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Oriented components and their separations

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Abstract

There is a tight connection between connectedness, connected components, and certain types of separation spaces. Recently, axiom systems for oriented connectedness were proposed leading to the notion of reaches. Here, we introduce production relations as a further generalization of connectivity spaces and reaches and derive associated systems of oriented components that generalize connected components in a natural manner. The main result is a characterization of generalized reaches in terms of equivalent separation spaces.

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1. INTRODUCTION

Already in the 1940's, A. D. Wallace asked whether topological concepts can be axiomatized starting from a notion of connectivity or an associated

concept of separation [29], the latter being the complement of a generalization of proximity [24]. Ch. Ronse characterized the separations that are equivalent to abstract connectivities [20]. These results were generalized further in [26]. Since connectedness is an intrinsically symmetric notion, the theory requires that separations satisfy a symmetry axiom.

Tankyevych *et al.* [28] recently introduced so-called semi-connections as a generalized model of connected components in directed graphs. Ronse explored this concept in more detail [22] as a generalization of connectivity openings [20, 23] and discussed some fundamental properties of the equivalent notion of oriented components. The latter form a system of pairs (p, Q) with the interpretation that "every point of Q is reachable from p within Q". This construction is insufficient, however, to capture the natural connectivity structure of chemical reaction networks and directed hypergraphs in general. The key point is that in a chemical reaction, the "output molecules" depend on a set of "input molecules" rather than on a single input molecule. This suggests to generalize the work of [28, 22] to pairs (P, Q) such that every point of Q can be reached from the start set P within Q.

This formalization of reachability does not appear to be connected to concepts familiar from topology in an obvious manner. On the other hand, reaches are rather natural generalizations of connectivity structures, and the latter have been shown to be equivalent to certain generalized proximities in [20, 26]. It is the purpose of this contribution to show that there is also a 1-1 correspondence of reachability structures general enough to encompass chemical reaction networks, and thus directed hypergraphs, and a suitable class of generalized separations or, equivalently, proximities.

To this end we consider two binary relations \succ and \mid on $2^X \times 2^X$ that we interpret as follows: $P \succ Q$ means that P can produce Q, i.e., Q are the points eventually reachable from P. Production relations capture the salient structure of (directed) hypergraphs, which to our knowledge rarely have been considered with regard of their topological properties [10]. On the other hand, we think of $A \mid B$ as "A is separated from B". The negation of separation relations are *proximity* relations, $A \delta B$, which are well studied in the literature as a starting point for constructing topological theories [24, 13, 14, 18]. Before we turn to establishing the formal connection between production relations and separations, we briefly argue that production relations are an interesting notion to study in their own right.

2. PRODUCTION RELATIONS IN THE REAL WORLD

The paradigmatic examples of production relations derive from chemical reactions. Given a set X of molecular types, usually called compounds or reactants, chemical reactions describe the transformation of subsets into each other. An example is the burning of methane in oxygen, which produces carbon dioxide and water $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$. An important property of systems of chemical reactions is that the products can undergo further reactions, for instance with each other, e.g. $CO_2 + H_2O \rightarrow H_2CO_3$, or with additional

reactants, say $CO_2 + H_2 \rightarrow CO + H_2O$. Chemical reactions thus can be concatenated into overall reactions such as $CH_4 + 2O_2 \rightarrow H_2CO_3 + H_2O$. As long as we are only interested in which molecules can be transformed into each other, we can neglect the multiplicities (called stoichiometric coefficients) and think of reactions as a relation on 2^X . In our example $\{CH_4, O_2\} \rightarrow \{CO_2, H_2O\}$, and so on.

An important question in the analysis of reaction networks is to understand which compounds can eventually be generated from which initial conditions. In particular in the field of biochemistry, there are also large databases of the chemical reactions that together describe the metabolic network of a cell [8]. In a more general setting rules that describe which reactions are possible and which are not can be specified in the form of graph grammars. These can then be used to computationally generate large chemical networks [1]. Reachability in such a network amounts to asking whether, given a set Q of compounds of interest and set P of starting molecules, it is possible to produce Q by a sequence of consecutive reactions $P' \to Q'$ where initially $P' \subseteq P$ and always $Q' \subseteq Q$ must hold. In subsequent steps we also allow the educts P' to be contained in the union of the products of earlier steps. This construction naturally leads to the notion of what we call here the production relation $P \succ$ Q. Since chemical reactions may run in parallel, reachability must be "additive" in the sense that $P_i \succ Q_i$ for all $i \in I$ should imply $\bigcup_i P_i \succ \bigcup Q_i$. The re-use of products for consecutive reactions leads us to conclude that $P \succ Q$ and $S \succ T$ for some $S \subseteq Q$ must imply $P \succ Q \cup T$. In fact, we will be content with essentially these two properties when we formally define production relations in the next section.

A somewhat different motivation for the same formal construction comes from evolutionary algorithms. Here, the problem is to optimize a cost function $f: X \to \mathbb{R}$ over some set X using a search operator that produces from a set of parents $A \subseteq X$ a set of offsprings c(A). The same framework of course also models real evolution in biology [27, 25]. In the simplest case, mutations transform individual genotypes into their mutant offsprings, thus imposing a graph structure on X. In the usual setup of evolutionary strategies [19] and genetic algorithms [11], however, recombinants of two parents are used, i.e., the structure of the search space is determined implicitly by the relations of the form $\{x, y\} \to R_{xy}$. Such relations have been investigated extensively under the name transit functions [16, 5], which serve as generalizations of betweenness relations and abstract convexities. The cost function $f: X \to \mathbb{R}$ together with the topological structure on X implied by the search spaces give rise to "fitness landscapes" [30], in which concepts such as local minima, saddle points, and basins of attraction are well defined. These notions are inherently topological in nature and require only the definition of connected sets on X [9, 12, 26]. Search operators are not necessarily symmetric, however. Most recombination operators used in evolutionary computation tend to reduce diversity in the "search population" and thus are inherently directional. It is of interest, therefore, to consider reachability as a generalization of connectedness.

In general, production relations naturally appear in all types of generative systems. When generation rules apply to individual elements, as in the case of mutations of gene sequences, reaches in the sense of [28] and [22] are obtained. Generative grammars and (term) rewriting systems could also be viewed in this way. Alternatively, generation rules apply to sets or multisets of elements rather than individual elements. A proper description then requires production relations in the sense of this contribution. Within computer science this pertains in particular to large classes of "chemistry-like" formal systems such as Berry's Chemical Abstract Machine [3]. Certain constructions in natural languages, such the well known property of the German language to produce new nouns by concatenations of nouns, or the self-assembly of macromolecular complexes may serve as further examples.

3. Separations, Productions, and Oriented Components

3.1. Galois Correspondence. To relate the production relation \succ and a separation relation | with each other, we introduce another relation \emptyset on $(2^X \times 2^X) \times (2^X \times 2^X)$ that expresses when a pair (A, B) splits a pair (P, Q):

$$(3.1) \qquad (A,B) \ \emptyset \ (P,Q) \iff P \cup Q \subseteq A \cup B, \ P \subseteq B, \ \text{and} \ Q \cap A \neq \varnothing$$

The negation of \emptyset will be written as $\hat{\phi}$. Thus we have $(A, B) \stackrel{*}{\oplus} (P, Q)$ if and only if $P \cup Q \not\subseteq A \cup B$, or $P \notin B$, or $A \cap Q = \emptyset$. The relation $\hat{\phi}$ is a very natural way of connecting \succ and |: If $P \succ Q$ there is no $A \mid B$ that splits Pfrom Q, and $A \mid B$ means that there is no $P \succ Q$ that "reaches" from B to A. Fig. 1 illustrates the interesting case.

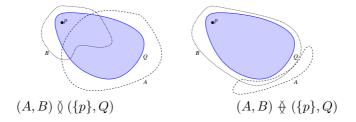


FIGURE 1. Illustration of the splitting relation 0 between two pairs of subsets.

