Tracelet Hopf Algebras and Decomposition spaces (Extended Abstract)

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Tracelets are the intrinsic carriers of causal information in categorical rewriting systems. In this work, we assemble tracelets into a symmetric monoidal decomposition space, inducing a cocommutative Hopf algebra of tracelets. This Hopf algebra captures important combinatorial and algebraic aspects of rewriting theory, and is motivated by applications of its representation theory to stochastic rewriting systems such as chemical reaction networks.

1 Introduction

Double-Pushout (DPO) [13] and more generally compositional categorical rewriting systems [1, 6] provide a versatile and mathematically sound framework for modeling complex transition systems, with a paradigmatic example being the modeling of reaction systems in biochemistry [10] and in organic chemistry [7]. The specification of an individual rewriting operation (*direct derivation*) in essence amounts to providing a rewrite rule, i.e., a span of monomorphisms, that acts as a sort of template for the operation, together with a *match*, which permits to specify the location within a host object where the local replacement operation is to be performed. In practical applications, it is often the case that the rewriting rules themselves involve only comparatively small graph-like objects. In contrast, the host objects to which the rewrites are applied could easily be several orders of magnitude larger, so that an enormous number of matches may be possible for a given rule and a given host object.

A natural and powerful approach to overcome this fundamental problem consists in focusing on the combinatorial, statistical and structural properties of *interactions* of rewriting rules within derivation traces, and to aim for a classification of traces in terms of "interaction patterns". Unlike in compositional diagrammatic calculi such as in particular the theory of string diagrams, the key obstacle for such a type of analysis in rewriting theories resides in the fact that two given rules may in general interact in a multitude of ways, i.e., there does not exist a notion of deterministic rule composition. Instead, as first demonstrated in [4] and further developed in [1, 9, 7, 6], it is necessary to define a notion of non-deterministic rule composition via a form of recursive application of the concurrency theorem, which then indeed permits to reason statically about classes of rule compositions. Taking inspiration from the notion of *pathways* in chemical reaction systems, this approach was then further refined in [2] to the notion of *tracelets*, which in essence act as the carriers of causal information in derivation sequences.

The main objective of the present paper is to establish a principled mathematical approach to formalize the *combinatorics* of tracelets. Generalizing results of [5] on rewriting systems over directed multi-graphs to the categorical rewriting theory setting, we will demonstrate that it is indeed the notion of *combinatorial Hopf algebras* that naturally captures the rich structure of tracelets. Apart from a rewriting-theoretic construction of the Hopf algebras (Section 5), we report on our original discovery

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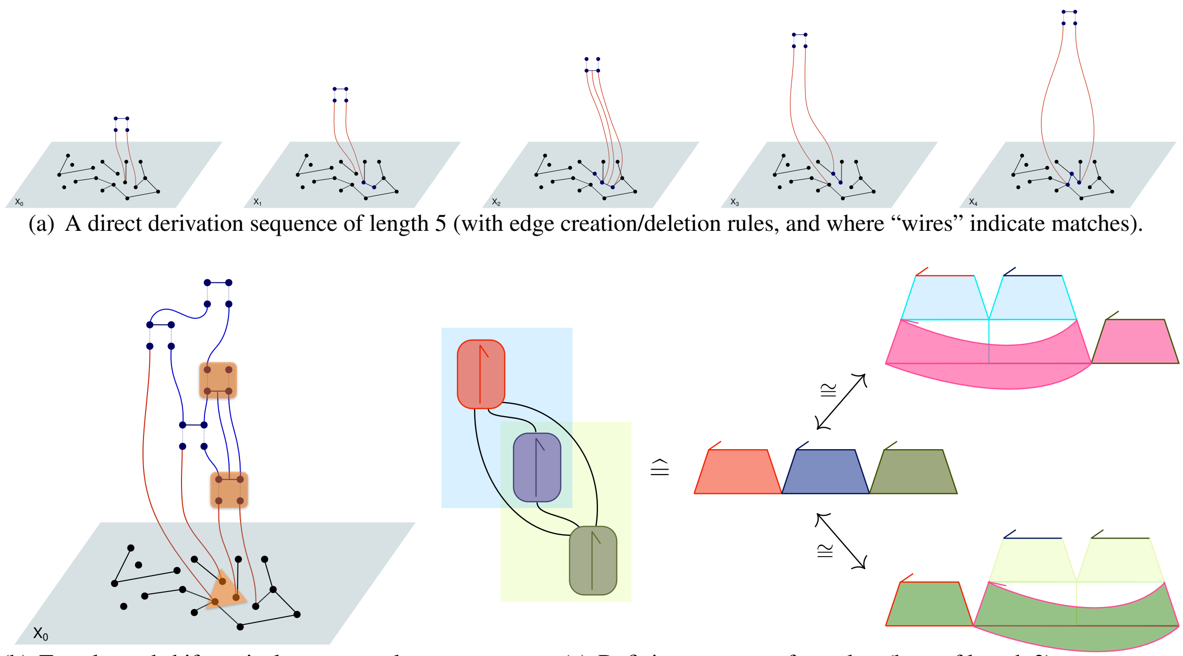


(a) A direct derivation sequence of length 5 (with edge creation/deletion rules, and where “wires” indicate matches).

(b) Tracelet and shift equivalence example.

(c) Defining property of tracelets (here of length 3).

Figure 1: An illustration of graph rewriting sequences (top) and of the tracelet picture (bottom).

that this at first sight seemingly ad hoc construction is in fact interpretable in terms of the theory of *decomposition spaces* (Sections 3 and 4). Our motivation for this approach has been the analogy between the inductive definition of tracelets and the decomposition-space axioms in homotopy combinatorics. The benefit of this ‘detour’ is to situate the tracelet Hopf algebra in a general framework covering most combinatorial Hopf algebras, thereby exhibiting the constructions and proofs as instances of general ideas.

Decomposition spaces were introduced in combinatorics by Gálvez, Kock and Tonks [16, 17] as a far-reaching homotopical generalization of posets for the purpose of incidence algebras and Möbius inversion, and independently by Dyckerhoff and Kapranov [12] in homological algebra and representation theory, motivated mainly by the Waldhausen S-construction and Hall algebras. Classically, since the work of Rota [22] in the 1960s, incidence algebras were defined from posets through the process of decomposing intervals, a construction which can fruitfully be formulated in terms of the nerve of a poset. However, a great many combinatorial co- and Hopf algebras are not of incidence type, meaning that they are not the incidence coalgebra of a poset. The basic observation of [16] is that simplicial objects more general than nerves of posets admit the incidence coalgebra construction, allowing most of the basic features of the theory to carry over — and that most combinatorial Hopf algebras do arise as incidence Hopf algebras of (monoidal) decomposition spaces.

