An Overview of Hopf Algebras of Trees 
and Their Actions on Functions

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Abstract

We provide an expository account of some of the Hopf algebras 
that can be defined using trees, labeled trees, ordered trees and heap 
ordered trees. We also describe some actions of these Hopf algebras on 
algebra of functions.

1 Introduction

There is growing interest in Hopf algebras defined from trees, permutations, 
and other combinatorial structures. In this paper, we provide an expository 
account of some of the Hopf algebras that can be defined using trees, labeled 
trees, ordered trees and heap ordered trees. We also describe some actions 
of these Hopf algebras on algebra of functions.

We assume that the reader is familiar with the basic definitions and 
properties of Hopf algebras, as covered, for example, in [14].

This paper is based in part on [9].

2 Hopf Algebras of Rooted Trees

2.1 Products of Trees

Throughout this paper, \( k \) will be a field of characteristic 0 such as the real 
numbers or the complex numbers.

Definition 2.1 By a tree we will mean a finite rooted tree. Let \( T \) be the 
set of finite rooted trees, and let \( kT \) be the \( k \)-vector space that has \( T \) as a 
basis.
In this section, we define an algebraic structure on $kT$ that was introduced in [3]. Suppose that $t_1, t_2 \in T$ are trees. Let $s_1, \ldots, s_r$ be the children of the root of $t_1$ and let $B_-(\cdot)$ denote the operator that operates on a tree and removes the root to produce a forest of trees:

$$B_-(t_1) = \{s_1, \ldots, s_r\}.$$

If $t_2$ has $n + 1$ nodes (counting the root), there are $(n + 1)^r$ ways to attach the $r$ subtrees of $t_1$ that have $s_1, \ldots, s_r$ as roots to the tree $t_2$. To do this, make each $s_i$ the child of some node of $t_2$. We let

$$B_+(s_1, \ldots, s_r; t_2).$$

denote this operation that attaches a forest of trees $s_1, \ldots, s_r$ to the nodes of a tree $t_2$ in all possible ways to produce a set of trees.

The product $t_1t_2$ of the trees $t_1$ and $t_2$ is defined to be the sum of these $(n + 1)^r$ trees. We summarize this in the following definition:

**Definition 2.2** The product of the trees $t_1 \in T$ and $t_2 \in T$ is defined to be

$$t_1t_2 = \sum B_+(B_-(t_1); t_2) \in kT.$$
2.2 Coproducts of Trees

We now define a coalgebra structure on the vector space $kT$:

$$\Delta(t) = \sum_{X \subseteq B_-(t)} B_+(X; e) \otimes B_+(B_-(t) \setminus X; e)$$

$$\epsilon(t) = \begin{cases} 
1 & \text{if } t \text{ is the tree whose only node is the root}, \\
0 & \text{otherwise}.
\end{cases}$$

Here, if $X \subseteq Y$ are multisets, $Y \setminus X$ denotes the set theoretic difference.

It is easily checked that the definition of a coproduct is satisfied, so that $kT$ is a cocommutative coalgebra.

This coalgebra and the algebra given in Example 3.1 with $X$ being the set of trees whose root has exactly one child, are duals of each other as graded vector spaces, with a tree with $n + 1$ nodes being of degree $n$, and the degree of a monomial $x_{i_1} \cdots x_{i_p}$ being the sum of the degrees of $x_{i_1}, \ldots, x_{i_p}$. The fact that coassociativity for this coalgebra is trivial gives an easy proof of the associativity of the algebra in Example 3.1.
2.3 Connes–Kreimer Hopf Algebra

Another algebra of trees was described in [2] in 1998 that is defined as follows:

If $T$ is the set of rooted trees, form expressions $a_1 \cdots a_k$, where $a_i \in T$. This is clearly a commutative algebra of monomials, which we denote $CK$.