More formally, we have the Galois connection comprising the two maps

(3.2)
$$\phi: 2^{2^{X} \times 2^{X}} \to 2^{2^{X} \times 2^{X}}, \ \{(P,Q) | P \succ Q\} \mapsto \{(A,B) | A \mid B\}$$
$$\theta: 2^{2^{X} \times 2^{X}} \to 2^{2^{X} \times 2^{X}}, \ \{(A,B) | A \mid B\} \mapsto \{(P,Q) | A \not\succeq B\}.$$

where the induced relations | and $\dot{\succ}$, resp., are defined by

(3.3)
$$A \mid B \iff (A, B) \notin (P, Q) \quad \forall (P, Q) \in 2^X \text{ with } P \succ Q$$
$$P \not\succ Q \iff (A, B) \notin (P, Q) \quad \forall (A, B) \in 2^X \text{ with } A \mid B$$

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The theory of Galois connections implies that $\theta(\phi)$ and $\phi(\theta)$ are closure operations on $2^{2^X \times 2^X}$ defining from a | and \succ relations $\ddot{|} := \phi(\dot{\succ}) = \phi(\theta(|))$ and $\dot{\succ} := \theta(\dot{|}) = \theta(\phi(\succ))$, resp., that are in 1-1 correspondence. In other words, θ and ϕ induce a bijection between $\operatorname{img} \theta$ and $\operatorname{img} \phi$. We are interested, therefore, in the properties of relations | and \succ that correspond to elements of $\operatorname{img} \theta$ and $\operatorname{img} \phi$, respectively.

3.2. **Basic Properties.** Throughout this section we write $\dot{|}:=\phi(\succ)$ for the separation relation induced by a given production relation \succ ; conversely $\dot{\succ}:=\theta(|)$ denotes the production relation induced by a given separation relation |. We start from an arbitrary production relation \succ and strive to identify the properties of $\dot{|}$ that are necessary for membership in img ϕ .

Theorem 3.1. Given an arbitrary production relation \succ , the corresponding relation $\dot{\mid}$ satisfies for all $A, B \in 2^X$:

- (S0) $\varnothing \mid B$ for all B.
- (S1) $A' \subseteq A, B' \subseteq B, and A \mid B \text{ implies } A' \mid B'.$
- (SR1) $A \mid C \text{ and } B \mid A \cup C \text{ implies } A \cup B \mid C.$
- (SR2) $A_i \cup B_i = Z$ and $A_i \mid B_i$ for all $i \in I$ implies $\bigcup_{i \in I} A_i \mid \bigcap_{i \in I} B_i$

Proof. (S0) follows immediately from the definition of \mathcal{A} .

(S1) Suppose $A' \subseteq A$ and $B' \subseteq B$. From $A \mid B$ we know that for all $P \succ Q$ with $P \cup Q \subseteq A \cup B$ and $P \subseteq B$ holds $Q \cap A = \emptyset$. The pairs $P \succ Q$ satisfying $P \cup Q \subseteq A' \cup B'$ and $P \subseteq B'$ are a subset of the latter. Furthermore, they also satisfy $Q \cap A' = \emptyset$. Thus $A' \mid B'$ holds.

(SR1) Suppose $A \mid C$ and $B \mid A \cup C$ are satisfied but $A \cup B \mid C$ does not hold, i.e., there is a production $P \succ Q$ with $P \subseteq C$, $Q \subseteq A \cup B \cup C$, and $(A \cup B) \cap Q \neq \emptyset$. Suppose first that $Q \cap B = \emptyset$; then $A \mid C$ implies $Q \cap A = \emptyset$. The desired production therefore must satisfy $Q \cap B \neq \emptyset$. Since $P \subseteq C$ implies $P \subseteq A \cup C$ we infer from $B \mid A \cup C$ that $Q \cap B = \emptyset$, a contradiction. Thus $A \cup B \mid C$ cannot be violated.

(SR2) Suppose $A_i \cup B_i = Z$ and $A_i \mid B_i$ holds for all $i \in I$. Consider all $P \succ Q$ with $P \cup Q \subseteq Z$ and $P \subseteq B_i$ for all $i \in I$, i.e., $P \subseteq \bigcap_i B_i$. By assumption, $Q \cap A_i = \emptyset$ for all i and thus $Q \cap \bigcup_i A_i = \emptyset$. Therefore $\bigcup_i A_i \mid \bigcap B_i$.

A space satisfying (S0) and (S1) can be seen as the most general form of a separation space generalizing even further the setting of Wallace [29]. The axioms (SR1) and (SR2), on the other hand, appeared in Ronse's characterization of separation spaces that are defined by connectedness [20].

Now we take the converse point of view. Starting from an arbitrary "separation" relation | we determine properties of the production relation \succeq that is defined by the map θ to obtain necessary conditions for membership in img θ .

Lemma 3.2. Given an arbitrary separation relation |, the corresponding relation \succ satisfies

- (O) $P \stackrel{\cdot}{\succ} \emptyset$.
- (U) If $P_i \succeq Q_i$ for all $i \in I$ then $\bigcup P_i \succeq \bigcup Q_i$. (union property)
- (T) If $P \succeq Q$, $S \subseteq Q$, and $S \succeq T$ then $P \succeq Q \cup T$. (transitivity)
- (T+) If $P \succeq Q$, $S \subseteq Q \subseteq T$ and $P \cup S \succ T$ then $P \succeq T$. (source closure)

Proof. (O) Given any collection of A|B we always have $A \cap Q = \emptyset$ if $Q = \emptyset$, i.e., $(A, B) \notin (P, \emptyset)$ holds for all $P \in 2^X$.

(U) Suppose $P_i \succeq Q_i$ for some family $i \in I$. Thus, for all $A \mid B$ with $P_i \subseteq B$ and $P_i \cup Q_i \subseteq A \cup B$ holds $A \cap Q_i = \emptyset$. In particular, therefore, every $A \mid B$ satisfying $\bigcup_{i \in I} P_i \in B$ and $\bigcup_{i \in I} P_i \cup \bigcup_{i \in I} Q_i \subseteq A \cup B$ therefore also satisfies $\bigcup_{i \in I} Q_i \cap A = \emptyset$, and therefore $\bigcup_{i \in I} P_i \succeq \bigcup_{i \in I} Q_i$ holds.

(T) Suppose $P \succeq Q$, $S \subseteq Q$ and $S \succeq T$. Suppose $P \succeq Q \cup T$ does not hold, i.e., there is a separation $A \mid B$ with $P \cup Q \cup T \subseteq A \cup B$, $P \subseteq B$, and $(Q \cup T) \cap A \neq \emptyset$. We observe that $Q \cap A \neq \emptyset$ contradicts $P \succeq Q$, hence $Q \cap A = \emptyset$, which implies $Q \subseteq B$ and therefore also $S \subseteq B$. Therefore $A \cap T \neq \emptyset$ contradicts $S \succeq T$, i.e., no such separation $A \mid B$ can exist, and $P \succeq Q \cup T$ must be true.

(T+) Suppose $P \succeq Q$ and $P \cup S \succeq T$ holds for $S \subseteq Q \subseteq T$. Note that $P \cup S \succ T$ implies by (U) also $P \cup S \succ T \cup Q$, hence we may choose T such that $Q \subseteq T$. Now suppose for contradiction that $P \succeq T$ does not hold. Then there is a $A \mid B$ with $P \cup T = A \cup B$ such that $P \subseteq B$ and $T \cap A \neq \emptyset$. Since $P \succeq Q$ we have $A \cap Q = \emptyset$ and thus $Q \subseteq B$, which further implies $S \subseteq B$. From $P \cup S \succeq T$ we know that $A' \cap T = \emptyset$ holds for all $A' \mid B'$ with $S \cup P \subseteq B'$ and $A' \cup B' = P \cup Q$. This is in particular also true for $A \mid B$, a contradiction. \Box

Axiom (U) generalizes the "union property" of [22]. It allows multiple production to be "applied" at the same time. The transitivity axiom (T) encapsulates the idea that Q is an "attractor" that is reached eventually.

Lemma 3.3. If (O) and (U) holds, then (T+) implies (T).

Proof. Suppose $P \succ Q$ and $S \subseteq Q$ and $S \succ T$. By (U) also have $P \cup S \succ Q \cup T$. Setting $T' = Q \cup T$ we have $S \subseteq Q \subseteq T'$ and $P \cup S \succ T'$. Now (T+) implies $P \succ T'$, i.e., $T \succ Q \cup T$, and thus (T) holds.

We next observe that it is sufficient to consider the relationship of \succ and \mid on a given subset $Y \in 2^X$. To this end we define for a given separation relation \mid and all pairs $(P, Q) \in 2^X \times 2^X$ the collections

(3.4)
$$\mathfrak{S}(P,Q) := \{ (A,B) \in 2^X \times 2^X | A \cup B = P \cup Q, P \subseteq B, \text{ and } A \mid B \}.$$

of separated pairs on $Y = P \cup Q$. The production relation $\dot{\succ}$ can be specified completely by the sets $\mathfrak{S}(P,Q)$ by virtue of the following simple condition:

Lemma 3.4. $P \succeq Q$ if and only if $Q \cap A = \emptyset$ for all $(A, B) \in \mathfrak{S}(P, Q)$.

