GROUPOIDS AND FAÀ DI BRUNO FORMULAE FOR GREEN FUNCTIONS IN BIALGEBRAS OF TREES

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ABSTRACT. We prove a Faà di Bruno formula for the Green function in the bialgebra of P-trees, for any polynomial endofunctor P. The formula appears as relative homotopy cardinality of an equivalence of groupoids.

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INTRODUCTION

This paper is a contribution to the combinatorial understanding of renormalisation in perturbative quantum field theory. It can be seen as part of the general programme, pioneered by Joyal and Baez–Dolan (and in a sense already by Grothendieck), of gaining insight into combinatorics, especially regarding symmetries, by upgrading from finite sets to suitably finite groupoids. We derive Faà di Bruno formulae in bialgebras of trees by realising them as relative homotopy cardinalities of equivalences of groupoids. An attractive aspect of this approach is that all issues with symmetries are handled completely transparently by the groupoid formalism, and take care of themselves throughout the equivalences without appearing in the calculations. This is made possible

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by our novel and consistent use of *homotopy sums*. The general philosophy is that sums weighted by inverses of symmetry factors always arise as groupoid cardinalities of homotopy sums. It is our hope that these kinds of techniques can be useful more generally in perturbative quantum field theory, and related areas.

Our starting point is the seminal work of van Suijlekom on Hopf algebras and renormalisation of gauge field theories [36], [37], [38]. Among several more important results in his work, the following caught our attention: for each interaction label v of a quantum field theory, the Connes-Kreimer Hopf algebra of Feynman graphs contains a formal series Y_v satisfying the multi-variate 'Faà di Bruno' formula

(1)
$$\Delta(Y_v) = \sum_{n_1 \cdots n_k} Y_v Y_{v_1}^{n_1} \cdots Y_{v_k}^{n_k} \otimes p_{n_1 \cdots n_k}(Y_v),$$

where $p_{n_1\cdots n_k}$ is the projection onto graphs containing n_i vertices of type v_i . The series Y_v is the renormalised (combinatorial) 1PI Green function

$$Y_v = \frac{G_v}{\prod_{e \in v} \sqrt{G_e}},$$

where

$$G_v = 1 + \sum_{\operatorname{res}\Gamma = v} \frac{\Gamma}{|\operatorname{Aut}\Gamma|}$$

is the bare Green function of all connected 1PI graphs Γ with residue v, the product is over the lines of the one-vertex graph v, and where the denominators

$$G_e = 1 - \sum_{\operatorname{res}\Gamma = e} \frac{\Gamma}{|\operatorname{Aut}\Gamma|}$$

constitute a renormalisation factor, cf. the Dyson formula (see [23, Ch. 8]) or [25, Ch. 7]). Van Suijlekom's proof of the formula is a matter of expanding everything, keeping track of several different combinatorial factors associated to graphs, and comparing them with the help of the orbit-stabiliser theorem. (The formula is Proposition 12 of [38], but the bulk of the proof is contained in various lemmas in [36] where the combinatorial factors involved are computed.)

Interest in Green functions in Hopf algebras of graphs is due in particular to the fact that, unlike the individual graphs, the Green functions actually have a physical interpretation. The Faà di Bruno Hopf algebra plays an important role in Hopf algebra approach to renormalisation, and many different relationships between it and the Hopf algebras of graphs or trees have been uncovered. One reason for the importance of the Faà di Bruno Hopf algebra is the general idea, expressed for example by Delamotte [13], that in the end renormalisation should be a matter of reparametrisation, i.e. substitution of power series. Already Connes and Kreimer [11] constructed a Hopf algebra homomorphism from the Faà di Bruno Hopf algebra (or rather the Connes– Moscovici Hopf algebra) to the Hopf algebra of Feynman graphs in the case of ϕ^3 in six space-time dimensions. Bellon and Schaposnik [4] were perhaps the first to explicitly write down the Faà di Bruno formula, in a form

$$\Delta(a) = \sum_{n} a^n \otimes a_n,$$

very pertinent to the formula we establish in the present paper. Recently the Faà di Bruno formula has been exploited by Ebrahimi-Fard and Patras [15] in the development of exponential renormalisation. Their paper contains also valuable information on the relationship with the Dyson formula.

It seems unlikely that a formula like this can exist for the Green function in the Hopf algebra of *trees* — indeed, the symmetry factors of the trees involved are not related to the combinatorics of grafting in the same way as symmetry factors of graphs are related to insertion of graphs (except in very special cases, such as considering only iterated one-loop self-energies in massless Yukawa theory in four dimensions, an example considered by many authors, e.g. [12], [6], [32]).

In the present paper we work with *operadic trees* instead of the combinatorial trees of the usual (Butcher)–Connes–Kreimer Hopf algebra — this is an essential point: operadic trees are more closely related to Feynman graphs, and have meaningful symmetry factors in this respect, cf. [29] (see also 8.12 below).

Our main theorem (7.3) at the algebraic level establishes the Faà di Bruno formula

(2)
$$\Delta(G) = \sum_{n} G^{n} \otimes p_{n}(G)$$

for the Green function $G = \sum_T T / |\operatorname{Aut}(T)|$ in the bialgebra of *P*-trees, for any polynomial endofunctor *P*.

The proof we give is very conceptual: the equation appears as an equivalence of groupoids, and all the symmetry factors are hidden and take care of themselves. A few remarks may be in order here to explain how this works.

A basic construction in combinatorics is to split a set into a disjoint union of parts: given a map of sets $E \to B$, the 'total space' E is the sum of the fibres:

$$E = \sum_{b \in B} E_b.$$

The same formula holds for groupoids, with the appropriate homotopy notions: given a map of groupoids $E \to B$, there is a natural equivalence

$$E \simeq \int^{b \in B} E_b.$$

The integral sign denotes the *homotopy sum* of the family (see 3.6) (and the fibres are homotopy fibres). Up to non-canonical equivalence it can be computed as

$$\simeq \sum_{b \in \pi_0 B} E_b / \operatorname{Aut} b,$$

revealing the symmetry factors, but our point is that homotopy sums interact very nicely with homotopy pullbacks, making the formalism look exactly as if we were dealing just with sets, and it is never necessary to mention the symmetry factors explicitly.

Our main theorem (5.7) at the groupoid level states the following equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$:

(3)
$$\int^{T \in \mathbf{T}} \operatorname{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T},$$

which is essentially a double-counting formula. Here $\operatorname{cut}(T)$ is the discrete groupoid of cuts of a tree, N is an (*I*-coloured) set, \mathbf{F}_N is the groupoid of forests with root profile N, and $_N \mathbf{T}$ is the groupoid of trees with leaf profile N. More precisely, if \mathbf{F} and \mathbf{T} are the groupoids of P-forests and P-trees, then \mathbf{F}_N and $_N \mathbf{T}$ are the homotopy fibres over N of the root and leaf functors respectively. The algebraic Faà di Bruno formula (2) is obtained just by taking homotopy cardinality (relative to $\mathbf{F} \times \mathbf{T}$) on both sides of the equivalence (3).

In order to arrive at a level of abstraction where the arguments become pleasant and the essential features are in focus, we have moved away quite a bit from the starting point mentioned above, and at the moment we have not quite succeeded in deriving van Suijlekom's formula from ours (or conversely). Depending on the choice of polynomial endofunctor P, our formula specialises to various formulae of independent interest, such as formulae for planar trees or binary trees. Our motivating example of polynomial endofunctor P, explained at the end of the paper, is defined in terms of interaction labels and 1PI graphs for any quantum field theory. Via work in progress by the second-named author [29] establishing a bialgebra homomorphism to this bialgebra of P-trees from the bialgebra of graphs, we hope in subsequent work to be able to derive van Suijlekom's formula from the Faà di Bruno formula of the present paper.

Outline of the paper. Section 1 and 2 are mostly motivational. We begin in Section 1 by revisiting the classical Faà di Bruno Hopf algebra, gradually recasting it in more categorical language, starting with composition of formal power series, then the incidence algebra viewpoint (cf. [14]), then finally the category of surjections (cf. [24]). We work with the non-reduced *bi*algebra rather than with the reduced *Hopf* algebra. This is an important point. In Section 2 we briefly revisit

the (Butcher)–Connes–Kreimer Hopf algebra of trees, introduce an operadic version of it that we need, and state one version of the main theorem for the bialgebra of operadic trees and the corresponding Green function.

The theory of groupoids is at the same time our main technical tool and the most important conceptual ingredient in our approach. Section 3 recalls a few notions, fixing terminology and notation for homotopy pullbacks, fibres, quotients and sum, in the hope of rendering the paper accessible to readers without a substantial background in category theory. In Section 4 we set up the formalism of operadic trees and forests, in terms of polynomial endofunctors, following [26]. This formalism is needed in particular to be able to talk about decorated trees — P-trees for a polynomial endofunctor P — at the level of generality needed to cover the examples envisaged.

In Section 5 we establish our main result, the equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$:

$$\int^{T \in \mathbf{T}} \operatorname{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}$$

already mentioned. Most of the arguments are formal consequences of general properties of groupoids; the only thing we need to prove by hand is the equivalence

$$\mathbf{C} \simeq \mathbf{F} imes_{\widetilde{\iota}} \mathbf{T}$$

between trees with a cut and pairs consisting of a forest and a tree such that the roots of the forest 'coincide' with the leaves of the tree (Lemma 5.5). In a precise sense, this is the essence of the Hopf algebra of trees.

Section 6 reviews and extends appropriate notions of groupoid cardinality, following Baez–Dolan [2] and Baez–Hoffnung–Walker [3]. In particular, we establish the basic properties of relative cardinality with respect to a morphism of groupoids. In Section 7 we finally prove the Faà di Bruno formula in the bialgebra of trees by taking cardinality of the groupoid equivalence of Section 5.