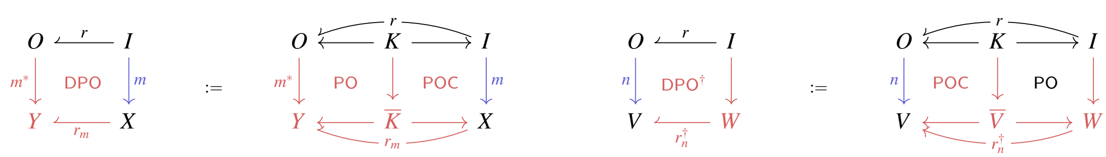
2 Double-Pushout rewriting and tracelet theory

Consider a rewriting system of undirected multi-graphs such as the one depicted in Figure 1(a), with some elementary rules that link and unlink vertices with edges. Starting from some initial graph X_0, each rewriting step (*direct derivation*) consists in choosing a rewriting rule together with an occurrence (*match*) of the input motif (drawn at the bottom of the rule diagrams) within the graph that is rewritten. Sequences of rewrites (*derivation traces*) have a rich intrinsic structure, arising from the highly non-trivial *interactions* of rules in a sequence through their matches, rendering a *compositional* interpretation of derivation traces a highly non-trivial task. To wit, consider the diagram in Figure 1(b), which provides a sort of movie-script depiction of the five-step derivation trace depicted in the top part of the figure. For clarity, red wires are used to indicate inputs to rules that are present in the original configuration X_0, while blue wires indicate inputs to rules that have originated from outputs of preceding rules.

The main purpose of the theory of *tracelets* [2] then consists in rendering mathematically precise the meaning of this intuitive picture. In particular, according to the *Tracelet Characterization Theorem* [2, Thm. 2], each derivation trace of length n is uniquely characterized by a *tracelet* of length n (cf. the sub-diagram consisting of the five rules and all blue wires in Figure 1(b)) and a *match* of the tracelet into the initial configuration X_0 (depicted as red wires in Figure 1(b)). Crucially, the compositional structure of tracelets offers a form of static causal analysis via algebraic relations such as commutator relations. This type of analysis takes advantage of algebraic relations such as *shift equivalence*, which in the example of Figure 1(b) amounts to the observation that the rules in the boxes highlighted in orange may be freely moved "along the wires" so as to exchange their order (i.e., without changing the overall effect of the rewriting sequence). Finally, as sketched via the highlighted triangle pattern that is produced via the rewriting sequence in the example, tracelets permit to statically reason about the combinatorics of pattern-counting problems in an efficient manner (cf. [3] for a prototype of such an analysis in the setting of counting patterns in planar rooted binary trees).

As depicted in Figure 1(c), a tracelet of length 3 exhibits already quite a non-trivial compositional structure, in that as sketched the internal structure of partial overlaps of rule inputs and outputs in such a tracelet is not of a purely sequential nature; to wit, the diagram encodes a special kind of trace of length 3, with the defining property that it may be equivalently (up to isomorphisms) be obtained via nested composition operations. It is in this particular sense that tracelets offer a *minimal* causal presentation of the structure of rewriting sequences, since via the equivalences to nested pairwise composition operations, they permit to efficiently express n-step sequences as just a special type of derivation sequences.

2.1. Categorical rewriting theory. For simplicity, we will focus here on the variant of tracelet theory for so-called *Double-Pushout (DPO) rewriting*, and for rewriting rules without application conditions (referring to [2] for the general theory[1]). Throughout this paper, let $\mathbf{C}$ denote an *adhesive category* [20] assumed to be *finitary* (in the sense of [11], i.e., with only finitely many subobjects for each object up to isomorphisms), and assumed to possess a strict initial object $\varnothing \in \mathsf{obj}(\mathbf{C})$. *Rewriting rules* are defined as spans of monomorphisms $r = (O \leftarrow o - K - i \rightarrow I)$, also denoted for brevity as $r = (O \leftharpoonup I)$. In the tradition of rewriting theory, we refer to such rules as *linear rules* (with "linear" referring to the nature of the span as a span of monos), and denote the class of all such rules as $\mathsf{Lin}(\mathbf{C})$. For every $r \in \mathsf{Lin}(\mathbf{C})$ and object $X \in \mathsf{obj}(\mathbf{C})$, let $\mathcal{M}_r(X)$ denote the *set of (DPO-admissible) matches of r into X*, where $m \in \mathcal{M}_r(X)$ iff m is a monomorphism and the *pushout complement* marked POC in the left-most diagram exists:



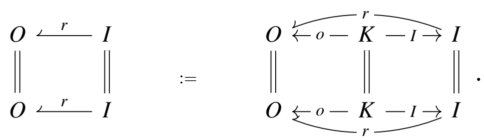
(1)

[1] Available generalizations include the type of rewriting (with *Sesqui-Pushout* semantics an alternative option), the choice of base-categories (with $\mathcal{M}$-*adhesive categories* [14] a more general option), as well as the inclusion of constraints and application conditions into the compositional rewriting semantics (cf. also [6]).

Note that in an adhesive category, pushouts along monomorphisms (here marked PO) are guaranteed to exist; in contrast, pushout complements (here marked POC) may fail to exist, since not every composable pair of arrows can be completed into a pushout square. Moreover, r_m and $Y = r_m(X)$ are evidently only defined up to universal isomorphisms. It is customary to refer to the data of the aforementioned diagram as a *direct derivation*. For later convenience, taking advantage of the symmetry of the definition, we mark by $\mathsf{DPO}^\dagger$ diagrams that arise as DPO-type direct derivations in the "opposite direction", i.e., "against" the direction of rules (here, from left to right; cf. the right-most diagram above).

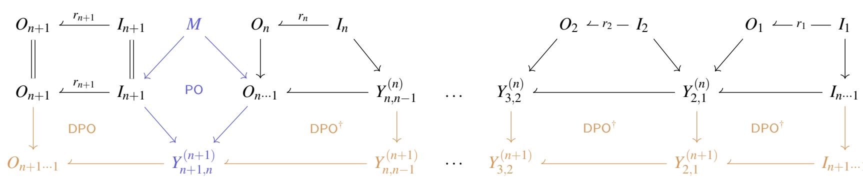
2.2. Tracelets. The class of *tracelets* $\mathcal{T}$ for DPO-type type rewriting over $\mathbf{C}$ is defined recursively:

- *Tracelets of length* 1: for every rule $r = (O \leftharpoonup I) \in \mathsf{Lin}(\mathbf{C})$, define $T(r) \in \mathcal{T}_1$ as a diagram



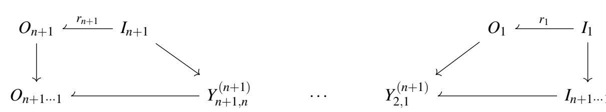
(2)