Proof. By definition, we have $P \succeq Q$ if and only if $(A, B) \notin (P, Q)$ for all $(A, B) \in 2^X$ with $A \mid B$. If $P \not\subseteq B$ or $P \cup Q := Y \not\subseteq A \cup B$ then $(A, B) \notin (P, Q)$ always holds, i.e., these pairs never impose a condition and therefore they can be ignored. Now consider the remaining case $P \subseteq B$ and $Y \subseteq A \cup B$. Thus $(A, B) \notin (P, Q)$ holds if and only if $A \cap Q = \emptyset$. Set $A' = A \cap Y$ and $B' = B \cap Y$ and observe that $P \subseteq B \cap Y$ iff $P \subseteq B'$ and $Q \cap A = Q \cap (A \cap Y) = Q \cap A'$. Therefore, $(A, B) \notin (P, Q)$ if and only if $(A', B') \notin (P, Q)$ and $A \cap Q = \emptyset$ if and only if $A' \cap Q = \emptyset$. Since $A \mid B$ implies $A' \mid B'$ by (S1) we conclude that $P \succeq Q$ holds if and only if $(A', B') \notin (P, Q)$ and $A' \mid B'$. The latter statement is equivalent expressed as $Q \cap A'' = \emptyset$ for all $(A'', B'') \in \mathfrak{S}(P, Q)$. □

Now let us fix Z and $P \subseteq Z$ and suppose $Q \cup P = Z$. As a consequence of (SR2) there is a unique "extremal" separation $A^*|B^*$ with $A^* \cup B^* = Z$ and $P \subseteq B^*$, which is defined by

(3.5)
$$A^* = \bigcup_{(A,B)\in\mathfrak{S}(P,Q)} A \text{ and } B^* = \bigcap_{(A,B)\in\mathfrak{S}(P,Q)} B$$

since $A \cap Q = \emptyset$ and $P \subseteq B$ for all $(A, B) \in \mathfrak{S}(P, Q)$.

Corollary 3.5. Suppose $A^* \mid B^*$ as defined by $\mathfrak{S}(P,Q)$ as in equ.(3.5). Then we have $P \succeq Q$ if and only if $Q \cap A^* = \emptyset$.

Proof. By lemma 3.4, $P \succeq Q$ if and only if $Q \cap A = \emptyset$ for all $(A, B) \in \mathfrak{S}(P, Q)$. By equ.(3.5) this is equivalent to $A^* \cap Q = \emptyset$.

The key observation here is that $A^*|B^*$ depends only on P and Z but not on the exact choice of Q as long as $Z \setminus P \subseteq Q \subseteq Z$. Thus $P \succeq Q$ implies $A^* \subseteq P \setminus Q$. Furthermore, $Q \cap A^* = \emptyset$ implies the same condition also for all subsets Q' of Q. Since the corollary holds as long as $Q' \cup P = Q \cup P = Z$, we have in particular the following implication:

(A) $P \succeq Q$ implies $P \succeq Q'$ for all Q' satisfying $Q \setminus P \subseteq Q' \subseteq Q$.

We will give a more intuitive interpretation of property (A) in the following section.

3.3. Oriented Components. For every pair $(P,Q) \in 2^X \times 2^X$ we define the set

(3.6)
$$Q[P] = \bigcup \left\{ Q' \in 2^X \mid Q' \subseteq Q, \ P' \subseteq P \text{ and } P' \succ Q' \right\}$$

The map $\gamma : 2^X \times 2^X \to 2^X : (P,Q) \mapsto Q[P]$ generalizes the openings that play a central role e.g. in topological approaches to image analysis [23, 20, 15]. The sets Q[P] will be referred to as (generalized) oriented components.

Lemma 3.6. Suppose \succ is a production relation satisfying (U). Then

- (o1) $Q[P] \subseteq Q$. (contraction)
- (o2) $P' \subseteq P$ and $Q' \subseteq Q$ implies $Q'[P'] \subseteq Q[P]$. (isotony)
- (o3) (Q[P])[P] = Q[P]. (idempotency)

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Proof. Property (o1) is an immediate consequence of the definition.

If P shrinks in equ.(3.6) then the union runs over fewer productions, and thus Q[P] cannot increase, i.e., $P' \subseteq P$ implies $Q[P'] \subseteq Q[P]$. The same argument can be applied if Q is reduced, hence $Q' \subseteq Q$ implies $Q'[P] \subseteq Q[P]$. Now (o2) follows by combining the two inclusions.

Fix P and Q. By definition every $Q' \subseteq Q$ with $P' \subseteq P$ and $P' \succ Q'$ implies $Q' \subseteq Q[P]$. Thus replacing Q in the r.h.s. of equ.(3.6) by Q[P] does not change the collection of sets. Since this substitution turns the definition of Q[P] into the definition of (Q[P])[P], property (o3) holds.

We call a map $2^X \times 2^X \to 2^X : (P,Q) \mapsto Q[P]$ that satisfies (o1), (o2), and (o3) a generalized opening. It defines a production relation by means of

$$(3.7) P \succ Q if and only if Q[P] = Q.$$

An immediate consequene is the following

Fact 3.7. If \succ satisfies (O) and (U) then $P \succ Q[P]$ for all $P, Q \in 2^X$.

Lemma 3.8. If $(P,Q) \mapsto Q[P]$ is a generalized opening, then the corresponding production relation \succ satisfies (O) and (U).

Proof. Setting $Q = \emptyset$ we have $\emptyset[P] = \emptyset$, i.e., $P \succ Q$.

Suppose Q[P] = Q and $P \subseteq P'$. Then isotony w.r.t. P implies $Q = Q[P] \subseteq Q[P'] \subseteq Q$, and thus Q[P'] = Q. Now consider an arbitrary family \mathcal{F} of pairs (P,Q) satisfying Q[P] = Q and let $P^* = \bigcup \{P | (P,Q) \in \mathcal{F}\}$. We have $Q[P] = Q[P^*]$ for all $(P,Q) \in \mathcal{F}$. Isotony w.r.t. to Q and condition (o1) now imply

$$\bigcup_{Q:(P,Q)\in\mathcal{F}}Q = \bigcup_{Q:(P,Q)\in\mathcal{F}}Q[P^*] \subseteq \left(\bigcup_{Q:(P,Q)\in\mathcal{F}}Q\right)[P^*] \subseteq \bigcup_{Q:(P,Q)\in\mathcal{F}}Q.$$

With the abbreviation $Q^* := \bigcup_{(P,Q) \in \mathcal{F}} Q$ we therefore have $Q^*[P^*] = Q^*$. In other words, $P \succ Q$ for all $(P,Q) \in \mathcal{F}$ implies $P^* \succ Q^*$, i.e., (U) holds. \Box

Theorem 3.9. Eqns.(3.6) and (3.7) define a bijection between relations \succ satisfying (O) and (U) on 2^X and maps $2^X \times 2^X \to 2^X$ satisfying (o1), (o2), and (o3).

Proof. It is shown e.g. in [22] that there is a bijection between the openings γ_P : $(P,Q) \mapsto Q[P]$ and the set systems with the union property $\mathcal{F}_P := \{Q | P \succ Q\}$ for fixed P. The theorem now follows directly from lemma 3.6 and lemma 3.8, whose proofs also establish the correspondence $P \succ Q \Longrightarrow P' \succ Q$ for all $P \subseteq P'$ and $Q[P] = Q \Longrightarrow Q[P'] = Q$ for all $P \subseteq P'$

Let us now turn to additional properties of production relations that derive from separations. Property (T) translates into a simple transitivity condition for generalized openings. The following lemma parallels Prop. 2 of [22]: **Lemma 3.10.** Let \succ be a production relation satisfying (O) and (U) and let $(Q, P) \mapsto Q[P]$ be the corresponding generalized opening. Then axiom (T) is equivalent to

(o4) $S \subseteq Q[P]$ implies $Q[S] \subseteq Q[P]$.

Proof. Suppose (T) holds. From $P \succ Q[P]$, $S \succ Q[S]$, and $S \subseteq Q[P]$ we conclude $P \succ Q[P] \cup Q[S] \subseteq Q$. By maximality of the oriented connected components we therefore have $Q[P] \cup Q[S] \subseteq Q[P]$, i.e., $Q[S] \subseteq Q[P]$, i.e., (o4) holds.