The coalgebra structure of $CK$ is defined as follows: we introduce the notion of cut. A cut is a set of removed edges. Given a tree $t$, an admissible cut of $t$ is one with at most one removed edge on each path from the root to any leaf. For a cut $C$ we let $R^C(t)$ to be the resulting piece containing the root, and $P^C(t)$ to be the monomial consisting of the other pieces. Then define

$$\Delta(t) = t \otimes 1 + \sum_C P^C(t) \otimes R^C(t).$$

There is an isomorphism

$$\chi : kT \to CK^*$$

from the Hopf algebra $kT$ to the graded dual of $CK$ satisfying

$$\langle \chi(t), a \rangle = (B_-(t), a) = (t, B_+(a)),$$

where $t \in kT$ and $a \in CK$. Here $(\cdot, \cdot)$ is an inner product defined on $CK$ that depends upon a factor determined by the symmetry of the arguments. For the definition of this inner product and a proof of this fact, see [11].

2.4 Labeled Trees, Ordered Trees and Heap Ordered Trees

It is easy to extend the definition of multiplication of trees from the vector space whose basis is the set of finite rooted trees to the vector space whose basis is the set of finite labeled rooted trees: simply label each node except the root with a label and keep the labels attached to the nodes when applying the operators $B_-$ and $B_+$. As shown in [5] this yields a Hopf algebra.

Similarly, the same definition of the product and coproduct applies to the vector space whose basis is the set of finite ordered trees, as well as to the vector space whose basis is the set of finite ordered, labeled trees. Both produce Hopf algebras. See [5] for details.

Later in this paper, we will need the Hopf algebra of heap ordered trees, which we define following [8]:

Definition 2.3 A standard heap ordered tree on $n + 1$ nodes is a finite, rooted tree in which all nodes except the root are labeled with the numbers $\{1, 2, 3, \ldots, n\}$ so that:
1. each label $i$ occurs precisely once;

2. if a node labeled $i$ has children labeled $j_1, \ldots, j_k$, then $i < j_1, \ldots, i < j_k$.

We denote the set of standard heap ordered trees on $n + 1$ nodes by $\mathcal{T}_n$. Let $k\mathcal{T}_n$ be the vector space over the field $k$ whose basis is the set of trees in $\mathcal{T}_n$, and let

$$k\mathcal{T} = \bigoplus_{n \geq 0} k\mathcal{T}_n.$$ 

Definition 2.4 A heap ordered tree is a rooted tree in which every node (including the root) is given a different positive integer label such that condition 2. of Definition 2.3 is satisfied.

A heap ordered tree differs from a standard heap ordered tree in that the root is also labeled, and that the labels can be taken from a larger set of positive integers. The number of distinct heap ordered trees on $n + 1$ nodes is $n!$. Heap ordered trees occur naturally when studying permutations and differential operators, as we shall see below.

2.5 Summary – Hopf Algebras of Trees

To summarize, with the product and coproduct as defined above, the vector spaces whose bases are (i) the set of rooted trees, (ii) labeled rooted trees, (iii) ordered trees, (iv) labeled ordered trees, (v) heap ordered trees, and (vi) labeled heap ordered trees are all Hopf algebras (see [5]).

In Section 4, we show that there is an isomorphism from the Hopf algebra of heap ordered trees to a Hopf algebra on permutations. In Section 5, we show how Hopf algebras of rooted labeled trees arise naturally when computing with derivations on the $k$-algebra of functions from $k^n$ to $k$. In Section 6, we show how Hopf algebras of rooted, ordered, labeled trees arise naturally when computing with derivations on the $k$-algebra of $C^\infty$ functions on a $C^\infty$ manifold.

3 Shuffle Algebras

The definitions and basic properties about shuffle algebras that we summarize in this section will be needed later.

A shuffle of the sequences $(i_1, \ldots, i_m)$ and $(j_1, \ldots, j_n)$ is a permutation $\sigma$ of $(k_1, \ldots, k_{m+n}) = (i_1, \ldots, i_m, j_1, \ldots, j_n)$ satisfying: if $p < q$, $\sigma(i_p) = k_r$, 

\[ \sigma(i_p) = k_r, \]
and $\sigma(i_q) = k_s$, then $r < s$; if $p < q$, $\sigma(j_p) = k_r$, and $\sigma(j_q) = k_s$, then $r < s$.