Examples of polynomial endofunctors giving rise to several kinds of trees are given in Section 8. In particular we relate our Faà di Bruno formulae with the classical one. In our final example we describe a polynomial endofunctor P defined in terms of Feynman graphs, which points towards transferring our results to bialgebras of graphs.

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1. The Faà di Bruno formula revisited

In this section we briefly review the classical Faà di Bruno bialgebra, first in terms of composition of power series, then in terms of partitions, and finally in terms of the groupoid of surjections.

1.1. Power series and the classical Faà di Bruno formula. Consider formal power series in one variable without constant term and with linear term equal to z:

$$f(z) = \sum_{n=0}^{\infty} \frac{A_n(f) z^n}{n!}$$
 $A_0 = 0, \ A_1 = 1.$

These form a group under substitution of power series, sometimes denoted $\text{Diff}(\mathbb{C}, 0)$, as the series can be regarded as germs of smooth functions tangent to the identity at 0. The classical Faà di Bruno Hopf algebra \mathcal{H} is the polynomial algebra on the symbols

$$a_n := A_n/n!, \quad n \ge 2,$$

viewed as linear forms on $\text{Diff}(\mathbb{C}, 0)$,

$$\langle a_n, f \rangle = a_n(f) = A_n(f)/n!, \qquad a_n \in \mathbb{C}[[z]]^*$$

The comultiplication is defined by

$$\langle \Delta(a_n), f \otimes g \rangle = \langle a_n, g \circ f \rangle,$$

and the counit by $\varepsilon(a_n) = \langle a_n, \mathbf{1} \rangle$. An explicit formula for Δ can be obtained by expanding

(4)
$$(g \circ f)(z) = \sum_{n=1}^{\infty} a_n(g) \left(\sum_{m=1}^{\infty} a_m(f) z^m\right)^n,$$

and involves the Bell polynomials. So far \mathcal{H} is a bialgebra; it acquires an antipode by general principles by observing that it is a connected graded bialgebra: the grading is given by

$$\deg(a_k) = k - 1.$$

We refer to Figueroa and Gracia-Bondía [16] for details on this classical object and its relevance in quantum field theory.

The formula for Δ can be packaged into a single equation, by considering the formal series

$$A = 1 + \sum_{k \ge 2} \frac{A_k}{k!} = 1 + \sum_{k \ge 2} a_k \quad \in \mathbb{C}[[a_2, a_3, \ldots]].$$

The comultiplication extends to series, and now takes the following form:

$$\Delta(A) = A \otimes 1 + \sum_{k \ge 2} A^k \otimes a_k$$

The values of Δ on the individual generators a_k can be extracted from this formula.

1.2. The (non-reduced) Faà di Bruno bialgebra. For our purposes it is important to give up the condition $a_1 = 1$. In this case, substitution of power series does not form a group but only a monoid, and the algebra is just a bialgebra rather than a Hopf algebra. We denote it by $\mathcal{F} = \mathbb{C}[a_1, a_2, a_3, \ldots]$. The definition of the comultiplication is still the same, and again it can be encoded in a single equation, involving now the formal series

$$A = \sum_{k \ge 1} \frac{A_k}{k!} = \sum_{k \ge 1} a_k \quad \in \mathbb{C}[[a_1, a_2, a_3, \ldots]].$$

The resulting form of the Faà di Bruno formula is the Leitmotiv of the present work:

Proposition. 1.3 (Classical Faà di Bruno identity). *The formal series* A satisfies

$$\Delta(A) = \sum_{k \ge 1} A^k \otimes a_k.$$

We stress that the bialgebra \mathcal{F} (with grading deg $(a_k) = k - 1$) is not connected: \mathcal{F}_0 is spanned by the powers of a_1 , all of which are group-like. One can obtain the classical Hopf algebra \mathcal{H} by imposing the relation $a_1 = 1$, which is easily seen to generate a bi-ideal.

1.4. Note on grading convention. Since $deg(a_k) = k - 1$, it is common in the literature to employ a different indexing, shifting the index so that it agrees with the degree. With the shifted index convention, the Faà di Bruno formula then reads

$$\Delta(A) = \sum_{n \ge 1} A^{n+1} \otimes a_n.$$

This is the convention used by van Suijlekom and many others, and explains the extra factor Y_v in the formula (1) quoted above. Beware that this convention means that certain indices are allowed to start at -1 and when it is said that $p_n(G)$ is the part of the Green function corresponding to graphs with n vertices, it actually means n+1 vertices.

While the shifted indexing convention can have its advantages, it is important for us to keep the indexing as above, so that the exponent in A^k matches the index in a_k . As we pass to more involved Faà di Bruno formulae, this will always express a type match: the outputs of one operation (the exponent) matching the input of the following (the subscript).

1.5. Faà di Bruno Hopf algebra in terms of partitions. The coefficients — the Bell polynomials which we did not make explicit — count partitions. In fact, it is classical (Doubilet [14], 1975) that the Hopf algebra \mathcal{H} can be realised as the reduced *incidence bialgebra* of the family of posets given by partitions of finite sets.

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The partitions of a finite set S form a lattice, in which $\sigma \leq \tau$ when σ is a refinement of τ . Consider the family of all intervals $[\sigma, \tau] := \{\rho \mid \sigma \leq \rho \leq \tau\}$ in partition lattices of finite sets, and declare two intervals equivalent if they are isomorphic as abstract posets. This is an order-compatible equivalence relation, meaning that the comultiplication formula

$$\Delta([\sigma,\tau]) = \sum_{\rho \in [\sigma,\tau]} [\sigma,\rho] \otimes [\rho,\tau]$$

is well-defined on equivalence classes. Disjoint union of finite sets defines furthermore a multiplication on these equivalence classes. If a_k is the interval given by the partition lattice of a set with $k \ge 2$ elements, then any interval is equivalent to a finite product of such a_k and this product expression is unique up to isomorphism of the sets involved.

The reduced incidence coalgebra on the vector space spanned by all equivalence classes (that is, the polynomial ring on the classes a_k , $k \geq 2$) is naturally isomorphic to the Faà di Bruno Hopf algebra \mathcal{H} .

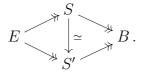
In order to get the 'nonreduced' bialgebra \mathcal{F} , one has to consider a finer equivalence relation: define an interval $[\sigma, \tau]$ to have $type 1^{\lambda_1}2^{\lambda_2}\cdots$ if λ_k is the number of blocks of τ that consist of exactly k blocks of σ , and declare two intervals equivalent if they have the same type. Every interval is isomorphic as a poset to a type-equivalent product of (possibly trivial) maximal intervals, yielding a 'nonreduced' incidence algebra isomorphic to \mathcal{F} . The technicalities involved here can be avoided by considering surjections instead of partitions.

1.6. Faà di Bruno in terms of surjections. Considering surjections $E \twoheadrightarrow B$ of nonempty finite sets, one can get the bialgebra \mathcal{F} directly. As a vector space it has as basis the isomorphism classes of surjections. The multiplicative structure is given by disjoint union, and since any surjection is the disjoint union of *connected* surjections $a_k = (\{1, \ldots, k\} \twoheadrightarrow \{1\})$, we have $\mathcal{F} \cong \mathbb{C}[a_1, a_2, \ldots]$.

The comultiplicative structure is given by

$$\Delta(E \twoheadrightarrow B) = \sum_{\substack{[E \twoheadrightarrow S \twoheadrightarrow B] \in \\ \pi_0 \operatorname{Fact}(E \twoheadrightarrow B)}} (E \twoheadrightarrow S) \otimes (S \twoheadrightarrow B).$$

Here the sum is over the components of the *factorisation groupoid* $Fact(E \rightarrow B)$, which has as objects the factorisations of $E \rightarrow B$ into two surjections $E \rightarrow S \rightarrow B$, and as morphisms the diagrams:



The relation with partitions is clear: a surjection $E \twoheadrightarrow B$ induces a partition of the set E, and a partition of E induces a surjection to the

set of parts. This correspondence provides an equivalence between the groupoid \mathbf{S} of surjections and that of sets-with-a-partition.

To obtain the Faà di Bruno Hopf algebra \mathcal{H} we identify surjections with equivalent factorisation groupoids, rather than just isomorphic surjections. Thus invertible surjections are all equivalent, as they have trivial factorisation groupoids. This relation is clearly generated by the equation $(1 \rightarrow 1) = (\emptyset \rightarrow \emptyset)$, that is, $a_1 = 1$.

The construction of the Faà di Bruno bialgebra in terms of the groupoid of surjections seems to be due to Joyal [24]. It is in the spirit of incidence algebras of Möbius categories introduced by Leroux [34], and studied recently by Lawvere and Menni [33]. However, the category of surjections is not a Möbius category, since it contains non-trivial isomorphisms. In our forthcoming paper [18] we extend the classical theory of incidence algebras and Möbius categories by allowing groupoid coefficients in order to cover the category of surjections, and also the category of trees in Section 4 below.

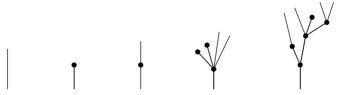
2. The bialgebra of trees, and the Main Theorem

2.1. The bialgebra of rooted trees of Connes and Kreimer [31], which in essence was studied already by Butcher [9] in the early 70s, is the free algebra \mathcal{H} on the set of isomorphism classes of *combinatorial trees* (defined for example as finite connected graphs without loops or cycles, and with a designated root vertex). The comultiplication is given on generators by

$$\begin{array}{cccc} \Delta: \mathcal{H} & \longrightarrow & \mathcal{H} \otimes \mathcal{H} \\ T & \longmapsto & \sum_{c} P_{c} \otimes S_{c}, \end{array}$$

where the sum is over all admissible cuts of T; the left-hand factor P_c is the forest (interpreted as a monomial) found above the cut, and S_c is the subtree found below the cut (or the empty forest, in case the cut is below the root). Admissible cut means: either a subtree containing the root, or the empty set. \mathcal{H} is a connected bialgebra: the grading is by the number of nodes, and \mathcal{H}_0 is spanned by the unit. Therefore, by general principles (see for example [16]), it acquires an antipode and becomes a Hopf algebra.

