp} = v_n^{\flat} \in W^{\mathsf{c}}$ and $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$, we get that $\gamma \mathcal{A}_{*-}^W \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} \lambda$, hence that $\gamma \mathcal{A}_{*-}^W \lambda_{n-1} = v_n^{\flat} \in W^{\mathsf{c}}$ and $(v_n^{\flat}, \lambda) \in \mathcal{E}^{-1}$, we get that $\gamma \mathcal{A}_{*-}^W \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} \lambda_{W^{\mathsf{c}}} \mathcal{E}^{-1} \lambda_{W^{\mathsf{c}}} \mathcal{E}^{-1} \subset \mathcal{A}_{*-}^W$ and we have that $\mathcal{B}^{-W} \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} = (\mathcal{E}^{-1} \Delta_{W^{\mathsf{c}}})^* \mathcal{E}^{-1} \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} \subset \mathcal{B}^{-W}$ which implies that $\mathcal{A}_{*-}^W \Delta_{W^{\mathsf{c}}} \mathcal{E}^{-1} \subset \mathcal{A}_{*-}^W$. On the other hand, the extended-oriented path ρ ends with -1, as it is the case for ρ'' . We conclude that the extended-oriented path ρ of length n satisfies the case 2 of \mathcal{H}_n , since it ends with -1 and its endpoints are such that $\gamma \mathcal{A}_{*-}^W \lambda$. Therefore, we have proven the case 2 of the induction assumption \mathcal{H}_n for the extended-oriented paths of length n.

This ends the proof.

References

- [ABC⁺22] Reynald Affeldt, Yves Bertot, Cyril Cohen, Marie Kerjean, Assia Mahboubi, Damien Rouhling, Pierre Roux, Kazuhiko Sakaguchi, Zachary Stone, Pierre-Yves Strub, and Laurent Théry. MathCompAnalysis: Mathematical components compliant analysis library. Technical Report Version 0.5.4, 2022.
- [AGT20] Reynald Affeldt, Jacques Garrigue, and Saikawa Takafumi. Reasoning with conditional probabilities and joint distributions in Coq. Technical report, 2020.
- [CDH21] Jean-Philippe Chancelier, Michel De Lara, and Benjamin Heymann. Conditional separation as a binary relation, 2021. Preprint.
- [CDLS06] Robert G Cowell, Philip Dawid, Steffen L Lauritzen, and David J Spiegelhalter. Probabilistic networks and expert systems: Exact computational methods for Bayesian networks. Springer Science & Business Media, 2006.
- [DCH21] Michel De Lara, Jean-Philippe Chancelier, and Benjamin Heymann. Topological conditional separation, 2021. Preprint.
- [Die18] Reinhard Diestel. *Graph theory*, volume 173 of *Graduate Texts in Mathematics*. Springer, Berlin, fifth edition, 2018. Paperback edition of [MR3644391].
- [GMT16] Georges Gonthier, Assia Mahboubi, and Enrico Tassi. A Small Scale Reflection Extension for the Coq system. Research Report RR-6455, Inria Saclay Ile de France, 2016.
- [HDC21] Benjamin Heymann, Michel De Lara, and Jean-Philippe Chancelier. Causal inference theory with information dependency models, 2021. Preprint.

- [LDLL90] S. L. Lauritzen, A. P. Dawid, B. N. Larsen, and H.-G. Leimer. Independence properties of directed Markov fields. *Networks*, 20(5):491–505, 1990.
- [Pea86] Judea Pearl. A constraint propagation approach to probabilistic reasoning. In Laveen N. Kanal and John F. Lemmer, editors, Uncertainty in Artificial Intelligence, volume 4 of Machine Intelligence and Pattern Recognition, pages 357–369. North-Holland, 1986.
- [Pea95] Judea Pearl. Causal diagrams for empirical research. *Biometrika*, 82(4):669–688, 1995.
- [PM18] Judea Pearl and Dana Mackenzie. The book of Why: the new science of cause and effect. Basic Books, 2018.
- [Wan10] Jinfang Wang. A universal algebraic approach for conditional independence. Annals of the Institute of Statistical Mathematics, 62:747–773, 2010.
- [YKS⁺16] Rutaro Yamaguchi, Ken Kin, Shugo Shimoyama, Manabu Hagiwara, Mitsuharu Yamamoto, and Jinfang Wang. Formalization of the conditional independence using Coq/SSReflect. Technical report, 2016.