- *Tracelets of length* $n+1$: denoting by $\mathcal{T}_n$ (for $n \geq 1$) the class of trecelets of length n, the class $\mathcal{T}_{n+1}$ is defined to consist of diagrams as below, where $r_k = (O_k \leftharpoonup I_k) \in \mathsf{Lin}(\mathbf{C})$ are linear rules (for $k = 1, \ldots, n+1$), where the top right part of the diagram encodes a tracelet $T \in \mathcal{T}_n$ of length n, where $\mu = (I_{n+1} \leftarrow M \rightarrow O_{n\cdots 1})$ is a span of monos, with the cospan $I_{n+1} \rightarrow Y^{(n+1)}_{n+1,n} \leftarrow O_{n\cdots 1}$ its pushout, and such that the direct derivations marked DPO and $\mathsf{DPO}^\dagger$ exist:



(3)

Then this data defines a tracelet $T(r_{n+1}) \,{}^{\mu}\!\angle\, T$ of length $n+1$ (the *tracelet composition* of $T(r_{n+1})$ with T along μ) uniquely up to universal isomorphisms (see comments below) as

$T(r_{n+1}) \,{}^{\mu}\!\angle\, T :=$ 

(4)

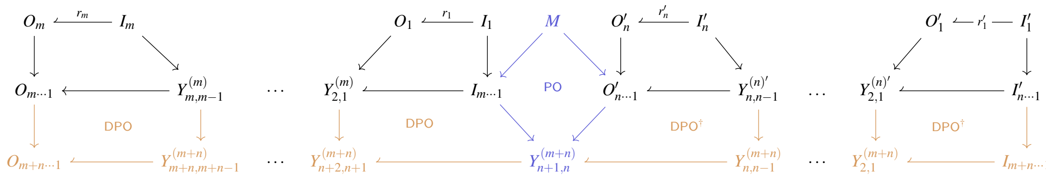
For later convenience, we will sometimes speak of the commutative square adjacent to rule r_i in a tracelet as the *ith plaquette*. Let $\mathcal{T} := \cup_{n\geq 1}\mathcal{T}_n$ denote the class of all (finite-length) tracelets. For later convenience, we also introduce the notations $\mathsf{in}(T) := I_{n\cdots 1}$ ("input interface" of $T \in \mathcal{T}_n$), $\mathsf{out}(T) := O_{n\cdots 1}$ ("output interface" of $T \in \mathcal{T}_n$), $\mathsf{MT}_{T(r_{n+1})}(T)$ (for "matches", i.e., admissible partial overlaps μ of the length-1 tracelet $T(r_{n+1})$ with the tracelet $T \in \mathcal{T}_n$) and $[[T]]$ for the so-called *evaluation* of the tracelet T, which for $T \in \mathcal{T}_n$ is defined with notations as in the top right of (4) as

$$[[T]] := (O_{n\cdots 1} \leftharpoonup I_{n\cdots 1}) = (O_{n\cdots 1} \leftharpoonup Y^{(n)}_{n,n-1}) \circ \cdots \circ (Y^{(n)}_{2,1} \leftharpoonup I_{n\cdots 1})\,. \tag{5}$$

Here, $\circ$ denotes the operation of *span composition* (considered up to span isomorphisms).

Up to this point, one might say that DPO-type tracelets are some form of data structure that encodes a certain form of *sequential compositions* of rewriting rules. This point of view is augmented via the following definition, which finally reveals tracelets as a particular notion of compositional diagrams.

2.3. Tracelet composition. Let $T \in \mathcal{T}_m$ and $T' \in \mathcal{T}_n$ be two tracelets of length m and n, respectively (for $m,n > 0$). Let $\mu := (I_{m\cdots 1} \leftarrow M \rightarrow O'_{n\cdots 1})$ be a partial overlap (of the "input interface" $I_{m\cdots 1}$ of T with the "output interface" $O'_{n\cdots 1}$ of T') whose pushout $I_{m\cdots 1} \rightarrow Y^{(m+n)}_{n+1,n} \leftarrow O'_{n\cdots 1}$ satisfies that in the diagram below, all direct derivations marked DPO and DPO†, respectively, exist:



(6)

In this case, we write $\mu \in \mathsf{MT}_T(T')$ to say that μ is a (DPO-admissible) *match* of T into T', and we define the *composition* of T with T' along μ as

$$T \,{}^{\mu}\!\angle\, T' :=$$

(7)

The definition of tracelets and their composition might appear somewhat ad hoc at first sight, yet it is very natural if viewed in diagrammatic form. To this end, consider the example of a tracelet of length 3 such as in Figure 1(c). The "wires" in the schematic diagram that link individual length-1 tracelets encode the partial overlaps; as indicated, the tracelet of length 3 may be realized recursively by either determining the partial overlap of the first and the second sub-tracelet, composing, and then determining the resulting overlap of the composite tracelet of length 2 with the third tracelet of length 1, or (equivalently as it will turn out) by computing the composition of the third and second tracelets of length 1, and of that composite with the first tracelet of length 1. This so-called *associativity property* of tracelet composition is at the heart of the algebraic properties of tracelets. It will be further illustrated when we now pass to discuss tracelets in the framework of decomposition spaces.

3 The decomposition space of rewrite rules

In this section we describe a decomposition space $\mathbf{X}_\bullet$ of rewrite rules (for a fixed rewrite system in a fixed adhesive category $\mathbf{C}$ as above), whose incidence algebra is the rule algebra.

3.1. Decomposition spaces. A decomposition space [12, 16] is a simplicial groupoid $X_\bullet : \mathbb{\Delta}^{\mathrm{op}} \rightarrow \boldsymbol{Grpd}$ satisfying a certain exactness property designed precisely to allow the incidence coalgebra construction, classically defined for posets. The nerve of a poset or a category is an example of a decomposition space. Where categories encode composition, decomposition spaces owe their name to encoding more generally decomposition. Many situations where compositionality is hard to achieve can be dealt with instead with decompositions, as is often the case in combinatorics, where combinatorial structures can be split into smaller ones without the ability to compose [18, 15]. Often non-deterministic composition structures can be turned around and constitute instead a decomposition.

There are different ways to formulate the decomposition-space axioms. One (simplified) version states that for any endpoint-preserving monotone map $\alpha : [2] \twoheadrightarrow [n]$, defining a decomposition of any

n-simplex into an n_1-simplex and an n_2-simplex, the natural square

$$\begin{array}{ccc} X_n & \longrightarrow & X_{n_1} \times X_{n_2} \\ \downarrow & \lrcorner & \downarrow \text{long edges} \\ X_2 & \xrightarrow[\text{short edges}]{} & X_1 \times X_1 \end{array} \tag{8}$$

is a (homotopy) pullback. It says that an n-simplex can be reconstructed from the two smaller simplices of the decomposition together with the information of a gluing of the long edges of the two simplices onto the short edges of a base 2-simplex.

This condition is considerably weaker than the Segal condition (which characterizes categories, hence composition rather than just decomposition), which says that a single-vertex overlap between the two smaller simplices is enough to perform the gluing. In the decomposition-space case, the base 2-simplex is required as a kind of context for the gluing.

3.2. Groupoids of tracelets. An *isomorphism* between two tracelets of length n is by definition a family of object-wise isomorphisms between the involved objects in $\mathbf{C}$ making all squares commute. We denote by $\mathbf{X}_n$ the groupoid of all tracelets of length n. (In particular, the only tracelet of length 0 is the empty one (which evaluates to the trivial rule), so $\mathbf{X}_0 = \{*\}$.)