Conversely suppose (o4) is satisfied. Assume $P \succ Q$, $S \succ T$ and $S \subseteq Q$. Thus we have Q[P] = Q and T[S] = T and further $Q[P] \subseteq (Q \cup T)[P]$, $S \subseteq (Q \cup T)[P]$, and $T \subseteq (Q \cup T)[S]$. Now (o4) implies $(Q \cup T)[S] \subseteq (Q \cup T)[P]$ and therefore $T \subseteq (Q \cup T)[P]$. Taken together we have $Q \cup T \subseteq (Q \cup T)[P]$ and thus $Q \cup T = (Q \cup T)[P]$. This translates to $P \succ Q \cup T$, i.e., (T) holds.

Property (T+) becomes a transitivity condition in the arguments:

Lemma 3.11. If \succ satisfies (O) and (U) and $(Q, P) \mapsto Q[P]$ is the corresponding generalized opening, then (T+) is equivalent to

(t+) If $R \subseteq Q[P]$ then $Q[P \cup R] = Q[P]$.

Proof. Suppose (T+) holds. Substituting Q by Q[P] and T by $T[P \cup S]$ transforms (T+) to: $S \subseteq Q[P] \subseteq T[P \cup S]$ and $P \cup S \succ T[P \cup S]$ implies $P \succ T[P \cup S]$. For the first precondition observe that $Q[P] \subseteq T[P \cup S]$ implies $Q[P] = (Q[P])[P] \subseteq (T[P \cup S])[P] \subseteq T[P]$, and hence in particular $S \subseteq Q[P] \subseteq T[P]$. The second precondition is always true and thus can be omitted. The definition of generalized oriented components, finally, implies $T[P \cup S] \subseteq T[P]$ because $T[P \cup S] \subseteq T$. On the other hand $T[P] \subseteq T[P \cup S]$ by isotony. Thus $S \subseteq T[P]$ implies $T[P] = T[P \cup S]$.

Conversely, assume $P \succ Q$, $S \subseteq Q \subseteq T$, and $P \cup S \succ T$. Therefore $Q = Q[P] \subseteq T[P]$ and thus $S \subseteq T[P]$ and $T[P \cup S] = T$. By (t+) we therefore have $T[P \cup S] = T[P]$. By definition $P \succ T[P]$, and thus T = T[P], i.e., $P \succ T$, i.e., (T+) holds.

In analogy to Lemma 3.3 we have the following

Fact 3.12. If (o2) holds, then (t+) implies (o_4) .

Proof. Assume (t+) and suppose $S \in Q[P]$. Then $Q[S] \subseteq Q[P \cup S] = Q[P]$, i.e., (o4) holds

Condition (A) is also easily translated to the language of generalized oriented components:

Lemma 3.13. If \succ satisfies (O) and (U) and $(Q, P) \mapsto Q[P]$ is the corresponding generalized opening, then (A) is equivalent to

(a) $Q[P] = (P \cup Q)[P] \cap Q.$

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Proof. Suppose ≻ satisfies (A). The set Z[P] is uniquely defined and by (o2) $Q[P] \subseteq Z[P]$ for all $Q \subseteq Z$ and by (o1) we have $Q[P] \subseteq Z[P]$, and thus $Q[P] \subseteq Z[P] \cap Q$. If $Q \cup P = Z$ then (A) implies $P \succ Z[P] \cap Q$ which in turn guarantees $Z[P] \cap Q \subseteq Q[P]$; hence $Q[P] = Z[P] \cap Q$ whenever $P \cup Q = Z$. Substituting $Z = P \cup Q$ establishes (a).

To see the converse set $Z = P \cup Q$ and assume (a), i.e., $Q[P] = Z[P] \cap Q$ for all Q satisfying $Z \setminus P \subseteq Q \subseteq Z$. By construction of the generalized oriented components we have $P \not\succ Q[P]$ and thus $P \not\succ Z[P] \cap Q$ for $Z \setminus P \subseteq Q \subseteq Z$. In particular for $Q \subseteq Z[P]$ this implies $P \not\succ Q$. On the other hand, $P \not\succ Q$ and $Q \subseteq Z$ implies $Q \subseteq Z[P]$. Therefore $P \succ Q$ implies $P \succ Q'$ for all Q' with $Z \setminus P \subseteq Q' \subseteq Q \subseteq Z[P]$, i.e., condition (A) holds. \Box

In this form, property (a) lends itself to a simple intuitive interpretation. It states that the generalized opening is completely defined by the $(Q \cup P)[P]$, i.e., the oriented components Q[P] with $P \subseteq Q$. This matches, of course, with the observation in the previous section that separations are defined by $Z = P \cup Q$ and P independent of the exact choice of Q. For later reference we finally record a simple consequence of property (a):

Lemma 3.14. If $(P,Q) \rightarrow Q[P]$ satisfies (o1) through (o4) and (a) then $P \setminus Q[P] = P \setminus Q'[P]$ for $Q \setminus P \subseteq Q' \subseteq Q \cup P$.

Proof. We set $Z = P \cup Q$ and hence $Z \setminus P \subseteq Q \subseteq Z$. By isotony we have $P \setminus Z[P] \subseteq P \setminus Q[P] \subseteq P \setminus (Z \setminus P)[P]) = P \setminus (Z[P] \cap (Z \setminus P)) = P \setminus Z[P] \cup P \setminus (Z \setminus P) = P \setminus Z[P]$; here the first equality uses (a). Thus $P \setminus Q'[P]$ does not depend on the choice of Q' between $Z \setminus P = Q \setminus P \subseteq Q' \subseteq P \cup Q$. \Box

3.4. **Bijection.** In order to show that there is a bijection between the production relations satisfying (O), (U), (T+), and (A) and the separation relations satisfying (S0), (S1), (SR1), and (SR2) it suffices to show that $\ddot{|} = \phi(\theta(|)) = |$ or $\ddot{\succ} = \theta(\phi(\succ)) = |$.

Consider the map $2^X \times 2^X \to 2^X$: $(P,Q) \mapsto Q(P)$ such that

(3.8)
$$Q(P) = Q \setminus \left\{ A \in 2^X | (A, B) \in \mathfrak{S}(P, Q) \right\} = Q \setminus A^*$$

Lemma 3.15. The map $(P,Q) \mapsto Q(P)$ satisfies (01), (02), (03), (a), (t+), and thus also (04).

Proof. (o1). $Q(P) \subseteq Q$ follows directly from the definition of Q(P).

(o2). Suppose $P' \subseteq P, A \cup B = P \cup Q, P \subseteq B$, and $A \mid B$. Thus $(A, B) \in \mathfrak{S}(P,Q)$. Set $Y' = P' \cup Q$. By isotony, $A \cap Y' \mid B \cap Y'$ and thus $(A \cap Y', B \cap Y') \in \mathfrak{S}(P',Q)$. Therefore $Y' \cap A^* := Y' \cap \bigcup \{A \mid (A, B) \in \mathfrak{S}(P,Q)\} = \bigcup \{Y' \cap A \mid (A \cap Y', B \cap Y') \in \mathfrak{S}(P',Q) =: Y' \cap \tilde{A}.$ By definition, $Q(P) = Q \setminus A^* = Q \setminus (Q \cap A^*) = Q \setminus (Y' \cap A^*)$ where we have used $Q \subseteq Y'$. Analogously we have $Q(P') = Q \setminus \tilde{A} = Q \setminus (Y' \cap \tilde{A})$. Therefore $Q(P') \subseteq Q(P)$.

Next consider $Q' \subseteq Q$ and set $Y' = P \cup Q'$. From $A \cup B = P \cup Q$ and $P \subseteq B$ we infer $(A \cap Y') \cup B = P \cup Q'$ and $A \cap Q' \mid B$. Therefore $Q' \cap \{A \mid (A, B) \in \mathfrak{S}(P, Q)\} \subseteq \{A \cap Y' \mid (A \cap Y', B) \in \mathfrak{S}(P, Q')\} = Q' \cap$ $\{A|(A \cap Y', B) \in \mathfrak{S}(P, Q')\} = Q' \cap \{A|(A, B) \in \mathfrak{S}(P, Q')\},$ which in turn implies $Q'(P) \subseteq Q(P)$. Therefore (o2) holds.

(a). We have $Q(P) := Q \setminus A^* = (Z \setminus A^*) \cap Q = Z(P) \cap Q = (P \cup Q)(P)$ because $Z(P) = Z \setminus A^*$, $Q \subseteq Z$ and $P \cup Q = Z$, and thus (a) is satisfied.