2.2. Operadic trees. For the present purposes it is crucial to work with *operadic trees* instead of combinatorial trees; this amounts to allowing loose ends (leaves). A formal definition is given in 4.2. For the moment, the following drawings should suffice to exemplify operadic trees — as usual the planar aspect inherent in a drawing should be disregarded:



Note that certain edges (the *leaves*) do not start in a node, and that one edge (the obligatory *root edge*) does not end in a node. A node without incoming edges is not the same thing as a leaf; it is a nullary operation (i.e. a constant), in the sense of operads. In operad theory, the nodes represent operations, and trees are formal combinations of operations. The small incoming edges drawn at every node serve to keep track of the arities of the operations. Furthermore, for coloured operads, the operations have type constraints on their inputs and output, encoded as attributes of the edges.

The trees appearing in BPHZ renormalisation are naturally operadic, as the nodes and edges come equipped with decorations by the graphs encoded. This is briefly explained in Example 8.12, following [29].

2.3. The bialgebra of operadic trees (cf. [28]). A *cut* of an operadic tree is defined to be a subtree containing the root — note that the arrows in the category of operadic trees are arity preserving (4.3), meaning that if a node is in the subtree, then so are all the incident edges of that node.

If $c: S \subset T$ is a subtree containing the root, then each leaf e of S determines an ideal subtree of T (4.3), namely consisting of e (which becomes the new root) and all the edges and nodes above it. This is still true when e is a leaf of T: in this case, the ideal tree is the trivial tree consisting solely of e. Figuratively, this means that for operadic trees cuts are not allowed to go above the leaves, and that cutting an edge does not remove it, but really cuts it(!). Note also that the root edge is a subtree; the ideal tree of the root edge is of course the tree itself. This is the analogue of the cut-below-the-root in the combinatorial case. For a cut $c: S \subset T$, define P_c to be the forest consisting of all the ideal trees generated by the leaves of S.

Let \mathcal{B} be the free algebra (that is, the polynomial ring) on the set of isomorphism classes of operadic trees, with comultiplication defined on the generators by

$$\begin{array}{cccc} \Delta:\mathcal{B} & \longrightarrow & \mathcal{B}\otimes\mathcal{B} \\ T & \longmapsto & \sum_{c:S\subset T} P_c\otimes S. \end{array}$$

As for combinatorial trees, \mathcal{B} becomes a graded bialgebra, but it is not connected since \mathcal{B}_0 is spanned by all powers of the trivial tree |. These are grouplike, so one could obtain a connected bialgebra by imposing the equation | = 1.

2.4. The Green function. In the completion of \mathcal{B} (that is, the power series ring), the series

$$G := \sum_{T} \delta_{T} / \left| \operatorname{Aut}(T) \right|$$

is called the *Green function*, in analogy with the (combinatorial) Green function of Feynman graphs. The sum is over all isomorphism classes of (operadic) trees, and there is a formal symbol δ_T for each isomorphism class of trees.

The following Faà di Bruno formula for the Green function in the bialgebra of (operadic) trees is a special case of our main theorem (7.3).

Theorem. 2.5. Write $G = \sum_{n \in \mathbb{N}} g_n$, where g_n is the summand in the Green function corresponding to trees with n leaves. Then

$$\Delta(G) = \sum_{n \in \mathbb{N}} G^n \otimes g_n.$$

The more general formula we prove is valid for P-trees for any polynomial endofunctor P. In addition to the naked trees considered so far, this covers many examples such as planar trees, binary trees, cyclic trees (Example 8.2), as well as the trees decorated by connected 1PI graphs of a quantum field theory (Example 8.12).

It is essential that we use operadic trees. There seems to be no reasonable Green function for combinatorial trees, since their symmetry factors are not related to the combinatorics of grafting.

We now first need to review some standard groupoid theory, then introduce more formally the trees and P-trees we treat, before coming to the proofs.

3. Groupoids

We recall some standard facts about groupoids, emphasising the use of the correct *homotopy* notions of the basic constructions such as pullback, fibre, quotient and sum. Although each of these notions can be traced a long way back (e.g. [21], [22], [8]), the consistent use of them in applications to combinatorics seems to be new. It is the systematic use of homotopy sums that makes all the symmetry factors 'disappear'.

3.1. Basics. A groupoid is a category in which every arrow is invertible. A morphism of groupoids is a functor, and we shall also need their natural isomorphisms. The set of isomorphisms classes, or components, of a groupoid X is denoted $\pi_0 X$. Many sets arising in combinatorics and physics, such as 'the set of all trees', are actually sets of isomorphism classes of a groupoid. For each object x the vertex group, denoted $\pi_1(x)$ or Aut(x), consists of all the arrows from x to itself. The notation π_0, π_1 is from topology. The homotopy viewpoint

of groupoids is an important aspect, as all the good notions to deal with them are homotopy notions (e.g. homotopy pullback, homotopy fibres, homotopy quotients, etc.), as we proceed to recall.

3.2. Equivalence. An equivalence of groupoids is just an equivalence of categories, i.e. a functor admitting a pseudo-inverse. Pseudo-inverse means that the two composites are not necessarily exactly the identity functors, but are only required to be isomorphic to the identity functors. A morphism of groupoids is an equivalence if and only if it induces a bijection on π_0 , and an isomorphism at the level of π_1 . A groupoid X is called *discrete* if it is equivalent to a set (that is, its vertex groups are all trivial), and *contractible* if it is equivalent to a singleton set.

3.3. Pullbacks. Recall that the *homotopy pullback* [8] or *fibre product* of a diagram of groupoids

$$X \xrightarrow{g} S \xleftarrow{f} Y$$

is the groupoid $X \times_S Y$ whose objects are triples (x, y, ϕ) with $x \in X$, $y \in Y$ and $\phi : fx \to gy$ an arrow of S, and whose arrows are pairs $(\alpha, \beta) : (x, y, \phi) \to (x', y', \phi')$ consisting of $\alpha : x \to x'$ an arrow in Xand $\beta : y \to y'$ an arrow in Y such that $g(\beta)\phi = \phi'f(\alpha) : fx \to gy'$.

Following [22, 2.6.2], one can say that the homotopy pullback and the projections to X and Y can be characterised up to canonical equivalence by a universal property: it is the 2-terminal object in a category of diagrams of the form

$$W \longrightarrow Y$$

$$\downarrow \simeq \downarrow^{g}$$

$$X \longrightarrow S$$

where 2-terminal means that the comparison map is not unique but rather that the comparison maps form a contractible groupoid.

3.4. Fibres. The notion of fibre is a special case of pullback, and again we need the homotopy version. The homotopy fibre E_b of a morphism $p: E \to B$ over an object b in B is the following homotopy pullback:

Here $\lceil b \rceil : 1 \rightarrow B$ is the inclusion morphism, termed the *name* of *b*.

For a morphism $b \to b'$ there is a canonical functor $E_b \to E_{b'}$, as one sees from the explicit description of fibres as pairs $(e, \phi : pe \cong b)$ and their isomorphisms. Thus we have a strict functor

(5)
$$F: B \to \mathbf{Grpd}, \quad F(b) = E_b.$$

Henceforth the words pullback and fibre will always mean the homotopy pullback and homotopy fibre, since these notions are invariant under equivalence (unlike the strict notions).

3.5. Homotopy quotient. Whenever a group G acts on a groupoid X, the homotopy quotient X/G (often denoted X//G, and known also as orbit groupoid [7, Ch. 11], semi-direct product [8], [10, II.5], and weak quotient [2], [3]) is the groupoid described as follows. Its objects are those of X. An arrow in X/G from x to y is a pair (g, ϕ) with $g \in G$ and $\phi : x.g \to y$ an arrow in X. Intuitively, X/G is obtained from X by sewing in a path in X for each object x and each (non-identity) element of the group. If X = 1, a singleton, then 1/G is the groupoid with a single object 1 and vertex group G. This groupoid may also be denoted BG, analogous to the classifying space in topology.

3.6. Grothendieck construction and homotopy sum. A family of sets indexed by a set B can be described either as a map $f : E \to B$ (the members of the family are the fibres $E_b := f^{-1}(b)$) or as a map $F : B \to \mathbf{Set}$ (the members are then the values F(b)). Similarly, as we proceed to recall, a family of groupoids indexed by a groupoid B can be described in two equivalent ways: either as a functor $B \to \mathbf{Grpd}$, or as a map of groupoids $E \to B$.

Given a functor $F : B \to \mathbf{Grpd}$, the Grothendieck construction (see SGA1 [21], Exp.VI, §8) produces a new groupoid E (actually the homotopy colimit of F) together with a map $E \to B$. The objects of Eare pairs (b, x) where $b \in B$ and $x \in F(b)$; an arrow from (b, x) to (b', x')is a pair (σ, ϕ) where $\sigma : b \to b'$ is an arrow of B, and $\phi : (F\sigma)(x) \to x'$ is an arrow of F(b'). The map $E \to B$ is the projection. The groupoid E is called the *homotopy sum* of the family F, and is denoted

$$\int^{b\in B} F(b).$$

This construction is mutually inverse to the construction in (5) of the functor $F: B \to \mathbf{Grpd}$ from a map $E \to B$.