Theorem 3.3. *The groupoids $\mathbf{X}_n$ assemble into a simplicial groupoid $\mathbf{X}_\bullet : \mathbb{\Delta}^{\text{op}} \to$ **Grpd** (whose face and degeneracy maps we proceed to describe below).*

Recall that a simplicial structure amounts to face maps d_i and degeneracy maps s_i as in the diagram

$$\mathbf{X}_0 \;\underset{\leftarrow d_0}{\overset{\leftarrow d_1}{\xrightarrow{s_0}}}\; \mathbf{X}_1 \;\begin{smallmatrix} \leftarrow d_2 \\ s_1 \rightarrow \\ \leftarrow d_1 \\ s_0 \rightarrow \\ \leftarrow d_0 \end{smallmatrix}\; \mathbf{X}_2 \;\begin{smallmatrix} \leftarrow d_3 \\ s_2 \rightarrow \\ \leftarrow d_2 \\ s_1 \rightarrow \\ \leftarrow d_1 \\ s_0 \rightarrow \\ \leftarrow d_0 \end{smallmatrix}\; \mathbf{X}_3 \qquad \cdots \tag{9}$$

subject to the *simplicial identities*: $d_i s_i = d_{i+1} s_i = 1$ and

$$d_i d_j = d_{j-1} d_i, \quad d_{j+1} s_i = s_i d_j, \quad d_i s_j = s_{j-1} d_i, \quad s_j s_i = s_i s_{j-1} \qquad (i < j).$$

The bottom and top face maps generate the class of *inert maps*, whereas the inner face maps and the degeneracy maps generate the class of *active maps*, for which we use the special arrow symbol $\rightarrowtail$. These two classes of maps play a special role in the theory; see [16], where more conceptual characterizations are given.

3.4. Description of the face maps. The *top face map* $d_n : \mathbf{X}_n \to \mathbf{X}_{n-1}$ (resp. the *bottom face map* $d_0 : \mathbf{X}_n \to \mathbf{X}_{n-1}$) is defined via (1) performing *tracelet surgery* to exhibit the tracelet as a composition of the first (the last) rule with an $(n-1)$-tracelet, followed by (2) extracting the length-$(n-1)$ tracelet. This is illustrated in Figure 1(c) for the case of $n = 3$, with d_0 (d_3) defined to return the tracelet shaded in light blue (in light yellow).

Recall from Section 2.2 that a *plaquette in position i* of a given tracelet is defined as the ith direct derivation, i.e., the commutative subdiagram of the tracelet involving the ith rule (read from the right). Then the *inner face maps* $d_i : \mathbf{X}_n \to \mathbf{X}_{n-1}$ (for $0 < i < n$) replace the two plaquettes p_i and p_{i+1} in the chain with a single new plaquette p' having the same starting point as p_i and the same endpoint as p_{i+1}, by applying the "synthesis" part of the concurrency theorem to convert the sub-sequence of plaquettes p_{i+1} after p_i into a one-step direct derivation along the composite rule $p'_{i+1,i}$. The result of this operation is guaranteed to be a tracelet of length $n-1$. Referring once again to Figure 1(c) for an illustration of the case $n=3$, d_1 (d_2) are defined to return the tracelet shaded in green (in pink).

The *degeneracy maps* $s_i : \mathbf{X}_n \to \mathbf{X}_{n+1}$ (for $0 \le i \le n$) insert a copy of the trivial rule $\emptyset \leftarrow \emptyset \to \emptyset$ in the tracelet at position i.

In the form stated, $\mathbf{X}_\bullet$ is only a pseudo-simplicial groupoid. This means that the simplicial identities only hold up to (specified) isomorphism, and that there are coherence issues to deal with. The reason for this pseudo-ness is that composition of rules and tracelets, as involved in the face maps, is only well defined up to isomorphism, relying as it does on pushouts and pullbacks. To actually get well-defined face maps, it is necessary to make choices of these universal constructions, and these choices screw up the strict simplicial identities. (A well-known example of this phenomenon is how composition of spans by means of pullbacks defines a bicategory, not an ordinary category.)

This pseudo-ness is not at all a problem for the sake of decomposition-space theory, designed to be up to homotopy, and it does not affect the incidence algebra we construct from this decomposition space (which in any case is spanned by iso-classes of rewrite rules). Nevertheless it is very fruitful to provide also a strict model of $\mathbf{X}_\bullet$. The standard technique for constructing this (which goes back to insight from algebraic topology from the 1970s (notably Quillen,[2] Waldhausen, and Segal)) is to beef up the groupoid of n-simplices to something equivalent that contains all the (redundant) data involved in the face maps.

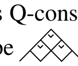
Specifically, a 2-simplex should not just be a 2-tracelet, but rather a 2-tracelet *together* with a choice of composite rule. In this way the middle face map $d_1 : \mathbf{X}_2 \to \mathbf{X}_1$ does not have to compute any composite by means of choices; it can simply return the choice already built in. The fact that these choices are unique up to universal isomorphisms says precisely that this bigger groupoid is equivalent to the original, and hence that the homotopy properties of the bigger simplicial groupoids are the same. In Figure 2(b) we see such a fully specified 2-simplex. The two short edges (01 and 12) are the two rules in a 2-tracelet, and the squares marked PO and POC are the plaquettes constituting altogether the 2-tracelet. The pullback square (blue, marked with PB) is not part of the data of the tracelet, but it is included in the fully specified notion of 2-simplex.

In degree 3 we arrive at the first point where there is an interesting simplicial identity to establish, namely commutativity of the square

$$\begin{array}{ccc} \mathbf{X}_3 & \xrightarrow{d_1} & \mathbf{X}_2 \\ {\scriptstyle d_2}\downarrow & & \downarrow{\scriptstyle d_1} \\ \mathbf{X}_2 & \xrightarrow[d_1]{} & \mathbf{X}_1, \end{array} \tag{10}$$

which in essence states that a sequential composition of three rules may be recovered equivalently from two steps of pairwise rule compositions in either of the nesting orders.