Before we proceed, we show that the sets Q(P) are separated from their complements in Q. From $A^* | B^*$, $Z \setminus A^* \subseteq B^*$ and $P \subset B^*$ we obtain $P \cup Z \setminus A^* \subseteq B^*$, which by isotony implies $A^* | P \cup Z \setminus A^*$. From $Z(P) = Z \setminus A^*$ we have $A^* = Z \setminus Z(P)$ and thus $Z \setminus Z(P) | Z(P) \cup P$. Isotony immediately yields $Q \cap (Z \setminus Z(P)) | (Q \cap Z(P)) \cup P$, which by (a) reduces to

(3.9)
$$Q \setminus Q(P) \mid Q(P) \cup P$$
 for all $P, Q \in 2^X$.

(t+) Let $R \subseteq Q(P)$ and set $A := Q \setminus Q(P)$ and $B := Q(P) \cup P$. By equ.(3.9), $A \mid B$ is a separation with $R \cup P \subseteq B$. Therefore $Q(R \cup P) \subseteq Q \setminus A = Q(P)$. By (o2) we have $Q(P) \subseteq Q(R \cup P)$; therefore $Q(R \cup P) = Q(P)$.

(o3) Suppose that there is a separation $A \mid C$ with $A \cup C = Z(P) \cup P$ and $P \subseteq C$. With $B := Z \setminus Z(P)$ we have $B \mid A \cup C$ and thus by (SR1) also $A \cup B \mid C$, i.e., $A \cup (Z \setminus Z(P)) \mid C$. Since this separation by definition is contained in $\mathfrak{S}(P,Q)$, we have $A \cup (Z \setminus Z(P)) \subseteq A^* = Z \setminus Z(P)$, i.e., $A \subseteq Z \setminus Z(P)$. Thus $A \cap Z(P) = \emptyset$. We conclude: (*) All separations $A \mid B$ with $A \cup B = Z(P) \cup P$ and $P \subseteq B$ satisfy $A \cap Z(P) = \emptyset$.

The definition of (Z(P))(P) and (*) together imply $Z(P) \subseteq (Z(P))(P)$. Thus (o1) implies (Z(P))(P) = Z(P). Now consider Q(P) with $P \cup Q = Z$. From (a) we have $Q(P) = Q \cap Z(P) \subseteq Z(P)$ and thus $Q(P) \cup P = Z$. Now (a) implies with $Q'(P) = Q' \cap Z(P)$ in particular also for Q' = Q(P), i.e., $(Q(P))(P) = Q(P) \cap Z(P)$. Since $Q(P) \subseteq Z(P)$ by (o2), we arrive at (Q(P))(P) = Q(P).

(o4). Property (t+) with R = Q(P) implies $Q(Q(P) \cup P) \subseteq Q(P)$ and thus by isotony of Q(.) we have $Q(Q(P)) \subseteq Q(Q(P) \cup P) \subseteq Q(P)$. Thus for any $S \subseteq Q(P)$, isotony also implies $Q(S) \subseteq Q(Q(P)) \subseteq Q(P)$.

Lemma 3.16. Let | satisfy (S0), (S1), (SR1), and (SR2), let \succeq be the derived production relation with generalized oriented connected components $(P,Q) \mapsto Q[P]$ and let $(P,Q) \mapsto Q(P)$ be the map defined in equ.(3.8). Then for all $P, Q \in 2^X$ holds Q(P) = Q[P].

Proof. By definition of Q(P) we have Q(P) = Q if and only if $A^* = \emptyset$, i.e., iff there is no separation $A \mid B$ with $P \in B$ and $A \neq \emptyset$, i.e., if and only if $P \succeq Q$. By Thm. 3.9 $(P,Q) \mapsto Q(P)$ bijectively maps to a unique production relation, which we have just seen is the same as $P \succeq Q$. The bijection between the production relation \succeq and the generalized opening $(P,Q) \mapsto Q[P]$ completes the proof. \Box

Theorem 3.17. There is a bijection between production relations \succ satisfying (O), (U), (T+), and (A) and separation relations satisfying (S0), (S1), (SR1), and (SR2).

Proof. It suffices to show that $A \mid B$ if and only if $A \mid B$. The fact that \mid and $\dot{\succ}$ are related by the Galois connection defined in equ.(3.3) then immediately implies the theorem.

Suppose $A \mid B$. For $A = \emptyset$ we trivially have $A \mid B$. Thus assume $A \neq \emptyset$ and set $Y = A \cup B$. From $A \mid B$ we know that $P \succeq Q$ with $P \subseteq B$ and $P \cup Q \subseteq Y$ must satisfy $Q \cap A = \emptyset$. In particular, the corresponding generalized oriented components satisfy $Q(P) \cap A = \emptyset$ for all $P \subseteq B$ and $Q \subseteq Y$ in particular $Y(B) \cap A = \emptyset$. By equ.(3.9) we have $Y \setminus Y(B) \mid Y(B) \cup B$. From $A \subseteq Y$ and $Y(B) \cap A = \emptyset$ we conclude $A \subseteq Y \setminus Y(B)$ and thus, by (S1) $A \mid Y(B) \cup B$ and finally $A \mid B$.

Conversely, assume $A \mid B$. Lemma 3.16 implies that the generalized connected components w.r.t. \succ are given by equ.(3.8). Now suppose $A \mid B$ does not hold. Then there is a $P \succeq Q$ with $P \cup Q \subseteq A \cup B$, $P \subseteq B$, and $Q \cap A \neq \emptyset$. This is impossible, however, since by construction $A \cap Y(B) = \emptyset$ and $Q \subseteq Y(B)$. Thus $A \mid B$.

We recall, finally, that axiom (A) means that $(P,Q) \to Q[P]$ and hence the relation \succ is uniquely defined by the $P \succ Q$ or Q[P] with $P \subseteq Q$. In other words, we might want to restrict the definition of production relations \succ and of generalized oriented components Q[P] to the domain $\{(P,Q)|P \subseteq Q \subseteq X\}$. In this condition axiom (A) becomes void and thus can be omitted.

4. PROPERTIES OF SEPARATION AND PRODUCTION RELATIONS

Throughout this section we assume | and \succ are connected by their natural bijection (3.3) and that the Q[P] are the equivalent generalized oriented components. In particular, | satisfies (S0), (S1), (SR1), and (SR2), \succ satisfies (O), (U), (A), (T+), and $(P,Q) \mapsto Q[P]$ satisfies (o1), (o2), (o3), (t+), and (a). Recall that axioms (o4) and (T), resp., also hold by Lemma 3.3 and Fact 3.12.

4.1. The Membership Property.

Theorem 4.1. The following three conditions are equivalent

- (SR0) $A \mid B$ implies $A \cup B \mid A \cap B$.

 - (m) If $P \subseteq Q$ then $P' \subseteq P \setminus Q[P]$ implies $Q[P'] = \emptyset$. (M) $P \succ Q$, $P' \succ Q'$, $P' \subseteq P \setminus Q$, and $Q' \subseteq Q$ implies $Q' = \emptyset$.

Proof. Suppose (SR0) holds, $A \mid B$ and $Z = A \cup B$. We have $B \succ Z[B]$ and thus $Z[B] \cap A = \emptyset$, i.e., $Z[B] \subseteq B \setminus A = Z \setminus A$. Furthermore, let $\{A_i | i \in I \}$ be the family of sets with $A_i \cup B = Z$ and $A_i \mid B$ and set $A = \bigcup_{i \in I} A_i$. By (SR2) we have $\hat{A} \mid B$. From $Z[B] \cap A_i = \emptyset$ for all I and $Z \setminus Z[B] \mid Z[B]$, which is a special case of equ.(3.9), we conclude $\hat{A} = Z \setminus Z[B]$. By (SR0) $A \cup B \mid A \cap B$, i.e., for every $P' \subseteq A \cap B$ holds $Z[P'] \cap (A \cup B) = Z[P'] \cap Z = \emptyset$, i.e., $Z[P'] = \emptyset$. This is true in particular also for all $P' \subseteq \hat{A} \cap B = B \cap (Z \setminus Z[B]) = B \setminus Z[B].$ By lemma 3.14 we have $B \setminus Z[B] = B \setminus Q[B]$, i.e., $P' \in B \setminus Q[B]$ implies $Q[P'] = Z[P'] = \emptyset.$

Conversely, suppose (m) holds but there is a pair $A \mid B$ such that $A \cup B \mid$ $A \cap B$ does not hold, i.e., there is a point $y \in A \cup B = Z$ and a $P' \in A \cap B$ with $y \in Q[P']$ for some $Q \subseteq Z$. From $A \mid B$ we have $Q[B] \subseteq B \setminus A$. Since $A \mid B$ we have $A \subseteq Z \setminus Z[B]$ and thus $P' \subseteq A \cap B \subseteq B \cap (Z \setminus Z[B]) = B \subseteq Z[B]$. Now property (m) implies $Z[P'] = \emptyset$. Since $Q[P'] \subseteq Z[P']$ we arrive at the desired contradiction.