Proposition. 3.7. Given a map of groupoids $f : E \to B$, the total space E is equivalent (over B) to the homotopy sum of its fibres:

$$E \simeq \int^{b \in B} E_b.$$

This can be computed (up to equivalence) as

$$E \simeq \sum_{b \in \pi_0 B} E_b / \operatorname{Aut}(b).$$

Proof. This is straightforward: one checks that the explicit construction of the homotopy pullback of f along id_B is actually isomorphic to the Grothendieck construction of the functor (5). Applying the first

result to the composite $E \to B \xrightarrow{\sim} \sum_{b \in \pi_0 B} 1/\operatorname{Aut}(b)$ one obtains the second. \Box

The following can be seen as a Fubini lemma:

Lemma. 3.8. Given morphisms of groupoids $X \xrightarrow{f} B \xrightarrow{t} I$, we have $\int_{a}^{b \in B} X_b \simeq \int_{a}^{i \in I} \left(\int_{a}^{b \in B_i} X_b \right)$

over I.

Again, the proof of the lemma is straightforward, yet it automatically takes care of a lot of automorphism yoga which without the setting of groupoids tends to become messy. Already spelling it out in (set) sums and group actions reveals that a lot is going on: The formula says

$$\sum_{b \in \pi_0 B} X_b / \operatorname{Aut}(b) \simeq \sum_{i \in \pi_0 I} \left(\sum_{b \in \pi_0 B_i} X_b / \operatorname{Aut}_i(b) \right) / \operatorname{Aut}(i).$$

Note that $\pi_0 B_i$ denotes the set of connected components of the fibre B_i which is typically different from the set of connected components of B that intersect the fibre: objects in the fibre might be connected only via arrows in B that are not in the fibre. Similarly, $\operatorname{Aut}_i(b)$ denotes the vertex group of b in the fibre B_i , not the whole vertex group $\operatorname{Aut}(b)$.

Applying Proposition 3.7 twice we get the following easy doublecounting lemma. It can be seen as the groupoid analogue of double counting in a bipartite graph, held by Aigner [1] as one of the most important principles in enumerative combinatorics.

Lemma. 3.9. Let A, B, U be groupoids, together with morphisms

 $B \longleftarrow U \longrightarrow A$

and write U_S , $_TU \subseteq U$ for the (homotopy) fibres over $S \in A$ and $T \in B$ respectively. Then there are equivalences of groupoids

$$\int_{-T}^{T \in B} U \simeq U \simeq \int_{-T}^{S \in A} U_S.$$

3.10. Slices. We shall need homotopy slices, sometimes called weak slices. The *slice category* $\mathbf{Grpd}_{/I}$ has as objects the morphisms $X \to I$, and arrows are triangles with a 2-cell, that is, a natural transformation:

$$(6) \qquad \qquad X \xrightarrow{} X \xrightarrow{} X$$

Arrows are composed by pasting such triangles.

Taking homotopy pullback along a morphism of groupoids $f: B' \to B$ defines a functor

$$f^*: \mathbf{Grpd}_{/B} \to \mathbf{Grpd}_{/B'}.$$

This has a homotopy left adjoint, defined by composition with f,

 $f_!: \mathbf{Grpd}_{/B'} \to \mathbf{Grpd}_{/B}$

and a homotopy right adjoint

 $f_*: \mathbf{Grpd}_{/B'} \to \mathbf{Grpd}_{/B},$

in the sense that there are natural equivalences of mapping groupoids

(7)
$$\mathbf{Grpd}_{B}(f_!E', E) \simeq \mathbf{Grpd}_{B'}(E', f^*E),$$

(8) $\mathbf{Grpd}_{/B'}(f^*E, E') \simeq \mathbf{Grpd}_{/B}(E, f_*E').$

3.11. *I*-coloured finite sets, or families of objects in *I*. Let **Bij** denote the groupoid of finite sets and bijections. Since a set may be regarded as discrete groupoid, we can consider **Bij** as a groupoid-enriched subcategory of Grpd. For a groupoid *I*, the groupoid of *I*-coloured sets is the slice category

$$\widetilde{I} := \mathbf{Bij}_{/I}.$$

Hence an *I*-coloured set is a groupoid morphism $X \to I$, where X is a finite set, and isomorphisms between them are are triangles with a 2-cell as in (6). If I = 1 is the one-point trivial groupoid, we recover the groupoid of (one-coloured) sets and bijections, $\tilde{1} \simeq \text{Bij}$.

The groupoid I can be considered also as the groupoid of families of objects in I. In this case, the finite set X plays a secondary role, it is merely an indexing set for the family. We use this viewpoint for example when we say that a forest is a family of trees. Formally, if **T** is the groupoid of trees (cf. below), then the groupoid of forests is

 $\mathbf{F} = \widetilde{\mathbf{T}}.$

It should be mentioned, although we will not need this fact, that \widetilde{I} is the free symmetric monoidal category on I.

4. Trees and forests

4.1. Polynomial functors. The theory of polynomial functors (for which we refer to [19]) is very useful to encode combinatorial structures, types and operations, and covers notions such as species and operads. Any diagram of groupoids

$$I \stackrel{s}{\leftarrow} E \stackrel{p}{\rightarrow} B \stackrel{t}{\rightarrow} I$$

defines a *polynomial endofunctor* as the composite (see 3.10)

$${f Grpd}_{/I} \xrightarrow{s^*} {f Grpd}_{/E} \xrightarrow{p_*} {f Grpd}_{/B} \xrightarrow{t_!} {f Grpd}_{/I}.$$

The intuition is that B is a collection of typed operations. The arity of an operation b is given by the size of the fibre E_b , the input types are the s(e) for $e \in E_b$, and the output type is t(b).

We shall see examples of polynomial functors in Section 8.

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4.2. Trees. It was observed in [26] that operadic trees can be conveniently encoded by diagrams of the same shape as polynomial functors. By definition, a *tree* is a diagram of finite sets

satisfying the following three conditions:

(1) t is injective

(2) s is injective with singleton complement (called the *root* and denoted 1).

With A = 1 + M, define the walk-to-the-root function $\sigma : A \to A$ by $1 \mapsto 1$ and $e \mapsto t(p(e))$ for $e \in M$.

(3) $\forall x \in A : \exists k \in \mathbb{N} : \sigma^k(x) = 1.$

The elements of A are called *edges*. The elements of N are called *nodes*. For $b \in N$, the edge t(b) is called the *output edge* of the node. That t is injective is just to say that each edge is the output edge of at most one node. For $b \in N$, the elements of the fibre $M_b := p^{-1}(b)$ are called *input edges* of b. Hence the whole set $M = \sum_{b \in N} M_b$ can be thought of as the set of nodes-with-a-marked-input-edge, i.e. pairs (b, e) where b is a node and e is an input edge of b. The map s returns the marked edge. Condition (2) says that every edge is the input edge of a unique node, except the root edge. Condition (3) says that if you walk towards the root, in a finite number of steps you arrive there. The edges not in the image of t are called *leaves*. The tree $1 \leftarrow 0 \rightarrow 0 \rightarrow 1$ is the *trivial tree* |.

4.3. Morphisms of trees (cf. [26]). A *tree embedding* is by definition a diagram

(10)
$$\begin{array}{c} A' \longleftrightarrow M' \longrightarrow N' \longrightarrow A' \\ \alpha \downarrow \qquad \qquad \downarrow^{-} \qquad \qquad \downarrow \qquad \qquad \downarrow^{\alpha} \\ A \longleftrightarrow M \longrightarrow N \longrightarrow A. \end{array}$$

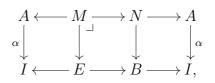
where the rows are trees. (It follows from the tree axioms that the components are injective.) The fact that the middle square is cartesian means that there is specified, for each node b of the first tree, a bijection between the incoming edges of b and the incoming edges of the image of b. In other words, a tree embedding is arity preserving.

A tree embedding is *root-preserving* when it sends the root to the root. In formal terms, these are diagrams (10) such that also the left-hand square is cartesian.

An *ideal embedding* (or an *ideal subtree*) is a subtree S in which for every edge e, all the edges and nodes above e are also in S. There is one ideal subtree generated by each edge in the tree. The ideal embeddings are characterised as having also the right-hand square of (10) cartesian.

Ideal embeddings and root-preserving embeddings admit pushouts along each other in the category **TEmb** of trees and tree embeddings [26]. The most interesting case is pushout over a trivial tree: this is then the root of one tree and a leaf of another tree, and the pushout is the grafting onto that leaf.

4.4. Decorated trees: *P*-trees. An efficient way of encoding and manipulating decorations of trees is in terms of polynomial functors [26] (see also [28, 27, 29, 30]). Given a polynomial endofunctor *P* represented by a diagram $I \stackrel{s}{\leftarrow} E \stackrel{p}{\rightarrow} B \stackrel{t}{\rightarrow} I$, a *P*-tree is a diagram



where the top row is a tree. The squares are commutative up to isomorphism, and it is important that the isos be specified as part of the structure. Unfolding the definition, we see that a *P*-tree is a tree whose edges are decorated in *I*, whose nodes are decorated in *B*, and with the additional structure of a bijection for each node $n \in N$ (with decoration $b \in B$) between the set of input edges of *n* and the fibre E_b , subject to the compatibility condition that such an edge $e \in E_b$ has decoration s(e), and the output edge of *n* has decoration isomorphic to t(b).

Standard examples of P-trees are given in Section 8, where we also consider groupoid-polynomial decorated trees arising naturally in quantum field theory, where in order to account for symmetries it is crucial that the representing diagram $I \leftarrow E \rightarrow B \rightarrow I$ be of groupoids, not just sets.

The category of *P*-trees is the slice category $TEmb_{/P}$. The notions of root-preserving and ideal embeddings work the same in this category as in TEmb, and again these two classes of maps allow pushouts along each other.

4.5. Forests. A forest can be defined as a family of trees, or equivalently as a finite sum of trees in the category of polynomial endofunctors. It is convenient to have also an elementary definition, similar to that of trees.