For the groupoids of bare tracelets, this simplicial identity cannot be strict, due to the choices of pushouts and pullbacks involved in composition of rules and tracelets. That the equation holds up to natural isomorphism is a nontrivial statement which involves the concurrency theorem (in the particular form called associativity theorem [9, 4, 5]). We explain how the same theorem implies the strict equation for the fully specified 3-simplices. This exhibits the beautiful geometry inherent in the associativity theorem. As always, the idea is that a fully specified 3-simplex should contain all information about all

[2]Historical remark: Bénabou (1963) had described a bicategory spans. Quillen used the techniques of big redundant n-simplices to exhibit the same structure as a *strict* simplicial groupoid, now called Quillen's Q-construction. Instead of having simply chains of n composable spans in degree n, he defined it to be diagrams of shape , that is composable spans, *together* with all the relevant pullbacks. Similar constructions were given in related situation by Waldhausen and Segal, and today the technique is standard in algebraic topology.

choices. In particular (in order for the four face maps to be forgetful) it should contain four 2-simplices of the form of Figure 2(b). A full picture of such a subdivided tetrahedron is given in Figure 2(e). One can chase through how this is built up from composition of tracelets, over specified overlaps: Consider the diagram depicted in Figure 2(c), which is formed by (1) a 2-simplex encoding a composition of two rules r_{21} and r_{10} into some rule r_{20}, and (2) another 2-simplex of which one "short edge" is the rule r_{20}, and which contains another rule r_{32} and the data of the composition of r_{32} with r_{20} into some rule r_{30}. Upon closer inspection, it is possible (via a number of somewhat intricate steps) to construct from this data the interior and the other two faces of a tetrahedron. To this end, one first invokes the "analysis" part of the DPO-type concurrency theorem in order to obtain, from the sub-diagram that encodes the one-step direct derivation of the object I_{03} along the composite rule $O_{20} \leftarrow K_{20} \rightarrow I_{20}$, the data of a sequence of two direct derivations along the "constituent" rules $O_{21} \leftarrow K_{21} \rightarrow I_{21}$ after $O_{10} \leftarrow K_{10} \rightarrow I_{10}$. This construction in particular delivers an object Z located in the interior of the tetrahedron. Over several further steps (involving pushout and pullback operations), it is then possible to fill the remaining two faces of the 3-simplex with the structure of two sequential rule compositions, ultimately resulting in the diagram of Figure 2(e). The fact that all these constructions are given by universal properties (pushouts and pullbacks, together with the axioms of adhesive categories) ensures that the groupoid of such fully specified 3-simplices is equivalent to the groupoid of bare 3-tracelets. The face maps are now obvious (or even tautological) and all the simplicial identities are clearly strict for this reason: they merely return data already contained in (the beefed-up version of) $\mathbf{X}_3$.

The higher simplices are increasingly cumbersome to describe, due to our limited vision of geometry in dimension higher than 3, but the principle is easy to follow: just include all information about all possible composites, and the overall geometric shape is always a geometric n-simplex whose edges are rules, whose 2-dimensional faces are as in Figure 2(b) and whose 3-dimensional faces are as in Figure 2(e).

The fact that in each dimension the bare tracelets contain information necessary and sufficient to reconstruct the full specified simplex is an expression of the central result of [2] that it is indeed tracelets that provide the minimal carriers of causal information in sequential rule compositions.

We proceed to establish that $\mathbf{X}_\bullet$ is a decomposition space. Since this is a homotopy invariant property, we may work with the simple version of groupoids of n-tracelets. Before the check, let us just note that $\mathbf{X}_\bullet$ is not a Segal space (a category), because of the non-deterministic nature of composition. Specifically, a 2-simplex cannot be reconstructed from knowing its two short edges.

Theorem 3.5. $\mathbf{X}_\bullet$ *is a decomposition space. This means that for all* $0 < i < n$ *the two squares*

$$\begin{array}{ccc} \mathbf{X}_{n+1} & \xrightarrow{d_{n+1}} & \mathbf{X}_n \\ {\scriptstyle d_i}\downarrow & & \downarrow{\scriptstyle d_i} \\ \mathbf{X}_n & \xrightarrow[d_n]{} & \mathbf{X}_{n-1} \end{array} \qquad\qquad \begin{array}{ccc} \mathbf{X}_{n+1} & \xrightarrow{d_0} & \mathbf{X}_n \\ {\scriptstyle d_{i+1}}\downarrow & & \downarrow{\scriptstyle d_i} \\ \mathbf{X}_n & \xrightarrow[d_0]{} & \mathbf{X}_{n-1} \end{array} \tag{11}$$

are (homotopy) pullbacks.

To check this, it is enough to show that the fibers of the maps pictured vertically are equivalent. We shall see that indeed all fibers of inner face maps are canonically identified with the fiber of $d_1 : \mathbf{X}_2 \rightarrow \mathbf{X}_1$.

3.6. Fiber calculations. Consider $d_1 : \mathbf{X}_2 \rightarrow \mathbf{X}_1$ which sends a pair of composable rules with minimal gluing (r_2, w, r_1) to the composite rule r'. The fiber over $r' \in \mathbf{X}_1$ is thus the groupoid of all (r_2, w, r_1) that compose to r'. We denote this groupoid $(\mathbf{X}_2)_{r'}$. Notice that the objects of $\mathbf{X}_2$ are composable pairs of plaquettes with the property that the intermediate point between the two plaquettes is a minimal gluing (of the output of rule r_1 with the input of rule r_2; in other words, the middle cospan in the two-step direct derivation sequence is a pushout of its own pullback).

Lemma 3.7. *The (homotopy) fiber of $d_i : \mathbf{X}_n \to \mathbf{X}_{n-1}$ (for $0 < i < n$) over a tracelet which in position i has a plaquette with rule r' is equivalent to the groupoid $(\mathbf{X}_2)_{r'}$. In particular, it does not depend on the whole plaquette p' under r', and it does not depend on the context in any way.*

One can now unpack the general construction of incidence algebras of decomposition spaces (cf. [16]) to establish:

Proposition 3.8. *The incidence algebra is the rule algebra of [9].*

This algebra is not our main focus in this work. Rather do we regard the decomposition space $\mathbf{X}_\bullet$ as a stepping stone towards more interesting decomposition spaces and Hopf algebras, notably the tracelet Hopf algebra.

4 Decomposition spaces of tracelets

So far we have defined the decomposition space $\mathbf{X}_\bullet$ of rules, whose incidence algebra is the rule algebra of [9]. We now proceed towards Hopf algebras spanned by tracelets.

The Hopf algebra of tracelets should be spanned by iso-classes of tracelets, which are now furthermore required to be *non-degenerate* as simplices of $\mathbf{X}_\bullet$. This means that the rules involved are not allowed to be the trivial rule.[3] The non-degenerate simplices of $\mathbf{X}_\bullet$ do not form a simplicial object, since inner faces of non-degenerate simplices are not always non-degenerate, but the outer face maps (the inert maps) survive (as a consequence of the decomposition-space axioms, see [17]), so as to define a presheaf

$$\vec{\mathbf{X}}_\bullet : \mathbb{\Delta}^{\mathrm{op}}_{\mathrm{inert}} \to \boldsymbol{Grpd}.$$

Left Kan extension along the inclusion functor $j : \mathbb{\Delta}_{\mathrm{inert}} \to \mathbb{\Delta}$ defines a new simplicial groupoid:

$$\mathbf{Y}_\bullet := j_! \vec{\mathbf{X}}_\bullet \ : \ \mathbb{\Delta}^{\mathrm{op}} \to \boldsymbol{Grpd}.$$