Suppose (m) holds, $P \succ Q$, $P' \succ Q'$, $P' \subseteq P \setminus Q[P]$, and $Q \subseteq Q'$. Then by definition, Q = Q[P] and Q' = Q'[P']. Isotony implies $Q'[P'] \subseteq Q[P']$. By (m) $Q[P'] = \emptyset$ and thus $Q' = \emptyset$, i.e., (M) holds.

Finally, suppose (M) holds. Consider $P' \subseteq P \setminus Q[P]$ and suppose $P' \succ Q'$ for some $Q' \subseteq Q$. By definition of generalized connected components, $Q' \subseteq$ $Q[P'] \subseteq Q$. From $P \succ Q[P']$ and (M) we conclude $Q[P'] = \emptyset$, i.e., (m) holds.

We shall see below that (m) corresponds to the "membership condition" employed in [22] in the context of oriented components: " $p \notin Q[\{p\}]$ implies $Q[\{p\}] = \emptyset$ " for $p \in Q$. Property (SR0), on the other hand, appeared in [26] as a condition for the existence of a bijection between connected components and symmetric separations.

4.2. The Point Source Property. Ronse's [22] work on oriented components can be embedded into the current framework by assuming that reachability from individual points completely specifies the production map. This property, which we call here the *point source property* is most easily expressed in terms of generalized oriented components as $Q[P] = \bigcup_{p \in P} Q[\{p\}].$

Theorem 4.2. The following three conditions are equivalent

- (SR2+) Let $A_i \cup B_i = Z$ and $A_i \mid B_i$ for all $i \in I$. Then $\bigcap A_i \mid \bigcup B_i$.
 - (D) If $P \succ Q$ and Q is maximal in $P \cup Q$ then there are $\{p\} \succ Q_p$ for $p \in P \text{ such that } \bigcup_{p \in P} Q_p = Q.$ (d) If $P \subseteq Q$ then $Q[P] = \bigcup_{p \in P} Q[\{p\}].$

Proof. (d) \Longrightarrow (SR2+). Suppose (d) holds, $A_i \cup B_i = Z$ and $A_i \mid B_i$ for all $i \in I$. From $A_i \mid B_i$ we known that for every $P \subseteq B_i$ we have, for every $Q \subseteq Z, Q[P] \cap A_i = \emptyset$ and thus in particular also $Q[\{p\}] \cap A_i = \emptyset$. For every $p \in \bigcup_{i \in I} B_i$ we therefore have $Q[\{p\}] \cap \bigcap_{i \in I} A_i = \emptyset$ and thus by (d) $Z[P] \cap \bigcap_{i \in I} A_i = \emptyset$ and therefore also $Q[P] \cap \bigcap_{i \in I} A_i = \emptyset$ for all $P \subseteq \bigcup_{i \in I} B_i$, and thus $\bigcap_{i \in I} A_i \mid \bigcup_{i \in I} B_i$.

 $(SR2+) \Longrightarrow (d)$. Fix Z and $P \subseteq Z$. Choose I so that $B_i = \{p\}$ and $A_i =$ $Z \setminus Z[\{p\}]$ for some $p \in P$. We have shown in the proof of Lemma (3.15) that $Z \setminus Z$ $Z[P] \mid Z[P] \cup P$. Therefore $A_i \mid B_i$ holds, and hence by (SR2+), also $\bigcap_{p \in P} (Z \setminus A_i)$ Z[P]) $|\bigcup_{p\in P} Z[\{p\}]$, i.e., $Z \setminus \bigcup_{p\in P} Z[\{p\}] |\bigcup_{p\in P} Z[\{p\}]$. Furthermore we know that $P \succ \bigcup_{p \in P} Z[\{p\}]$ by (U). By equ.(3.9) we have $Z \setminus \bigcup_{p \in P} Z[p]$ $P \cup \bigcup_{p \in P} Z[\{p\}]$. Now $P \succ Z[P]$ implies $Z[P] \cap Z \setminus \bigcup_{p \in P} Z[\{p\}] = \emptyset$, i.e., $Z[P] \subseteq \bigcup_{p \in P} Z[\{p\}], \text{ i.e., } Z[P] = \bigcup_{p \in P} Z[\{p\}]. \text{ Since } Z = Q \text{ for } P \subseteq Q, \text{ (d)}$ follows.

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(D) \Longrightarrow (d). Suppose $P \succ Z$ and assume that Z is maximal in $P \cup Z$. Thus $Z = (P \cup Z)[P]$. Set $Q = P \cup Z$. By construction Z = Q[P]. Property (D) implies that there are Q_p with $\{p\} \succ Q_p$ and $Q_p \subseteq Q$ such that $\bigcup_{p \in P} Q_p = Q[p]$. We have $Q_p \subseteq Q[\{p\}] \subseteq Q$ and thus $Q[P] = \bigcup_{p \in P} Q_p \subseteq \bigcup_{p \in P} Q[p] \subseteq Q[P]$, and hence $Q[P] = \bigcup_{p \in P} Q[p]$ whenever $P \subseteq Q$, i.e., (d) holds.

(d) \Longrightarrow (D) We may assume $P \subseteq Q$, thus Q[P] is the maximal set in $Q \cup P = Q$ satisfying $P \succ Q$. We simply choose $Q_p = Q[\{p\}]$. By construction $\{p\} \succ Q_p$ and $Q[P] = \bigcup_{p \in P} Q[\{p\}] = \bigcup_{p \in P} Q_p$.

Property (a) now implies $Q[P] = \bigcup_{p \in P} (Q \cup P)[\{p\}] \cap Q$ whenever $P \not\subseteq Q$. In general we only have

(4.1)
$$\bigcup_{p \in P} Q[\{p\}] \subseteq Q[P]$$

Equality is guaranteed only if $P \subseteq Q$.

Lemma 4.3. The following three axioms are equivalent for separation relations, production relations and generalized connected components satisfying the conditions of Thm. 3.17.

- (S0+) $A \mid \emptyset$ for all $A \in 2^X$.
 - (G) $\varnothing \succ Q$ implies $Q = \varnothing$.
 - (g) $Q[\varnothing] = \varnothing$.

Proof. Suppose (S0+) holds, i.e., $A \cap Q = \emptyset$ for all $A \in 2^X$ and all Q such that $\emptyset \succ Q$. Thus $Q = \emptyset$, i.e. (G) follows. Conversely suppose G holds. Then $A \mid \emptyset$ follows since $A \cap Q = \emptyset$ for $Q = \emptyset$.

Fact 4.4. Axiom (d) implies axiom (g).

Proof.
$$Q[\varnothing] = \bigcup_{p \in \varnothing} Q[\{p\}] = \varnothing$$
.

Lemma 4.5. If (d) holds, then (t) implies (t+).

4.3. **Reaches.** A reach [22] is a family $\mathfrak{R} \subseteq 2^X \times X$ satisfying the following three axioms:

- (r1) Let $\mathcal{F} \subseteq 2^X$ and $(F,p) \in \mathfrak{R}$ for all $F \in \mathcal{F}$. Then $(\bigcup_{F \in \mathcal{F}} F, p) \in \mathfrak{R}$. (union property)
- (r2) If $(Q, p) \in \mathfrak{R}$, $s \in Q$, and $(T, s) \in \mathfrak{R}$ then $(Q \cup T, p) \in \mathfrak{R}$. (transitivity) (r3) If $(p, F) \in \mathfrak{R}$ then $F = \emptyset$ or $p \in F$. (membership property)

As shown in [22] there is a bijection of set systems satisfying (r1) and systems of point openings, that is, maps $2^X \times X \to 2^X$, $(F,p) \mapsto F(p)$ satisfying the following three axioms for all $p \in X$ and all $F, F' \in 2^X$:

$$(p1) \ F(p) \subseteq F,$$

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(p2) $F' \subseteq F$ implies $F'(p) \subseteq F(p)$, (p3) (F(p))(p) = F(p),

 $(P^{\circ}) (1 (P)) (P) = (P),$

The bijection is established by virtue of

(4.2)
$$F(p) := \bigcup \{S | (S, p) \in \mathfrak{R} \text{ and } S \subseteq F\}$$
$$\mathfrak{R} = \{(F, p) | F = F(p)\}.$$

Now consider a production relation \succ satisfying (O), (U), (D), and (A) and the corresponding generalized opening. In this case Q[P] is completely determined by the $Q[\{p\}]$ with $p \in Q$. We can think of the $Q[\{p\}]$ as a point opening. Axiom (a) specializes to

(pa) If $p \notin F$ then $F(p) = (F \cup \{p\})(p) \setminus \{p\}$.

and uniquely defines the sets F(p) whenever $p \notin F$. An equivalent condition is (ra) If $p \in F$ and $(F, p) \in \mathfrak{R}$ then $(F \setminus \{p\}, p) \in \mathfrak{R}$.