By definition, a *(finite rooted) forest* is a diagram of finite sets

 $A \xleftarrow{s} M \xrightarrow{p} N \xrightarrow{t} A$

satisfying the following three conditions:

(1) t is injective

(2) s is injective; denote its complement R (the set of roots). With A = R + M, define the walk-to-the-roots function $\sigma : A \to A$ by being the identity on R, and $e \mapsto t(p(e))$ for $e \in M$.

(3) $\forall x \in A : \exists k \in \mathbb{N} : \sigma^k(x) \in R.$

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The interpretations of these axioms are similar to those following the definition of tree.

A forest embedding is by definition a diagram like (10), required now separately to be injective (whereas for trees this condition is automatic, for forests absence of the condition gives only etale maps).

A forest embedding is called a *root-preserving embedding* if it induces a bijection between the sets of roots. This is equivalent to being a sum of tree embeddings. By *ideal embedding* we understand an embedding such that the right-hand square of (10) is cartesian. This means that each edge and node above the subforest is also contained in the subforest. The most important example will be this: for a given tree S, the set of its leaves forms a forest, and the inclusion of this forest into S is an ideal embedding.

Just as for trees, root-preserving embeddings and ideal embeddings allow pushouts along each other (in the category of forests and forest embeddings). The important case is grafting a forest onto the leaves of a tree.

4.6. *P*-forests. The definition of *P*-forest is analogous to the definition of *P*-tree, and again the category of *P*-forest embeddings can be characterised as the finite-sum completion of $TEmb_{/P}$ inside the slice category $Poly_{/P}$.

5. FAÀ DI BRUNO EQUIVALENCE IN THE GROUPOID OF TREES

We fix a polynomial endofunctor P given by

$$I \leftarrow E \rightarrow B \rightarrow I.$$

Throughout this section the word 'tree' will mean P-tree, and 'forest' will mean P-forest. We denote the groupoids of P-trees and P-forests by \mathbf{T} and \mathbf{F} respectively.

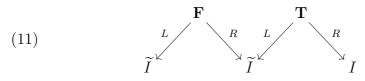
In this section we prove our main theorem, the equivalence of groupoids over $\mathbf{F}\times\mathbf{T}$

$$\int^{T \in \mathbf{T}} \operatorname{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}.$$

In Section 7 we will obtain the Faà di Bruno formula for the Green function in the bialgebra of trees by taking relative cardinality of both sides.

5.1. Leaves and roots. To any tree or to any forest we can associate its set of leaves. These are naturally *I*-coloured sets, and we have groupoid morphisms $L: \mathbf{T} \to \tilde{I}$ and $L: \mathbf{F} \to \tilde{I}$, called the *leaf maps*. Similarly, taking the root of a tree, and the set of roots of a forest, we have groupoid morphisms $R: \mathbf{T} \to I$ and $R: \mathbf{F} \to \tilde{I}$, called the *root maps*. We use two-sided subscript notation to indicate the fibres of

these maps,



Hence, we denote by \mathbf{T}_k the groupoid of trees with root colour $k \in I$ (or more precisely: with root colour isomorphic to k, and with a specified iso) and by \mathbf{F}_N the groupoid of forests whose set of roots is $N \in \tilde{I}$ (again, up to a specified iso). Similarly, for the fibres of L, we write ${}_N\mathbf{F}$ and ${}_N\mathbf{T}$ for the groupoids of forests and trees with leaf profile N. These are the groupoids of P-forests or P-trees with specified Ibijections between their leaves and N.

The groupoid of forests with a given *root profile* has the following characterisation:

Lemma. 5.2.

$$\mathbf{F}_N \simeq \mathbf{Grpd}_{I}(N, \mathbf{T})$$

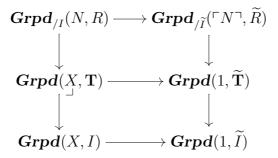
Proof. The forest root map $\mathbf{F} \to \widetilde{I}$ is the family functor applied to the tree root map, that is, $\widetilde{R} : \widetilde{\mathbf{T}} \to \widetilde{I}$. Hence we can write, by adjunction:

 $\mathbf{F}_N \simeq \lceil N \rceil^* \widetilde{R} \simeq \mathbf{Grpd}(1, \lceil N \rceil^* \widetilde{R}) \simeq \mathbf{Grpd}_{\widetilde{I}}(\lceil N \rceil, \widetilde{R}).$

It remains to establish the equivalence

$$\mathbf{Grpd}_{/\widetilde{I}}(\lceil N \rceil, R) \simeq \mathbf{Grpd}_{/I}(N, R).$$

Consider the commutative diagram



in which the vertical maps form the standard slice fibre sequences; the bottom vertical maps are postcomposition with R and \tilde{R} , respectively. Each of the horizontal maps sends a family to its name. Since the bottom square is a pullback, we conclude that the top map is an equivalence.

5.3. The groupoid of trees with a cut. In 2.3 we already defined a cut in a tree T to be a subtree S containing the root. For varying T, these form a groupoid \mathbf{C} : its objects are the root preserving inclusions $c: S \rightarrow T$, and its arrows are the isomorphisms of such inclusions, i.e. commutative diagrams

(12)
$$\begin{array}{c} T \xrightarrow{\tau} T' \\ c \\ S \xrightarrow{\sigma} S'. \end{array}$$

This groupoid comes equipped with canonical morphisms $m, r : \mathbf{C} \to \mathbf{T}$ and $w : \mathbf{C} \to \mathbf{F}$: when applied to a cut $c : S \to T$, the map m returns the total tree T, the map r returns the subtree (i.e. the tree S_c found below the cut), and the map w returns the forest P_c consisting of the ideal trees in T generated by the leaves of S. These maps and the morphisms L, R in (11) above form a commutative diagram

(13)
$$\begin{array}{c}
\mathbf{C} \xrightarrow{r} \mathbf{T} \\
w \\
\downarrow^{n} \\
\mathbf{T} \xrightarrow{-R} \\
\downarrow \\
\mathbf{F} \xrightarrow{-R} \\
\mathbf{F} \\
\mathbf{F} \\
\downarrow^{n} \\
\downarrow^{n} \\
\mathbf{F} \\
\downarrow^{n} \\
\downarrow^{$$

We denote by ${}_{T}\mathbf{C}$, \mathbf{C}_{S} and \mathbf{C}_{N} the fibres of the functors m, r and $L \circ r$. For a fixed tree T, the arrows of the groupoid ${}_{T}\mathbf{C}$ are

$$\begin{array}{c} T \stackrel{=}{\longrightarrow} T \\ \uparrow & \uparrow \\ R \stackrel{=}{\longrightarrow} R' \end{array}$$

and since the vertical maps are monomorphisms, we see that this groupoid has no nontrivial automorphisms, and hence is equivalent to a discrete groupoid which we denote by $\operatorname{cut}(T)$; we refer to its objects as the cuts of T. Thus $_T \mathbf{C} \simeq \pi_0(_T \mathbf{C}) = \operatorname{cut}(T)$ and the double-counting lemma 3.9 implies the following.

Lemma. 5.4. We have equivalences of groupoids

$$\int^{T \in \mathbf{T}} \operatorname{cut}(T) \simeq \int^{T \in \mathbf{T}} {}_{T} \mathbf{C} \simeq \mathbf{C} \simeq \int^{S \in \mathbf{T}} \mathbf{C}_{S} \simeq \int^{N \in \widetilde{I}} \mathbf{C}_{N}$$

The following Main Lemma states that the solid square face of (13) is a (homotopy) pullback square and enables us to identify the fibres \mathbf{C}_S and \mathbf{C}_N .

Lemma. 5.5. The canonical morphism to the product

$$(w,r)\colon \mathbf{C}\longrightarrow \mathbf{F}\times \mathbf{T}$$

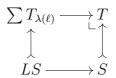
that sends $c: S \rightarrow T$ to (P_c, S_c) , induces an equivalence

$$\mathbf{C} \simeq \mathbf{F} \times_{\widetilde{I}} \mathbf{T}.$$

Proof. Starting with an object $(P, S, L(S) \stackrel{\lambda}{\cong} R(P))$ of the pullback, we construct a tree with a cut by *grafting.* The isomorphism λ may be regarded as a root-preserving embedding of forests

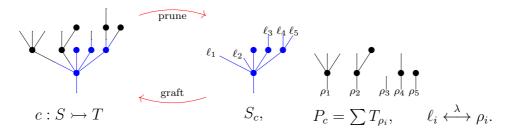
$$LS \rightarrowtail P = \sum_{\ell \in LS} T_{\lambda(\ell)},$$

and we construct the pushout in the category of forests of this map and the ideal subforest embedding $LS \rightarrow S$,



to obtain a root-preserving embedding $S \rightarrow T$ in the sense of 4.5. Note that since the forest S is a tree, T is again a tree. This assignment is functorial: an isomorphism (ρ, σ) from (P, S, λ) to (P', S', λ) induces an isomorphism of pushouts $\tau : T \cong T'$ extending σ as in (12).

In the reverse direction, we *prune* a root-preserving inclusion $S \rightarrow T$ to obtain $(\sum T_{\ell}, S, \mathrm{Id})$ where T_{ℓ} is the ideal subtree of T generated by the image of the leaf edge ℓ in T. An isomorphism of root-preserving inclusions (12) is sent to (τ, σ) where $\tau_{\ell} : T_{\ell} \rightarrow T'_{\tau\ell}$ is the restriction of τ to the ideal subtree T_{ℓ} .