This is a general construction that makes sense for any (complete) decomposition space, and by a result of Hackney and Kock [19] it always produces a decomposition space again. One can expand explicitly what its simplices are:

$$\mathbf{Y}_k = \sum_{\alpha:[k] \twoheadrightarrow [n]} \vec{\mathbf{X}}_n.$$

(The sum is over active maps.) In particular

$$\mathbf{Y}_0 = \mathbf{X}_0 \qquad \text{and} \qquad \mathbf{Y}_1 = \sum_{n \in \mathbb{N}} \vec{\mathbf{X}}_n.$$

So the new 1-simplices are the non-degenerate tracelets of any length. The higher simplices are 'subdivided tracelets'. To see this, recall that the decomposition space axioms can be written (cf. [16, Prop. 6.9]) as saying that for any active map $\alpha : [k] \twoheadrightarrow [n]$ the canonical square

$$\begin{array}{ccc} \mathbf{X}_n & \longrightarrow & \mathbf{X}_{n_1} \times \cdots \times \mathbf{X}_{n_k} \\ \downarrow & \lrcorner & \downarrow \\ \mathbf{X}_k & \longrightarrow & \mathbf{X}_1 \times \cdots \times \mathbf{X}_1 \end{array} \tag{12}$$

[3] By imposing this condition, we account directly for an equivalence relation imposed in [2] called 'equivalence up to trivial tracelets' (cf. Definition 5.2).

is a (homotopy) pullback. Here the vertical maps are active and the horizontal maps are combinations of inert maps. What the condition says is that it is possible to glue together k simplices (of different dimensions n_i) if just one has available a 'mould' to glue them together in, namely a k-simplex whose k principal edges match the long edges of the k simplices. (This is also the essence of the very definition of tracelet.)

An example of such a composition is depicted in Figure 2(c), in which a length-2 tracelet (depicted as the 2-simplex 012) is composed along the short edge 02 of the 2-simplex 023 with a tracelet of length 1 (here depicted as the edge 23). Figure 2(d) then depicts the method for computing the resulting tracelet of length 3, which itself is depicted in Figure 2(f).

Since non-degeneracy in a decomposition space can be measured on principal edges (cf. [17]), we also have the (homotopy) pullback

$$\begin{array}{ccc} \vec{\mathbf{X}}_n & \longrightarrow & \vec{\mathbf{X}}_{n_1} \times \cdots \times \vec{\mathbf{X}}_{n_k} \\ \downarrow & \lrcorner & \downarrow \\ \mathbf{X}_k & \longrightarrow & \mathbf{X}_1 \times \cdots \times \mathbf{X}_1 . \end{array} \tag{13}$$

We see that a k-simplex in $\mathbf{Y}_\bullet$ is the data of a tracelet τ of length k (not necessarily non-degenerate) together with a non-degenerate tracelet σ_i glued onto each of the principal edges of this base tracelet along their evaluation. (That is, the rule given by evaluating the tracelet σ_i must match the rule corresponding to the ith principal edge of τ.)

The corresponding algebra, given by the standard incidence algebra construction (cf. [16]), is spanned by isomorphism classes of non-degenerate tracelets, and the product of two tracelets is given by summing over all possible tracelet composites.

We now proceed to extend this structure into a Hopf algebra. This is not straightforward, because the decomposition space $\mathbf{Y}_\bullet$ is not monoidal under sum. A monoidal structure exists in degree 1, by declaring the product of two tracelets to be the composite along trivial overlap:

$$T \odot T' := T \overset{\emptyset}{\angle} T'.$$

But this definition is not compatible with higher simplices.

Our task is now to explain how this is fixed in a canonical way. The solution amounts to imposing the so-called *shift equivalence* relation on tracelets, an equivalence relation already important in rewriting theory. In the graphical interpretation it is about saying that for tracelets that are not connected, it should make no difference in which order they are applied. After passing to this equivalence relation, the monoidal structure $\odot$ will be well defined in all simplicial degrees. This final symmetric monoidal decomposition space of tracelets up to shift equivalence will be denoted $\mathbf{Z}_\bullet$. We shall go deeper into the notion of shift equivalence in Section 5 (and interested readers are referred to [8, 1, 6] for the full background information and details). Here we just state the following Proposition 4.2, which gives an alternative approach to shift equivalence.

A *splitting vertex* of a tracelet is an inner vertex for which the corresponding rule overlap is trivial. This property is invariant under precomposition with active maps. (That is, if $\sigma' = g(\sigma)$ for g an active map not eliminating vertex v, then v is splitting for σ' if and only if it is splitting for σ.) Second, there is a transitive property in connection with 'stages' in the sense of higher-order simplices of $\mathbf{Y}_\bullet$. Note that this transitive property does *not* imply that irreducibility is compatible with inert maps (outer face maps).

A non-degenerate tracelet $T \in \mathbf{Y}_1 = \sum_n \vec{\mathbf{X}}_n$ is *primitive* if it does not admit any splitting. (A higher-dimensional simplex $\sigma \in \mathbf{Y}_k$ (that is a subdivided tracelet) is primitive if its long edge is primitive in $\mathbf{Y}_1 = \sum_n \vec{\mathbf{X}}_n$ (that is, its underlying tracelet is primitive).)

Lemma 4.1. *Every maximal splitting of a given simplex has, up to isomorphism and permutation, the same primitive pieces.*

Proposition 4.2. *Tracelets are shift equivalent in the restricted sense of trivial overlaps if and only if they have the same factorization into primitives.*

Proposition 4.3. *Shift equivalence is compatible with the simplicial structure. This defines a simplicial groupoid $\mathbf{Z}_\bullet$ with $\mathbf{Z}_k = \mathbf{Y}_k/\sim$. This simplicial groupoid is a (locally finite) decomposition space.*

Note that if $\widetilde{\mathbf{Y}}_n$ denotes the groupoid of shift equivalence classes, then we have

$$\mathbf{Z}_k = \sum_{[k] \twoheadrightarrow [n]} \mathbf{Y}_k \times_{\mathbf{X}_1^k} \left(\widetilde{\mathbf{Y}}_{n_1} \times \cdots \times \widetilde{\mathbf{Y}}_{n_k}\right)$$

This makes sense: in the fiber product, the maps from the factors $\widetilde{\mathbf{Y}}_{n_i}$ return the long edge, which is invariant under shift equivalence.

Theorem 4.4. *There is a level-wise equivalence of groupoids*

$$\mathbf{Z}_k \simeq \mathsf{S}(\mathbf{Y}_k^{\mathrm{irr}}),$$

assembling into an equivalence of simplicial groupoids. here S is the free-symmetric-monoidal-category monad. In particular, $\mathbf{Z}_\bullet$ is symmetric monoidal under $\odot$.

Note that the primitive tracelets themselves do not form a simplicial groupoid, as the outer face map applied to a primitive tracelet is not necessarily primitive. But after we apply S, which is just a fancy way of saying ‘monomials of’ or ‘families of’, it does work.