We call a set system $\mathfrak{R} \subseteq 2^X \times X$ a *pre-reach* if it satisfies (r1) and (ra).

We note here that this construction differs from the definition in [22], where $F(p) = \emptyset$ is stipulated for $p \notin F$. In either case, however, $(F, p) \mapsto F(p)$ is uniquely determined by the subset $\{(F, p) | p \in F\}$ on which [22] and our definition does agree. Therefore there is an obvious 1-1 correspondence.

Lemma 4.6. There is a bijection between pre-reaches, i.e., set systems \mathfrak{R} on $2^X \times X$ satisfying (r1) and (ra) and production relations \succ on 2^X satisfying (O), (U), (A), and (D), by virtue of $(F, p) \in \mathfrak{R}$ if and only if $\{p\} \succ F$.

Proof. It is easier to argue in terms of the openings F(p) and the generalized oriented components Q[P], respectively. First we recall that Q[P] is uniquely determined by $(Q \cup P)[P]$ through property (a), i.e., the Q[P] with $P \not\subseteq Q$ are determined by those with $P \subseteq Q$. For the latter, however, property (d) implies that they are uniquely determined by the $Q[\{p\}]$ with $p \in Q$. If $p \notin Q$, property (a) again determines $Q[\{p\}]$. Since (a) coincides with (ra) for |P| = 1, it extends to equality $F(p) = F[\{p\}]$ to all $p \in X$. It follows that $F(p) = F[\{p\}]$ induces a bijection between openings satisfying (ra) and generalized openings satisfying (a) and (d). Indeed (o1), (o2), and (o3) trivially specialize to (p1), (p2), and (p3).

It remains to show that (p1), (p2), and (p3) together with (d) implies (o1), (o2), and (o3). For $P \subseteq Q$ we have $Q[P] = \bigcup_{p \in P} Q[\{p\}] \subseteq Q$ and otherwise $Q[P] = (Q \cup P)[P] \cap Q \subseteq Q$, i.e., (o1) holds.

Next suppose $P' \subseteq P$ and $Q' \subseteq Q$. By (ii) we have $(Q' \cup P')[p] \subseteq (Q \cup P)[p]$. Therefore $Q'[P'] = (Q' \cup P')[P'] \cap Q' = Q' \cap \bigcup_{p \in P'} (Q' \cup P')[p] \subseteq Q \cap \bigcup_{p \in P} (Q \cup P)[p] = Q \cap (Q \cup P)[P] = Q[P]$, i.e. (o2) holds.

In particular, we have $(Q[\{p\}])[\{p\}] \subseteq (Q[P])[\{p\}] \subseteq (Q[P])[P]$ for all $p \in P$ and therefore also $\bigcup_{p \in P} (Q[p])[\{p\}] \subseteq (Q[P])[P]$. Now suppose $P \subseteq Q$. Then (d) implies $Q[P] = \bigcup_{p \in P} Q[\{p\}]$ and (p3) implies $Q[P] = \bigcup_{p \in P} (Q[\{p\}])[\{p\}]$ and therefore $Q[P] \subseteq (Q[P])[P]$. Now (o2) implies the desired equality Q[P] =(Q[P])[P]. Finally, if $P \not\subseteq Q$ we have $(Q[P])[P] = (Q[P] \cup P)[P] \cap Q[P] =$ $\begin{array}{l} ((Q \cup P)[P] \cap Q)[P] \cap Q[P] \text{ By } (o2) \ ((Q \cup P)[P])[P] \cap Q[P] \subseteq ((Q \cup P)[P] \cap Q)[P]. \\ \text{On the other hand} \ ((Q \cup P)[P])[P] \cap Q[P] = (Q \cup P)[P] \cap Q[P] = Q[P], \text{ and} \\ \text{thus } Q[P] \subseteq (Q[P])[P]. \text{ Thus } (o3) \text{ holds.} \end{array}$

A family $\mathfrak{R} \subseteq 2^X \times X$ is transitive if

(rt) $(F,p) \in \mathfrak{R}, q \in F$ and $(G,q) \in \mathfrak{R}$ implies $(F \cup G, p) \in \mathfrak{R}$.

It is shown in [22] that if \Re satisfies (r1), then (rt) is equivalent to

(pt) $q \in F(p)$ implies $F(q) \subseteq F(p)$

for the corresponding system of point openings. In our setting we have the following, analogous result:

Lemma 4.7. Let \succ be a production relation satisfying (O), (U), and (D) and let \mathfrak{R} be the corresponding pre-reach. Then (r2) is equivalent to (T) and (T+).

Proof. Specializing (T) to single point sources yields $\{p\} \succ Q, s \in Q$, and $\{s\} \succ T$ implies $\{p\} \succ Q \cup T$, which translates to $(Q, p) \in \Re$, $s \in Q$, and $(T, s) \in \Re$ implies $(Q \cup T, p) \in \Re$, i.e, (r2). Now suppose $\{p\} \succ Q_p$ for all $p \in P, S \subseteq Q = \bigcup_{p \in P} Q_p$ and $s \succ T_s$ for $s \in S$. Then $P \succ Q$, and for every $s \in S$ there is p such that $s \in Q_p$ and therefore $\{p\} \succ Q_p \cup T_s$. Using $T = \bigcup_{s \in S} T_s$ and thus by (U) $S \succ T$, and applying (U) again yields $P \succ Q$, $S \subseteq Q$ and $S \succ T$ implies $P \rightarrow Q \cup T$, i.e., (T) holds. Finally, by Lemma 4.5 (D) and (T) imply (T+). □

In the presence of (r1), it is shown in [22] that (r3) is equivalent to $p \in Q(p)$ or $Q(p) = \emptyset$. This condition obviously clashes with (pa). The reason is that for $p \notin Q$, [22] stipulates $Q(p) = \emptyset$, while we have made another choice with condition (pa), which in turn is motivated by (A). Instead, we use the specialization of (m) to singleton sets P:

(pm) If $p \in Q$ then $p \in Q(p)$ or $Q(p) = \emptyset$

To see that (pm) is the proper specialization of (m) we simply note that for $P' = P = \{p\}$ we have $P' \subseteq P \setminus Q[P] = \{p\} \subseteq \{p\} \setminus Q[\{p\}]$ which translates to $p \notin Q[\{p\}]$.

Lemma 4.8. Let \succ be a production relation satisfying (O), (U), (A) and (D) and let \mathfrak{R} be the corresponding pre-reach. Then (M) and (pm) are equivalent.

Proof. We first show that (m) reduces to (pm) for $P = \{p\}$. Assume $p \in Q$. If $p \in Q[\{p\}]$ then $P' = \emptyset$; otherwise $P' = \{p\} = P$ and thus $p \notin Q[\{p\}]$. Now (m) implies $Q[P'] = Q[\{p\}] = \emptyset$, and hence (pm) follows.

Conversely, suppose (pm) holds and suppose $P \subseteq Q$. Then by (d) $Q[P] = \bigcup_{p \in P} Q[\{p\}]$. Let $\overline{P} = P \setminus Q[P]$. Then for $p' \in \overline{P}$ holds $p' \notin Q[P]$ and thus also $p' \notin Q[\{p'\}]$, hence (pm) implies $Q[\{p'\}] = \emptyset$. By (d) we have $Q[\overline{P}] = \bigcup_{p' \in \overline{P}} Q[\{p'\}] = \emptyset$. Isotony now implies $Q[P'] = \emptyset$ for all $P' \subseteq P \setminus Q[P]$, i.e., (m) holds.

We can summarize this discussion in this section in the following form:

Corollary 4.9. There is a bijection between the generalized oriented components satisfying (01), (02), (03), (04), (m), (a), and (d) and the system of point openings satisfying (p1), (p2), (p3), (pt), (pm), and (pa). The latter coincides for $p \in Q$ with the system of point openings that is equivalent to reaches in the sense of Ronse [22].