In other words, a shuffle of the sequences $(i_1, \ldots, i_m)$ and $(j_1, \ldots, j_n)$ is a permutation of $(i_1, \ldots, i_m, j_1, \ldots, j_n)$ that preserves the order of $(i_1, \ldots, i_m)$ and of $(j_1, \ldots, j_n)$.

We denote this shuffle by $\sigma(i_1, \ldots, i_m; j_1, \ldots, j_n)$.

**Definition 3.1 (shuffle product)** Let $X$ be a set of non-commuting variables, and let $A$ be the vector space with basis all monomials in the variables $\{x_1, \ldots, x_n\}$. Define a product on $A$ as follows. If $x_{i_1} \cdots x_{i_m}, x_{j_1} \cdots x_{j_n} \in A$, define

$$(x_{i_1} \cdots x_{i_r})(x_{j_1} \cdots x_{j_s}) = \sum_{\sigma} x_{\sigma(i_1)} \cdots x_{\sigma(i_m)} x_{\sigma(j_1)} \cdots x_{\sigma(j_n)},$$

where the sum is taken over all shuffles $\sigma(i_1, \ldots, i_r; j_1, \ldots, j_s)$.

The coproduct on $A$ is defined in the same way as for the free non-commutative algebra on the set $X$, given by

$$\Delta(x_i) = 1 \otimes x_i + x_i \otimes 1.$$ 

**Theorem 3.2** Fix a field $k$, and let $k\langle x_1, \ldots, x_n \rangle$ denote the vector space over $k$ in the non-commuting variables $x_1, \ldots, x_n$. Then the shuffle product defined above makes $k\langle x_1, \ldots, x_n \rangle$ into a Hopf algebra over $k$.

### 4 Hopf Algebras of Permutations

Let $\mathfrak{S}_n$ denote the symmetric group on $n$ symbols, let $k\mathfrak{S}_n$ denote the vector space over the field $k$ with basis $\mathfrak{S}_n$, and let

$$k\mathfrak{S} = \bigoplus_{n \geq 0} k\mathfrak{S}_n.$$ 

In this section, we define a Hopf algebra structure on $k\mathfrak{S}$ following [8]. We begin with some notation.

Let $(\sigma_1 \sigma_2 \cdots \sigma_k)$ denote the cycle in $\mathfrak{S}_n$ which sends $\sigma_1$ to $\sigma_2$, $\sigma_2$ to $\sigma_3$, $\ldots$, and $\sigma_k$ to $\sigma_1$. Every permutation is a product of disjoint cycles. If $(\sigma_1 \sigma_2 \cdots \sigma_k)$ is a cycle, then there is a string naturally associated with the cycle that we write $\sigma_1 \sigma_2 \cdots \sigma_k$.

Now let $\sigma = (s_1) \cdots (s_r) \in \mathfrak{S}_m$ and $\tau = (t_1) \cdots (t_t) \in \mathfrak{S}_n$ be two permutations, each written as a product of disjoint cycles. We denote the
corresponding strings by \( s_i = m_{i1} \cdots m_{ip_i} \) and \( t_j = n_{j1} \cdots n_{jq_j} \) respectively. We call the elements of \( \{n_{11}, \ldots, n_{\ell q}\} \) attachment points for the cycles \( (s_1), \ldots, (s_r) \) on the permutation \( \tau = (t_1) \cdots (t_\ell) \). We will also define \( \circ \) to be the \((n + 1)^{th}\) attachment point.

Also, if \( \sigma \) is a permutation on \( \{1, \ldots, k\} \), let \( \text{st}(\sigma, m) \) be the permutation on \( \{m + 1, \ldots, m + k\} \) that sends \( m + i \) to \( m + \sigma(i) \).