The upshot is now that the standard incidence algebra construction (cf. [16]) yields a Hopf algebra H of tracelets up to shift equivalence. This is the Hopf algebra we are really interested in, and towards which the previous ones were preliminary constructions. By Poincaré–Birkhoff–Witt, H is the enveloping algebra of the Lie algebra of primitive tracelets. In the next section we spell out the structure maps of this Hopf algebra in details.

5 The Hopf algebra of tracelets

The construction given of the tracelet Hopf algebra from the viewpoint of decomposition spaces gives it a certain canonical feel, but it requires a lot of machinery. However, the Hopf algebra can also be described directly (via an extension of the rule diagram Hopf algebra construction of [5], which was based upon relational calculus), which we briefly describe in this final section. Throughout, we fix a field $\mathbb{K}$ that will typically be chosen as either $\mathbb{R}$ or $\mathbb{C}$ (or, possibly, $\mathbb{Q}$). An essential prerequisite for our Hopf algebra construction is given by the following equivalence relations.

5.1. Shift equivalence (cf. [2]). Let $\equiv_S$ denote the equivalence relation on $\mathcal{T}$ defined as the reflexive symmetric transitive closure of the relation on pairwise composition operations on tracelets: let $T = T_B \,{}^{\mu}\!\angle\, T_A$ (for some admissible match $\mu = (I_B \leftarrow M \rightarrow O_A)$), and denote by $[[T_B]] = (O_B \leftarrow K_B \rightarrow I_B)$ and $[[T_A]] = (O_A \leftarrow K_A \rightarrow I_A)$ the evaluations of T_B and T_A, respectively. Suppose $[[T_B]]$ and $[[T_A]]$ are *sequentially independent* in the composition along μ, which entails that M is isomorphic to both the pullbacks of the cospans $K_B \rightarrow I_B \leftarrow M$ and $M \rightarrow O_A \leftarrow K_A$, respectively. In this situation we define the composite tracelet $\overline{T} = T_A \,{}^{\overline{\mu}}\!\angle\, T_B$ (for $\overline{\mu} = I_A \leftarrow M \rightarrow O_B$) to be *shift equivalent* to the tracelet $T = T_B \,{}^{\mu}\!\angle\, T_A$.

5.2. Normal form equivalence (cf. [2]). Let $\equiv_A$ denote an equivalence relation on $\mathcal{T}$ (so-called *abstraction equivalence*) whereby $T \equiv_A T'$ if T and T' are tracelets of the same length, and if moreover there exists an isomorphism $T \xrightarrow{\cong} T'$ (induced from isomorphisms on objects so that the resulting diagram commutes). Let $\equiv_T$ be defined as the reflexive symmetric transitive closure of a relation whereby for any $T \in \mathcal{T}$, we let $T \equiv_T T \uplus T_\varnothing \equiv_T T_\varnothing \uplus T$ (with $T_\varnothing := T(\varnothing \leftarrow \varnothing \rightarrow \varnothing) \in \mathcal{T}_1$, and where $\uplus := {}^{\mu_\varnothing}\angle$ denotes tracelet composition along trivial overlap). Then we define the *tracelet normal form* equivalence relation as $\equiv_N := rst(\equiv_A \cup \equiv_T \cup \equiv_S)$, i.e., as the reflexive symmetric transitive closure of the union of the aforementioned three relations.

Definition 5.3 (Primitive tracelets)**.** Denote by $\mathfrak{Prim}(\mathcal{T}_N)$ the set of *primitive tracelets*, defined as

$$\mathfrak{Prim}(\mathcal{T}_N) := \{[T]_{\equiv_N} | T \neq T_\varnothing \wedge \nexists T_A, T_B \neq T_\varnothing : T \equiv_N T_A \uplus T_B\}\,. \tag{14}$$

Primitive tracelets play a central role in our construction, since they are in a certain sense the smallest "indecomposable" building blocks of tracelets with respect to (de-)composition (just as primitive *rule diagrams* in [5]).

Proposition 5.4 (Tracelet normal form)**.** *Every tracelet $T \in \mathcal{T}$ is $\equiv_N$-equivalent to a* tracelet normal form *in the sense that $T_\varnothing \equiv_N T_\varnothing$, and*[4] *$\forall T \neq T_\varnothing : T \equiv_N \biguplus_{i\in I} T_i$, where $T_i \in \mathfrak{Prim}(\mathcal{T}_N)$ for all $i \in I$, and with I a (finite) index set.*

Definition 5.5 (Tracelet $\mathbb{K}$-vector space $\hat{\mathcal{T}}$)**.** Let $\hat{\mathcal{T}}$ be the $\mathbb{K}$-vector space spanned by a basis indexed by $\equiv_N$-equivalence classes, in the sense that there exists an isomorphism $\delta : \mathcal{T}_N \xrightarrow{\simeq} basis(\hat{\mathcal{T}})$ from the set[5] of $\equiv_N$-equivalence classes of tracelets $\mathcal{T}_N := \mathcal{T}/_{\equiv_N}$ to the set of basis vectors $basis(\hat{\mathcal{T}})$. We will use the notation $\hat{T} := \delta(T)$ for the basis vector associated to some class $T \in \mathcal{T}_N$. We denote by $Prim(\hat{\mathcal{T}}) \subset \hat{\mathcal{T}}$ the sub-vector space of $\hat{\mathcal{T}}$ spanned by basis vectors indexed by primitive tracelets.

Definition 5.6 (Tracelet algebra product and unit)**.** Let $\otimes \equiv \otimes_{\mathbb{K}}$ be the tensor product operation on the $\mathbb{K}$-vector space $\hat{\mathcal{T}}$. Then the *multiplication map* μ and the *unit map* η are defined via their action on basis vectors of $\hat{\mathcal{T}}$ as follows:

$$\mu : \hat{\mathcal{T}} \otimes \hat{\mathcal{T}} \rightarrow \hat{\mathcal{T}} : \hat{T} \otimes \hat{T}' \mapsto \hat{T} \diamond \hat{T}'\,, \qquad \hat{T} \diamond \hat{T}' := \sum_{\mu \in \mathsf{MT}_T(T')} \delta\left(\left[T\, {}^{\mu}\!\angle\, T'\right]_{\equiv_N}\right) \tag{15}$$

$$\eta : \mathbb{K} \rightarrow \hat{\mathcal{T}} : k \mapsto k \cdot \hat{T}_\varnothing\,. \tag{16}$$

Both definitions are suitably extended by (bi-)linearity to generic (pairs of) elements of $\hat{\mathcal{T}}$.