Proof. The first statement is a direct consequence of Lemmas 4.6, 4.7, and 4.8. By virtue of (pa) and the choice made in [22] to set $Q(p) = \emptyset$ whenever $p \notin Q$, the system of point openings is completely defined by $(Q, p) \mapsto Q(p)$ for $p \in Q$. Here $Q(p) = Q[\{p\}]$, i.e., the bijection is just the identity on this subset. \Box

Finally, we can relate reaches to separation spaces:

Corollary 4.10. There is a bijection between the generalized oriented components satisfying (o1), (o2), (o3), (o4), (m), (a), and (d) and separation spaces satisfying (S0), (S0+), (S1), (SR0), (SR1), (SR2), and (SR2+). The same is true for the reaches as defined in [22].

This result directly generalizes the 1-1 correspondence between connectivity spaces and *symmetric* separations satisfying the same axioms [26]. We will return to this point in section 4.5.

4.4. Disjunctiveness. Consider the following properties:

(S3) $A \mid B$ implies $A \cap B = \emptyset$.

- (P) $P \succ P$ for all $P \in 2^X$.
- (p) $P \subseteq Q$ implies $P \subseteq Q[P]$.

Lemma 4.11. Suppose | and \succ are corresponding separation and production relations, and let $\{Q[P]\}$ be the corresponding system of generalized oriented components. Then (S3), (P), and (p) are equivalent.

Proof. Suppose $A \mid B$. By assumption, we have in particular $B \succ B$. It follows immediately that $B \cap A = \emptyset$.

Conversely, assume $A \mid B$ implies $A \cap B = \emptyset$ and suppose $P \succ P$ does not hold for some $P \in 2^X$. Then there is $A \mid B$ such that $P \subseteq B$ and $P \cap A \neq \emptyset$, whence $A \cap B \neq \emptyset$, a contradiction.

Suppose $P \subseteq Q$. From $P \succ P$ we immediately conclude $P \subseteq Q[P]$. Conversely, consider $P \subseteq P[P]$. By isotony we have $P[P] \subseteq P$ and therefore P = P[P] and thus $P \succ P$.

Lemma 4.12. Suppose (p) holds. Then (m) is equivalent to (g) and, equivalently, (SR0) reduces to (S0+).

Proof. Since $P \subseteq Q[P]$ for all $P \subseteq Q$, we have $P' = P \setminus Q[P] = \emptyset$. Thus (m) reduces to $Q[\emptyset] = \emptyset$, i.e., axiom (g). Analogously, we can argue that (S3) simplifies (SR0) to $A \mid B$ implies $A \cup B \mid \emptyset$. By (S0) we have $\emptyset \mid B$ and thus $B \mid \emptyset$ for all $B \in 2^X$.

4.5. Symmetry Axioms. The natural symmetry axiom for separations is (S2) $A \mid B$ implies $B \mid A$.

Lemma 4.13. Suppose | satisfies (S2). Then (S0) and (S0+), (SR2) and (SR2+) are equivalent. Furthermore, (S2) and (SR2) implies (SR0).

Proof. $\emptyset \mid A$ implies $A \mid \emptyset$ for all $A \in 2^X$ and vice versa.

Suppose $A_i | B_i$ for all $\in I$ and (SR2) holds. Then by (S2) $B_i | A_i$. (SR2) ensures $\bigcup_{i \in I} B_i | \bigcap_{i \in I} A_i$. Using (S2) again we also have $\bigcap_{i \in I} A_i | \bigcup_{i \in I} B_i$, i.e., (SR2+) holds. The implication in the other direction is shown analogously.

Finally, if $A \mid B$ then by (S2) also $B \mid A$. Applying (SR2) with $Z = A \cup B$, $A_1 = A, B_1 = B, A_2 = B$, and $B_2 = A$ results in $A \cap B \mid B \cap A$, i.e., (SR0) holds.

As shown in [26], there is a bijection between the "partial connections" of [21] and separation spaces satisfying (S0), (S1), (S2), (SR0), (SR1), and (SR2). Equivalent constructions have been considered e.g. in [23, 7, 4, 17, 6], see [26] for a detailed overview. Lemma 4.13 above shows that the (SR0) axiom thus is redundant in [26] and can simply be omitted. The (S2) axiom, via (SR0) and (SR2+) implies both the membership property (M) and point definedness (D) for the corresponding production relation and the generalized oriented components, i.e., the (S2) axiom takes us automatically to the reaches of [22]. The symmetry condition for the corresponding oriented components can be paraphrased in our notation as

(s) If $p \in Q$ and $r \in Q[\{p\}]$ then $Q[\{p\}] \subseteq Q[\{r\}]$.

By (o4) we have $Q[\{r\}] \subseteq Q[\{p\}]$ for $r \in Q[\{p\}]$, and thus under our general assumptions axiom (s) is equivalent to $Q[\{p\}] = Q[\{r\}]$.

Lemma 4.14. (S2) is equivalent to (m), (d), and (s).

Proof. Suppose (S2) holds. By lemma 4.13 we have (SR2+) and (SR0), and thus (m) and (d). In particular either $x \in Q[\{x\}]$ or $Q[\{x\}] = \emptyset$ for all $x \in X$. Suppose $p \in Q$ and $r \in Q[\{p\}]$; by (o4) this implies $Q[\{r\}] \subseteq Q[\{p\}]$. Now there are two cases to consider.

(1) If $p \in Q[\{r\}]$ then (o4) implies $Q[\{p\}] \subseteq Q[\{r\}]$, and thus $Q[\{r\}] = Q[\{p\}]$. (2) Otherwise $p \notin Q[\{r\}]$. By equ.(3.9) we have $Q \setminus Q[\{r\}] \mid Q[\{r\}]$ and by (S2) also $Q[\{r\}] \mid Q \setminus Q[\{r\}]$. Since $p \in Q \setminus Q[\{r\}]$, the correspondence of separation and generalized oriented components implies $Q[\{p\}] \cap Q[\{r\}] = \emptyset$. The assumption $r \in Q[\{p\}]$ thus implies $r \notin Q[\{r\}]$ and thus by (m) $Q[\{r\}] = \emptyset$ and therefore $Q \mid \{r\}$. Using (S2) again implies $\{r\} \mid Q$ and thus $p \in Q$ implies $Q[\{p\}] \cap \{r\} = \emptyset$, i.e., $r \notin Q[\{p\}]$, a contradiction. Thus $r \in Q[\{p\}]$ implies $p \in Q[\{r\}]$.

Conversely, suppose (m), (d), and (s) hold. Suppose (S2) does not hold, i.e., there is $A \mid B$ with $A \cup B = Q$ but $B \mid A$ does not hold. Then for all $p \in B$ holds $Q[\{p\}] \cap A = \emptyset$ and there is some $y \in A$ such that $Q[\{y\}] \cap B \neq \emptyset$. Consider $x \in B \cap Q[\{y\}]$. From $x \in B$ we infer $Q[\{x\}] \cap A = \emptyset$. On the other hand, axiom (s) implies $Q[\{x\}] = Q[\{y\}]$ and thus $Q[\{y\}] \cap A = \emptyset$, whence $y \notin Q[\{y\}]$. Now (m) implies $Q[\{y\}] = \emptyset$, a contradiction. Thus (S2) must hold.

The axiom for production relations corresponding to (s) is

(S) If $\{p\} \succ S$ then $q \succ S$ for all $q \in S$.

If \succ corresponds to a reach, i.e., in addition to (O), (U), (T), and (A) we also have (D) and (M), then (S) is equivalent to (s) for the corresponding system of generalized oriented components [22].

CONCLUDING REMARKS

We have shown here that production relations are in 1-1 correspondence with a class of proximity spaces satisfying simple, rather natural axioms. This establishes a natural topological interpretation of directed hypergraphs in general and chemical reaction networks in particular. The usefulness of this correspondence is further supported by the equivalence of simple properties in both axiom systems.

Many open questions remain for future research. The natural morphisms between proximity spaces, proximal maps $f : (X, \delta) \to (Y, \delta)$, preserve proximity, i.e., $A \delta B$ implies $f(A) \delta f(B)$. It will be interesting to investigate the properties of the corresponding maps for production relations. These should be related to the "catenous functions" introduced in [17]. On this basis one can hope to investigate the natural product structures. This might be interesting for production relations defined on Cartesian products such as the sequence spaces (Hamming graphs) typically used to model molecular evolution.

The Wallace closure $w : 2^X \to 2^X$ associated with a proximity is usually defined as $x \in w(B)$ iff $\{x\} \delta B$. The Wallace closure can be viewed as a generalization of Kuratowski's closure function for topologies. We will explore this connection to generalized topologies in forthcoming work. Such closure functions have been used as an alternative way of associating a topological structure with chemical reaction networks [2]. Exactly how this approach is connected with the production relations used here remains to be explored in the future.

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