Corollary. 5.6. For $S \in \mathbf{T}$ and $N \in \widetilde{I}$ we have equivalences of groupoids

$$\mathbf{C}_{S} \simeq (\mathbf{F} \times_{\widetilde{I}} \mathbf{T})_{S} \simeq \mathbf{F}_{LS},$$
$$\mathbf{C}_{N} \simeq \mathbf{F}_{N} \times_{N} \mathbf{T}.$$

Combining the previous results, we arrive at our main theorem:

Theorem. 5.7. We have equivalences of groupoids

$$\int^{T \in \mathbf{T}} \operatorname{cut}(T) \simeq \int^{S \in \mathbf{T}} \mathbf{F}_{LS}$$
$$\simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}.$$

We can regard this as an equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$. For fixed T, the map from $\operatorname{cut}(T)$ to $\mathbf{F} \times \mathbf{T}$ is precisely

$$\sum_{c \in \operatorname{cut}(T)} 1 \xrightarrow{\lceil (P_c, S_c) \rceil} \mathbf{F} \times \mathbf{T} .$$

To emphasise this, we can reformulate the result as

(14)
$$\int^{T \in \mathbf{T}} \sum_{c \in \operatorname{cut}(T)} \{P_c\} \times \{S_c\} \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}$$

Extracting the algebraic version of the Faà di Bruno formula 7.3 from 5.7 will be a matter of taking cardinality in a certain sense, which we explain in the next section.

If we take the fibres of the equivalence given in Theorem 5.7, over a fixed colour $v \in I$, we obtain:

Corollary. 5.8. We have equivalences of groupoids

$$\int^{T \in \mathbf{T}_v} \operatorname{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}_v$$

6. GROUPOID CARDINALITY

6.1. Finiteness conditions and cardinality. A groupoid X is called *finite* when $\pi_0(X)$ is a finite set and each $\pi_1(x)$ is a finite group. A morphism of groupoids is called finite when all its fibres are finite.

The cardinality [2] of a finite groupoid (sometimes called groupoid cardinality or homotopy cardinality if there is any danger of confusion) is the nonnegative rational number given by the formula

$$|X| := \sum_{x \in \pi_0 X} \frac{1}{|\operatorname{Aut}(x)|}.$$

Here $|\operatorname{Aut}(x)|$ denotes the order of the vertex group at x. This is independent of the choice of the x in the same connected component since an arrow between two choices induces an isomorphism of vertex groups. It is clear that equivalent groupoids have the same cardinality.

If X is a finite set considered as a groupoid, then the groupoid cardinality coincides with the set cardinality. If G is a finite group considered as a one-object groupoid, then the groupoid cardinality is the inverse of the order of the group. We have the following fundamental formulae for cardinality of sums, products and homotopy quotients of groupoids:

$$\begin{split} |X + Y| &= |X| + |Y| \\ |X \times Y| &= |X| \times |Y| \\ |X/G| &= |X| / |G| \,, \end{split}$$

where X and Y are finite groupoids and G is a finite group acting on X.

6.2. Cardinalities of families. For the sake of taking cardinalities we shall need the following 'numerical' description of the groupoid \tilde{I} of families of objects in I, cf. 3.11.

Let v_1, \ldots, v_s be representatives of the isoclasses in I. Then every family

$$N: X \to I$$

is isomorphic to a sum (in the category of sets over I) of families of the kind $\lceil v_i \rceil : 1 \to I$. Hence for uniquely determined natural numbers n_i we have

$$N \cong \sum_{i=1}^{s} n_i \ulcorner v_i \urcorner.$$

It follows that

$$\pi_0(\widetilde{I})\simeq\mathbb{N}^s.$$

We compute the vertex group. The automorphism group of $\lceil v_i \rceil$: $1 \rightarrow I$ is $\operatorname{Aut}(v_i)$ and that of $n_i \lceil v_i \rceil$ is $n_i! \operatorname{Aut}(v_i)^{n_i}$, since each point contributes with a factor $\operatorname{Aut}(v_i)$, and since the points can also be permuted. Altogether, we have

(15)
$$\operatorname{Aut}(N) \cong \prod_{i=1}^{s} n_i! \operatorname{Aut}(v_i)^{n_i},$$

and the groupoid \widetilde{I} can be described as

$$\widetilde{I} \simeq \sum_{(n_1,\dots,n_s)\in\mathbb{N}^s} \frac{1}{\prod_i n_i! \operatorname{Aut}(v_i)^{n_i}}.$$

6.3. Relative cardinality. Relative cardinality refers to the situation where one groupoid X is relatively finite over another groupoid, i.e. we have a morphism $p: X \to B$ with finite fibres. This notion is from [3]. In this situation we define the *relative cardinality* of X relative to B,

$$|p| := |X|_B := \sum_{b \in \pi_0 B} \frac{|X_b|}{|\operatorname{Aut}(b)|} \cdot \delta_b,$$

in the completion of the Q-vector space spanned by symbols δ_b for $b \in \pi_0(B)$. The notation $|X|_B$ assumes the morphism $X \to B$ is

clear from the context. Since the morphism has finite fibres X_b , the coefficients are well-defined nonnegative rational numbers.

The vector space spanned by the δ_b is isomorphic to the space of functions $\pi_0 B \to \mathbb{Q}$ with finite support, and its completion is the function space $\mathbb{Q}^{\pi_0 B}$. For each $b \in \pi_0 B$ we identify the cardinality of the inclusion $\lceil b \rceil : 1 \to B$ with a function

$$\delta_b = |1|_{\ulcorner_b \urcorner} : \pi_0 B \longrightarrow \mathbb{Q}$$
$$x \longmapsto \begin{cases} 1 & \text{if } x \simeq b \\ 0 & \text{otherwise.} \end{cases}$$

Hence we identify the relative cardinality of $X \to B$ with the function

$$\begin{array}{rcl} \pi_0 B & \longrightarrow & \mathbb{Q} \\ b & \longmapsto & |X_b| \,/ \, |\mathrm{Aut}(b)| \,. \end{array}$$

6.4. Properties of relative cardinality. When taking relative cardinality of a product $p \times p' \colon X \times X' \to B \times B'$, the formal symbols are indexed by $(b, b') \in \pi_0 B \times \pi_0 B' \simeq \pi_0 (B \times B')$. We shall then use notation $\delta_b \otimes \delta'_b$ instead of $\delta_{(b,b')}$, so that $|p \times p'| = |p| \otimes |p'|$.

Consider the groupoid morphism $X \to X/G$ given by the action of a finite group on a groupoid. Then we have

$$|X/G|_{X/G} = \frac{|X|_{X/G}}{|G|}$$

Lemma. 6.5. For any action of a finite group G on a groupoid X and a finite morphism $X/G \to A$, we have

$$\left|X/G\right|_{A} = \left|X\right|_{A} / \left|G\right|$$

where |G| denotes the order of the group G.

We need the following transitivity property of relative cardinality:

Lemma. 6.6. Given groupoid morphisms $X \xrightarrow{p} B \xrightarrow{t} I$ with finite fibres, the relative cardinality of p is obtained from those of the restrictions $p_v : X_v \to B_v$,

$$|p| = |X|_B = \sum_{v \in \pi_0 I} \frac{|p_v|}{|\operatorname{Aut}(v)|}.$$

Also the relative cardinality of X over I is obtained from the relative cardinality over B by substituting $\delta_{t(b)}$ for each δ_b . That is:

$$|X|_I = \sum_{b \in \pi_0 B} \frac{|X_b|}{|\operatorname{Aut}(b)|} \,\delta_{t(b)}.$$

In particular, any groupoid can be measured over itself via the identity morphism $\text{Id}: X \to X$:

$$|X|_X = \sum_{x \in \pi_0 X} \frac{1}{|\operatorname{Aut}(x)|} \,\delta_x$$

Hence we get the following useful result.

Corollary. 6.7. For $p: X \to B$ we have

$$|X|_B = \sum_{x \in \pi_0 X} \frac{1}{|\operatorname{Aut}(x)|} \,\delta_{p(x)}.$$

6.8. Power series. Both the power series A from Section 1 and the Green function in 2.4 are examples of the following general situation. For X a groupoid with finite vertex groups, consider the relative cardinality of the map $X \hookrightarrow \widetilde{X}$, the full inclusion of X into the groupoid of families of objects in X (cf. 3.11). We have

$$\sum_{x \in \pi_0 \widetilde{X}} \frac{|X_x|}{|\operatorname{Aut}(x)|} \cdot \delta_x = \sum_{x \in \pi_0 X} \frac{1}{|\operatorname{Aut}(x)|} \cdot \delta_x,$$

since the summand is zero when $x \notin \pi_0 X$. As an element of the ring $\mathbb{Q}^{\pi_0 \widetilde{X}}$, this cardinality is

$$\begin{aligned} \pi_0 \widetilde{X} &\longrightarrow & \mathbb{Q} \\ x &\longmapsto & \begin{cases} 1/|\operatorname{Aut}(x)| & \text{if } x \in \pi_0 X \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

We observe the natural isomorphisms

$$\mathbb{Q}^{\pi_0 X} \cong \operatorname{Sym}(\mathbb{Q}^{\pi_0 X}) \cong \mathbb{Q}[[\delta_x]]_{x \in \pi_0 X}$$

between the ring of functions and the power series in symbols δ_x for $x \in \pi_0 X$. This restricts to an isomorphism between the subring of functions with finite support and the polynomial ring.

7. The Faà di Bruno formula in the bialgebra of trees

The polynomial functor P, represented by $I \leftarrow E \rightarrow B \rightarrow I$, remains fixed in this section, and we denote the groupoids of P-trees and Pforests by **T** and **F** respectively.