Proposition 5.7. *The morphisms μ and η define an* associative, unital $\mathbb{K}$-algebra $(\hat{\mathcal{T}}, \mu, \eta)$*, which we refer to as* tracelet algebra*.*

Definition 5.8 (Tracelet coproduct and counit)**.** Fixing the *notational convention* $\uplus_{i\in\emptyset} T_i := T_\varnothing$ for later convenience, let $T \equiv_N \uplus_{i\in I} T_i$ be the tracelet normal form for a given tracelet $T \in \mathcal{T}$ (where $T_i \in \mathfrak{Prim}(\mathcal{T}_N)$ for all $i \in I$ if $T \neq T_\varnothing$). Then the *tracelet coproduct* Δ and *tracelet counit* ε are defined via their action on basis vectors $\hat{T} = \delta(T)$ of $\hat{\mathcal{T}}$ as

$$\Delta : \hat{\mathcal{T}} \rightarrow \hat{\mathcal{T}} \otimes \hat{\mathcal{T}} : \hat{T} \mapsto \Delta(\hat{T}) := \sum_{X \subset I} \delta\left([\uplus_{x\in X} T_x]_{\equiv_N}\right) \otimes \delta\left(\left[\uplus_{y \in I\setminus X} T_y\right]_{\equiv_N}\right) \tag{17}$$

and $\varepsilon : \hat{\mathcal{T}} \rightarrow \mathbb{K} : \hat{T} \mapsto coeff_{\hat{T}_\varnothing}(\hat{T})$. Both definitions are extended by linearity to generic elements of $\hat{\mathcal{T}}$.

[4] We chose to make the case distinction explicit in order to emphasize that the normal form of a non-trivial tracelet $T \neq T_\varnothing$ does itself not contain trivial sub-tracelets, so that manifestly $T_i \in \mathfrak{Prim}(\mathcal{T}_N)$ in $T \equiv_N \uplus_{i\in I} T_i$. This is clearly the case, since invoking $\equiv_T$ on $\uplus_{i\in I} T_i$ would in effect remove any trivial constituent $T_i = T_\varnothing$.

[5] Here, we tacitly assume that the $\equiv_N$-equivalence classes indeed form a proper *set*, which is in all known applications the case since abstraction equivalence $\equiv_A$ is part of the definition of $\equiv_N$. For example, it is well known that the isomorphism classes of finite directed multigraphs indeed form a set.

Proposition 5.9. *The data* $(\hat{\mathfrak{T}}, \Delta, \varepsilon)$ *defines a* coassociative, cocommutative and counital coalgebra*.*

Proof. Since the construction of Δ and ε is the standard construction for a deconcatenation coalgebra (cf. e.g. [21]), the proof is omitted here for brevity. □

The algebra and coalgebra structures on $\hat{\mathfrak{T}}$ are compatible in the following sense:

Theorem 5.10 (Bialgebra structure)**.** *The data* $(\hat{\mathfrak{T}}, \mu, \eta, \Delta, \varepsilon)$ *defines a* bialgebra*.*

By virtue of the definition of the tracelet normal form, it is evident that both composition and decomposition of tracelets is compatible with a filtration structure given by the number of "connected components" in the following sense:

Theorem 5.11 (Compare [5], Sec. 3.4 and Thm. 3.2)**.** *The tracelet bialgebra* $(\hat{\mathfrak{T}}, \mu, \eta, \Delta, \varepsilon)$ *is filtered by*

$$\hat{\mathfrak{T}}^{(n)} := span_{\mathbb{K}} \left\{ \hat{T}_1 \uplus \ldots \uplus \hat{T}_n \middle| \hat{T}_1, \ldots, \hat{T}_n \in Prim(\hat{\mathfrak{T}}) \right\}, \tag{18}$$

and for this filtration it is connected ($\hat{\mathfrak{T}}^{(0)} := span_{\mathbb{K}}\{\hat{T}_{\varnothing}\}$)*. In particular, it acquires an antipode and becomes a Hopf algebra.*

Finally, yet again taking inspiration from [5], one may demonstrate that the tracelet Hopf algebra is isomorphic to a Hopf algebra that is well-known in the setting of the Heisenberg–Weyl diagram Hopf algebra and the Poincaré–Birkhoff–Witt theorem for "normal-ordering" of elements of the Hopf algebra:

Theorem 5.12. *Let* $\mathcal{L}_{\mathfrak{T}} := (Prim(\hat{\mathfrak{T}}), [.,.]_{\diamond})$ *denote the* tracelet Lie algebra*, where* $[\hat{T}, \hat{T}']_{\diamond} := \hat{T} \diamond \hat{T}' - \hat{T}' \diamond \hat{T}$ *is the* commutator operation *(w.r.t.* $\diamond$*). Then the tracelet Hopf algebra is isomorphic (in the sense of Hopf algebra isomorphisms) to the* universal enveloping algebra *of* $\mathcal{L}_{\mathfrak{T}}$*.*

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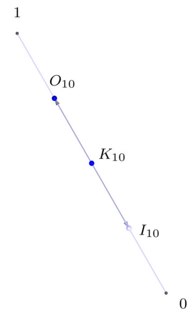
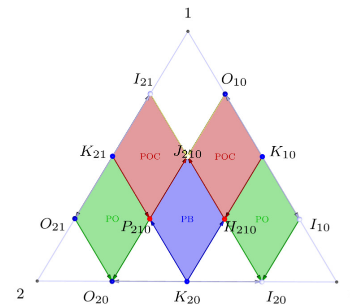
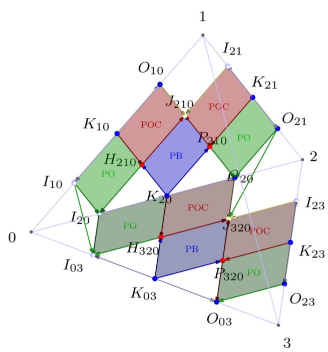


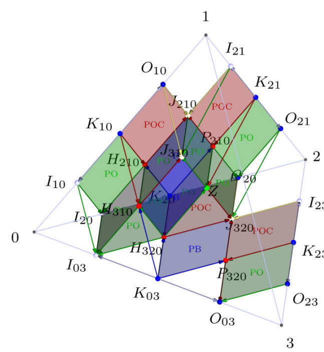
(a) 1-simplices



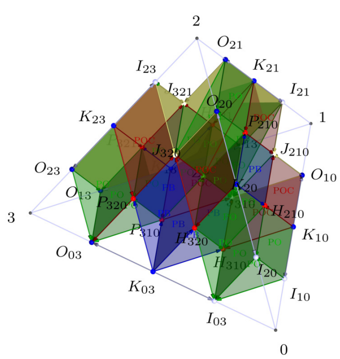
(b) 2-simplices



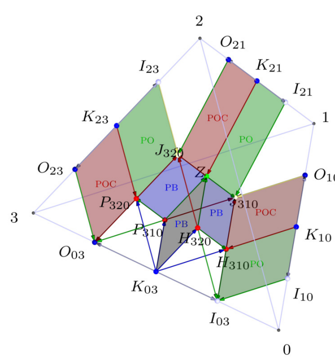
(c) From adjacent 2-simplices…



(d) … via the Concurrency Theorem…



(e) … to 3-simplices.



(f) Tracelets of length 3 and evaluation

Figure 2: Elements of Tracelet Decomposition Space theory (*Note:* in order to allow for a more in-detail inspection, the figures are hyperlinked to on-line interactive 3D views of the respective diagrams).

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