The definition of the product in the bialgebra is simpler if we introduce the standard order of a permutation, which is defined as follows:

**Definition 4.1** We say that a permutation \( \sigma \in \mathfrak{S}_m \) that is expressed as a product of cycles \( \sigma = (s_1) \cdots (s_r) \) is in standard order if the cycles \( (s_i) = (m_{i1} \cdots m_{ip_i}) \) are written so that

1. \( m_{i1} < m_{i2}, m_{i1} < m_{i3}, \ldots, m_{i1} < m_{ip_i} \)
2. \( m_{11} > m_{21} > m_{31}, \ldots, m_{i-1,1} > m_{i1} \)

In other words, a product of cycles \( \sigma = (s_1) \cdots (s_r) \) is written in standard order if each cycle \( (s_i) = (m_{i1} \cdots m_{ip_i}) \) starts with its smallest entry, and if the cycles \( (s_1), \ldots, (s_r) \) are ordered so that their starting entries are decreasing. A permutation can always be written in standard order since disjoint cycles commute, and since a single cycle is invariant under a cyclic permutation of its string.

We now define the heap product of two permutations.

**Definition 4.2** We define the heap product \( \sigma \# \tau \) of \( \sigma \in \mathfrak{S}_m \) and \( \tau \in \mathfrak{S}_n \) as follows:

1. Put \( \sigma \) and \( \tau \) in standard order;
2. Replace \( \sigma \) by \( \text{st}(\sigma, n) \);
3. Form terms as follows: if \( (s_i) \) is one of the cycles in \( \sigma \), attach the string \( s_i \) to any one of the \( n + 1 \) attachment points; if the attachment point is one of \( n_{11}, \ldots, n_{\ell q} \), say \( n_{jk} \), place the string \( s_i = m_{i1} \cdots m_{ip_i} \) to the right of \( n_{jk} \); otherwise (if the attachment point is \( \circ \) we multiply the term we are constructing by \( (s_i) \);
4. The product \( \sigma \# \tau \) is the sum of all the terms constructed in this way, taken over all the cycles in \( \sigma \) and over all attachment points.

Note that there are \((n + 1)^r\) terms in \( \sigma \# \tau \).
We now describe the coalgebra structure of $k \mathcal{S}$: Define a function $\text{st}(\pi)$ from permutations to permutations as follows: let $\pi = (s_1) \cdots (s_p) \in \mathcal{S}_n$ and let $L = \{\ell_1, \ldots, \ell_k\}$ be the labels (in order) which occur in the $s_i$. (If $\pi$ fixes $i$, we include a 1-cycle $(i)$ as a factor in $\pi$.) The permutation $\text{st}(\pi)$ is the permutation in $\mathcal{S}_k$ gotten by replacing $\ell_j$ with $j$ in $\pi$. For example, if $\pi = (13)(4)(57) \in \mathcal{S}_7$, then $\text{st}(\pi) \in \mathcal{S}_5$ equals $(12)(3)(45)$.

The coalgebra structure of $k \mathcal{S}$ is defined as follows. Let $\pi = (s_1) \cdots (s_k) \in \mathcal{S}_n$, and let $C = \{(s_1), \ldots, (s_k)\}$. If $X \subseteq C$ let $\rho(X) = \text{st}(\prod_{(s_i) \in C} (s_i))$. Note that if $\rho(X) \in \mathcal{S}_k$, then $\rho(C\setminus X) \in \mathcal{S}_{n-k}$. Define

$$\Delta(\pi) = \sum_{X \subseteq C} \rho(X) \otimes \rho(C\setminus X)$$

$$\epsilon(\pi) = \begin{cases} 1 & \text{if } \pi \text{ is the identity permutation in } \mathcal{S}_0, \\ 0 & \text{otherwise.} \end{cases}$$

The following theorem is proved in [8].

**Theorem 4.3** With the product and coproduct defined above, $k \mathcal{S}$ is a Hopf algebra.

It turns out that this Hopf algebra structure on $k \mathcal{S}$ is isomorphic to the Hopf algebra structure on heap-ordered trees defined above [8].

There are several other different Hopf algebra structures on permutations that can be defined, including the Malvenuto-Reutenauer Hopf algebra. The Malvenuto-Reutenauer is a non-commutative, non-cocommutative, self-dual, graded Hopf algebra. In contrast, the Hopf algebra on permutations defined above is non-commutative, cocommutative, graded Hopf algebra. For descriptions of these other Hopf algebras on permutations see [12], [10], [1].