7.1. The bialgebra of P-trees (cf. [28]). Consider the bialgebra given by the free algebra on the set of isomorphism classes of P-trees

$$\mathcal{B} = \mathbb{Q}[\delta_T]_{T \in \pi_0 \mathbf{T}}.$$

The constituent trees of a *P*-forest *F* define a monomial δ_F , and these monomials form a linear basis of \mathcal{B} . The comultiplication structure is given by

$$\Delta(\delta_T) = \sum_{c \in \operatorname{cut}(T)} \delta_{P_c} \otimes \delta_{S_c}.$$

The bialgebra of 2.3 is just the special case where P is the exponential functor of 8.1.

7.2. Definition of the Green functions of trees. In the completion of \mathcal{B} , the power series ring, we define the total Green function as the relative cardinality of $\mathbf{T} \to \widetilde{\mathbf{T}} = \mathbf{F}$:

$$G := \sum_{T \in \pi_0 \mathbf{T}} \frac{\delta_T}{|\operatorname{Aut}(T)|} \in \mathbb{Q}[[\delta_T]]_{T \in \pi_0 \mathbf{T}}.$$

In analogy with the situation in QFT, where there is one Green function for each possible residue (interaction label) in the theory, we also define an individual Green function for each possible (isomorphism class of) root colour $v \in \pi_0 I$,

$$G_v := \sum_{T \in \pi_0(\mathbf{T}_v)} \frac{\delta_T}{|\operatorname{Aut}_v(T)|}.$$

Here the automorphism group $\operatorname{Aut}_v(T)$ consists of those automorphisms of T which fix the root colour v. This is the relative cardinality of the inclusion $\mathbf{T}_v \to \mathbf{T} \to \mathbf{F}$.

It follows from Lemma 6.6 that we have the relationship

$$G = \sum_{v \in \pi_0 I} \frac{G_v}{|\operatorname{Aut}(v)|}.$$

Let $s := |\pi_0 I|$ be the number of colours, and let $\mathbf{n} = (n_1, \dots, n_s) \in \mathbb{N}^s$ be a multiindex, parametrising an isoclass of objects N in \widetilde{I} . Consider the relative cardinality of the inclusion of the homotopy fibre ${}_N \mathbf{T} \to \mathbf{T}$,

$$G_{\mathbf{n}} := \sum_{T \in \pi_0(N\mathbf{T})} \frac{\delta_T}{|\operatorname{Aut}_N(T)|}.$$

We also consider the summands of the Green function corresponding to all trees with n_v leaves of each colour $v \in \pi_0 I$,

$$g_{\mathbf{n}} := \sum_{T \in \pi_0 \mathbf{T}, \ LT \cong N} \frac{\delta_T}{|\operatorname{Aut} T|}$$

This is the relative cardinality of the *full subcategory* of \mathbf{T} whose objects are those trees T with leaf profile N. This is equivalent to the homotopy quotient $_{N}\mathbf{T}/\operatorname{Aut} N$ of the homotopy fibre by the canonical action of Aut N. Clearly,

$$g_{\mathbf{n}} = G_{\mathbf{n}} / |\operatorname{Aut} N|.$$

and hence

$$G = \sum_{\mathbf{n} \in \mathbb{N}^s} g_{\mathbf{n}}.$$

The comultiplication Δ extends to power series, and we can extract an algebraic Faà di Bruno formula from of our Theorem 5.7. **Theorem. 7.3.** The following Faà di Bruno formula holds for the Green function in the bialgebra of trees.

(16)
$$\Delta(G) = \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n}}.$$

Here $G^{\mathbf{n}}$ is to be interpreted as the product

$$G^{\mathbf{n}} = \prod_{v \in \pi_0 I} G_v^{n_v}.$$

To prove the theorem we first need a result about forests. Recall that the multiindices **n** classify the isomorphism classes of objects $N \in \tilde{I}$.

Lemma. 7.4. Let $N : X \to I$ be an object of \widetilde{I} of class $\mathbf{n} = (n_1, \ldots, n_s)$. Then

$$\mathbf{F}_N \simeq \prod_{i=1}^s \mathbf{T}_{v_i}^{n_i}.$$

Proof. Combining Lemma 5.2 with 6.2, we find

$$\mathbf{F}_{N} \simeq \mathbf{Grpd}_{/I}(X, R)$$

$$\simeq \mathbf{Grpd}_{/I}\left(\sum_{i=1}^{s} n_{i} \ulcorner v_{i} \urcorner, R\right)$$

$$\simeq \prod_{i=1}^{s} \mathbf{Grpd}_{/I} (\ulcorner v_{i} \urcorner, R)^{n_{i}}.$$

Now $\lceil v_i \rceil$ is the 'lowershriek' $\lceil v_i \rceil_!(1)$ and so by adjunction (7) we have

$$\simeq \prod_{i=1}^{s} \mathbf{Grpd}(1, \lceil v_i \rceil^* R)^{n_i} \simeq \prod_{i=1}^{s} \mathbf{T}_{v_i}^{n_i}.$$

Corollary. 7.5.

$$|\mathbf{F}_N| = G^{\mathbf{n}} = \prod_{i=1}^s G_{v_i}^{n_i}.$$

7.6. Proof of theorem **7.3.** The left-hand side $\Delta(G)$ of (16) is the relative cardinality of the left-hand side of (14) of theorem 5.7. It remains to show that the right-hand side of (16) is the relative cardinality of the right-hand side of (14). We have

$$\left| \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T} \right| = \sum_{N \in \pi_0 \widetilde{I}} \left| \mathbf{F}_N \right| \otimes \left|_N \mathbf{T} \right| / \left| \operatorname{Aut} N \right| = \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n}}.$$

7.7. Summands of Green functions. If $v \in I$ and $\mathbf{n} \in \mathbb{N}^s$ is a multiindex parametrising an isoclass of an object $N \in \tilde{I}$, define the Green function

$$g_{\mathbf{n},v} := |_N \mathbf{T}_v / \operatorname{Aut} N|$$
.

We have

$$g_{\mathbf{n}} = \sum_{v \in \pi_0 I} \frac{g_{\mathbf{n},v}}{|\operatorname{Aut}(v)|}$$

and hence

$$G = \sum_{\mathbf{n}} \sum_{v \in \pi_0 I} \frac{g_{\mathbf{n},v}}{|\operatorname{Aut}(v)|}.$$

Taking relative cardinality of Corollary 5.8 then gives

Theorem. 7.8. For $v \in I$ and $\mathbf{n} \in \mathbb{N}^s$ we have

$$\Delta(G_v) = \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n},v}.$$

This is the version that most closely resembles the multi-variate Faà di Bruno formula and the formula of van Suijlekom.

8. Examples

In this section we specialise to some standard examples of the polynomial endofunctor P, and compare with the classical Faà di Bruno bialgebra. Following [29] we also explain a polynomial endofunctor of certain graphs which was actually our motivating example, and which points towards transferring our results to bialgebras of graphs.

8.1. Naked trees. Consider the polynomial functor P represented by

$$1 \leftarrow \mathbf{Bij}' \to \mathbf{Bij} \to 1,$$

where **Bij**' denotes the groupoid of finite pointed sets and basepointpreserving bijections, and 1 denotes a singleton set. This is the exponential functor

$$P(X) = \exp(X) = \sum_{n \in \mathbb{N}} X^n / n!.$$

There is a fibre of each finite cardinality $n \in \mathbb{N}$, and for every tree $A \leftarrow M \rightarrow N \rightarrow A$ there is a unique *P*-decoration

$$A \longleftarrow M \longrightarrow N \longrightarrow A$$
$$\downarrow \qquad \qquad \downarrow^{\neg} \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$
$$1 \longleftarrow \mathbf{Bij'} \longrightarrow \mathbf{Bij} \longrightarrow 1$$

(since a node of arity n must map to $n \in \mathbf{Bij}$, and since the choices of where to map the incoming edges to the fibre over n are all uniquely isomorphic). It follows that in this case P-trees are essentially the same thing as the naked trees defined in 4.2 (in the precise sense that the groupoid of P-trees is equivalent to the groupoid of naked trees).

8.2. Cyclic trees. If P is the polynomial endofunctor

$$1 \leftarrow \mathbb{C}' \to \mathbb{C} \to 1,$$

where \mathbb{C} is the groupoid of finite cyclically ordered sets, and \mathbb{C}' is the groupoid of finite cyclically ordered pointed sets (in fact, canonically equivalent to the N' of the following example), then the notion of *P*-tree is that of cyclic tree.

8.3. Planar trees. Consider the polynomial functor P represented by

$$1 \leftarrow \mathbb{N}' \to \mathbb{N} \to 1,$$

where \mathbb{N} is the (discrete) groupoid of finite ordered sets, and \mathbb{N}' is the (discrete) groupoid of finite ordered sets with a marked point, so that the fibre of the middle map is naturally a linearly ordered set. This functor is the geometric series

$$P(X) = \frac{1}{1-X} = \sum_{n \in \mathbb{N}} X^n.$$

In this case the P-trees

$$\begin{array}{cccc} A & & & M & \longrightarrow N & \longrightarrow A \\ & & & & \downarrow^{-} & & \downarrow & & \downarrow \\ 1 & & & \mathbb{N}' & \longrightarrow \mathbb{N} & \longrightarrow 1 \end{array}$$

are naturally planar trees, since the cartesian square in the middle equips the incoming edges of each node in the tree with a linear order.

Note that the resulting bialgebra of planar trees is still commutative, unlike the planar-tree Hopf algebra studied by Foissy [17] and others. Since P-trees are rigid (this is true in general when P is represented by discrete groupoids), there are no symmetries, so the Green function is just the sum of all the formal symbols,

$$G = \sum_{T \in \pi_0 \mathbf{T}} \delta_T.$$

8.4. Planar binary trees. Consider now the diagram

$$\leftarrow 2 \rightarrow 1 \rightarrow 1$$

representing the polynomial functor $P(X) = X^2$. In this case *P*-trees are planar binary trees.

8.5. Injections. For the constant polynomial functor P(X) = 1, represented by

$$1 \leftarrow 0 \rightarrow 1 \rightarrow 1,$$

there are two possible *P*-trees:

$$x \qquad y \uparrow$$

P-forests are disjoint unions of these. The groupoid \mathbf{F} of *P*-forests is naturally equivalent to the groupoid whose objects are injections

between finite sets, and whose arrows are the isomorphisms between such. The associated Faà di Bruno bialgebra is $\mathbb{Q}[\delta_x, \delta_y]$, with the comultiplication given by

$$\Delta(\delta_x) = \delta_x \otimes \delta_x$$
$$\Delta(\delta_y) = 1 \otimes \delta_y + \delta_y \otimes \delta_x.$$

Expanding we find

$$\Delta(\delta_y^n) = \sum_{k \le n} \binom{n}{k} \delta_y^k \otimes \delta_y^{n-k} \delta_x^k.$$

After passing to the reduction (putting x = 1) we get the usual binomial Hopf algebra. The Green function is

$$G = \delta_x + \delta_y$$

with $g_0 = \delta_y$ and $g_1 = \delta_x$, and the Faà di Bruno formula is immediate. 8.6. Linear trees. The identity functor P(X) = X is represented by $1 \leftarrow 1 \rightarrow 1 \rightarrow 1$.

Now *P*-trees are linear trees. We take a variable x_n for the isoclass of the linear tree with n nodes, and find the comultiplication formula

$$\Delta(x_n) = \sum_{i=0}^n x_i \otimes x_{n-i}$$

this is the ladder Hopf algebra, studied for example in [35].

8.7. Trivial trees. Consider the polynomial functor

$$P = (I \leftarrow 0 \to 0 \to I).$$

where I is a discrete groupoid. The only P-trees are the trivial trees, one for each $x \in \pi_0 I$. The groupoids of P-trees and P-forests are I and \tilde{I} respectively. In $\mathbb{Q}[\pi_0 I]$ all generators are grouplike, and we have

$$G = \sum_{x \in \pi_0 I} x$$

$$\Delta(G) = \sum_{x \in \pi_0 I} x \otimes x = \sum_{x \in \pi_0 I} |I_x \times {}_xI| = \sum_{x \in \pi_0 \widetilde{I}} |\widetilde{I}_x \times {}_xI|$$

(This is the monoid algebra on the free commutative monoid on $\pi_0 I$.) 8.8. Effective trees. Consider the polynomial functor represented by

$$1 \leftarrow \mathbf{B}' \rightarrow \mathbf{B} \rightarrow 1$$
.

where **B** is the groupoid of non-empty finite sets and bijections (and **B'** the groupoid of non-empty finite pointed sets and basepoint-preserving bijections). The resulting endofunctor is $P(X) = \exp(X) - 1$. In this case *P*-trees are naked trees with no nullary operations, sometimes

called 'effective' trees. These are the key to understanding the relationship with the classical Faà di Bruno bialgebra, cf. 1.2, as explained below.

Since effective trees have no nullary nodes, they always have a nonempty set of leaves, and therefore the leaf map can be seen to take values in **B**. Furthermore, for each $n \in \mathbf{B}$, the homotopy fibre ${}_{n}\mathbf{T} \subset \mathbf{T}$ is discrete, since if an automorphism of a effective tree fixes the leaves then it fixes the whole tree.

The sub-bialgebra \mathcal{B}_{eff} of \mathcal{B} is the polynomial algebra on the isomorphism classes of effective trees.

8.9. Stable trees. In a similar vein, we can consider *P*-trees for the polynomial functor $P(X) = \exp(X) - 1 - X$, represented by

$$1 \leftarrow \mathbf{Y}' \to \mathbf{Y} \to 1,$$

where **Y** is the groupoid of finite sets of cardinality at least 2. These are naked trees with no nullary and no unary nodes, called *reduced trees* by Ginzburg and Kapranov [20]. We adopt instead the term *stable trees*. Clearly stable trees are effective, so $L : \mathbf{T} \to \mathbf{B}$ is a discrete fibration. In this case it is furthermore finite: for a given number of leaves there is only a finite number of isoclasses of stable trees.

8.10. The classical Faà di Bruno: surjections versus effective trees. As far as we know, the classical Faà di Bruno bialgebra of surjections is not a bialgebra of P-trees for any P. There is nevertheless a close relationship with the bialgebra of effective trees, which we now proceed to explain. The following construction works for any polynomial endofunctor without nullary operations.

Since effective trees have no nullary nodes, the leaf map can be seen as taking values in the groupoid **B** of non-empty finite sets. Pulling back along the leaf map $L : \mathbf{T} \to \mathbf{B}$

$$L^*: \mathbf{Grpd}_{/\mathbf{B}} \to \mathbf{Grpd}_{/\mathbf{T}},$$

sends $\lceil n \rceil : 1 \rightarrow \mathbf{B}$ to the inclusion of the discrete fibre ${}_{n}\mathbf{T} \rightarrow \mathbf{T}$. This yields a linear map

which extends to an algebra homomorphism

$$\Phi: \mathcal{F} = \mathbb{Q}[[A_n]]_{n \in \pi_0 \mathbf{B}} \longrightarrow \mathbb{Q}[[\delta_T]]_{T \in \pi_0 \mathbf{T}} = \mathcal{B}_{\text{eff}}.$$

Lemma. 8.11. The map Φ is a bialgebra homomorphism.

Proof. We already noted that Φ preserves the Green functions. Now

$$(\Phi \otimes \Phi)(\Delta(A)) = (\Phi \otimes \Phi)(\sum_{n} A^{n} \otimes a_{n})$$
$$= \sum_{n} (\Phi A)^{n} \otimes \Phi(a_{n})$$
$$= \sum_{n} G^{n} \otimes g_{n}$$
$$= \Delta(\Phi(A)).$$

It remains to recall that the comultiplication in \mathcal{F} is determined by the comultiplication of the Green function.

8.12. Trees of graphs. This final example is our main motivation for studying P-trees: forthcoming work of the second author [29] shows that (nestings of) Feynman graphs for a given quantum field theory can be considered as P-trees for a suitable finitary polynomial endofunctor P defined over groupoids. We briefly describe this polynomial endofunctor and its relation with graphs.

The relationship between trees and graphs in the Connes-Kreimer Hopf algebras is that the trees encode nestings of graphs. In the following figure,



the small combinatorial tree in the middle expresses the nesting of 1PI subgraphs on the left. It is clear that such combinatorial trees do not capture anything related to symmetries of graphs. For this, fancier trees are needed, as partially indicated on the right. First of all, each node in the tree should be decorated by the 1PI graph it corresponds to in the nesting [5], and second, to allow an operadic interpretation, the tree should have leaves (input slots) corresponding to the vertices of the graph. Just as vertices of graphs serve as insertion points, the leaves of a tree serve as input slots for grafting.

The decorated tree should be regarded as a recipe for reconstructing the graph by inserting the decorating graphs into the vertices of the graphs of parent nodes. The numbers on the edges indicate the type constraint of each substitution: the outer interface of a graph must match the local interface of the vertex it is substituted into. But the type constraints on the tree decoration are not enough to reconstruct the graph, because for example the small graph \checkmark decorating the lefthand node could be substituted into various different vertices of the graph \checkmark . The solution found in [29], which draws from insights from higher category theory [30], is to consider *P*-trees, for *P* a certain polynomial endofunctor over groupoids, which depends on the theory.

To match the figures above, we consider a theory in which there are two interaction labels \rightarrow and \prec ; let *I* denote the groupoid of all such one-vertex graphs. Let *B* denote the groupoid of all connected 1PI graphs of the theory that are primitive in the Hopf algebra of graphs. Finally let *E* denote the groupoid of such graphs with a marked vertex. The polynomial endofunctor *P* is now given by the diagram

$$I \xleftarrow{s} E \xrightarrow{p} B \xrightarrow{t} I,$$

where the map s returns the one-vertex subgraph at the mark, p forgets the mark, and t returns the residue of the graph, i.e. the graph obtained by contracting everything to a point, but keeping the external lines. A P-tree is hence a diagram

$$A \longleftarrow M \longrightarrow N \longrightarrow A$$

$$\alpha \downarrow \leftarrow \downarrow \ \ \downarrow \rightarrow \downarrow \rightarrow \downarrow \alpha$$

$$I \longleftarrow E \longrightarrow B \longrightarrow I,$$

with specified 2-cells, in which the first row is a tree in the sense of 4.2. These 2-cells carry much of the structure: for example the 2-cell on the right says that the 1PI graph decorating a given node must have the same residue as the decoration of the outgoing edge of the node — or more precisely, and more realistically: an isomorphism is specified (it's a bijection between external lines of one-vertex graphs). Similarly, the left-hand 2-cell specifies for each node-with-a-marked-incoming-edge $x' \in M$, an isomorphism between the one-vertex graph decorating that edge and the marked vertex of the graph decorating the marked node x'. Hence the structure of a *P*-tree is a complete recipe not only for which graphs should be substituted into which vertices, but also how: specific bijections prescribe which external lines should be identified with which lines in the receiving graph.

More precisely, the result of [29] states an equivalence of groupoids. In particular a P-tree has the same symmetry group as the graph (with its nesting) that it encodes, so that the Green functions match up, and in the end the Faà di Bruno formula in the bialgebra of P-trees can be transported to a certain bialgebra of graphs. However, this bialgebra of graphs is not quite the same as the standard Connes–Kreimer Hopf algebra of graphs, and we are not yet able to derive van Suijlekom's Faà di Bruno formula from our general framework. The main dificulty lies in getting a purely operadic encoding of the line insertions, allowed in the Connes–Kreimer Hopf algebra but not in our bialgebra of graphs. This issue is closely related to the renormalisation factors $1/\sqrt{G_e}$ mentioned in the Introduction.

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