## 5 H-Module Algebras for Labeled Trees

In this and the next section, we describe some actions of Hopf algebras of trees on $k$-algebras $R$ of functions. In this section, we consider the case of $k$-algebras $R$ of functions on a space $X = k^n$. For example, $R$ can be the space of polynomials, rational functions or $C^\infty$ functions on $X$. In the next section, we consider the more general case of $k$-algebras of functions on a $n$-dimensional algebraic group $X$ or a $n$-dimensional $C^\infty$ manifold $X$. 

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Let $R$ be a commutative $k$-algebra, and let $H$ be a $k$-bialgebra. The algebra $R$ is a left $H$-module algebra if $R$ is a left $H$-module for which
\[ h \cdot (ab) = \sum_{(h)} (h(1) \cdot a)(h(2) \cdot b), \]
where $h \in H$, $\Delta(h) = \sum_{(h)} h(1) \otimes h(2)$, and $a, b \in R$.

Consider the vector space spanned by finite rooted trees, each of whose nodes except for the root are labeled with one of the formal symbols \{ $E_1$, \ldots, $E_M$ \}. This generates an algebra using the product defined above that we denote $kT(E_1, \ldots, E_k)$ or, if no confusion is possible, simply by $kT$. Note that the same symbol may label more than one node of the tree.

Fix an $k$-algebra $R$ of functions and consider the situation where the $E_i$ are not formal symbols, but are differential operators of the form
\[ E_j = \sum_{\mu=1}^{n} a_{j}^{\mu}(x)D_{\mu}, \]
with $a_{j}^{\mu}(x) \in R$. Here $D_{\mu} = \partial/\partial x_\mu$. The algebra $R$ is typically either the algebra of polynomial functions $k[x_1, \ldots, x_n]$, the algebra of rational functions $k(x_1, \ldots, x_n)$, or the algebra of smooth functions $C^\infty(k^n, k)$.

Let $H$ denote a Hopf algebra of trees labeled with derivations of $R$. In this section, we define a natural action of $H$ on $R$ that turns $R$ into a $H$-module algebra.

**Definition 5.1** We define a map
\[ \psi : kT(E_1, \ldots, E_M) \longrightarrow R \]
as follows. Let $t \in kT(E_1, \ldots, E_M)$ have $k + 1$ nodes, and let $f \in R$. Number the non root nodes of $t$ from 1 to $k$. We define $\psi(t)f$ as follows: For the root, form the term
\[ T_0 = \frac{\partial^r f}{\partial x_{i_1} \ldots \partial x_{i_r}}, \]
where the $r$ children of the root are numbered $l_1, \ldots, l_r$.
For a nonroot node numbered $j$ and labeled with $E_{l_1}$, form the term
\[ T_k = \frac{\partial^r a_j^{l_1}(x)}{\partial x_{i_1} \ldots \partial x_{i_r}}. \]
Then
\[ \psi(t)f = \sum_{i_1, \ldots, i_k} T_k T_{k-1} \cdots T_1 T_0. \]
The following theorem [6] captures an important property of this $\psi$-map.

**Theorem 5.2** Fix derivations $E_j = \sum a^j_\mu D_\mu$ with $a^j_\mu \in R$, and $D_\mu = \frac{\partial}{\partial x^\mu}$.

Let $k<E_1,\ldots,E_M>$ be the free associative algebra generated by the formal symbols $E_1,\ldots,E_M$. Let $H = kT(E_1,\ldots,E_M)$ be the Hopf algebra consisting of rooted trees labeled with the derivations $E_j$. Let $\text{Diff}(E_1,\ldots,E_M)$ be the higher order derivations generated by the derivations $E_1,\ldots,E_M$.

Then with the $\psi$-map as defined above makes the following diagram commute:

$$
\begin{array}{ccc}
    k<E_1,\ldots,E_M> & \rightarrow & kT(E_1,\ldots,E_M) \\
    \downarrow & & \downarrow \psi \\
    \text{Diff}(E_1,\ldots,E_M) & & \text{Diff}(E_1,\ldots,E_M)
\end{array}
$$

The right arrow is the map induced by the fact that $k<E_1,\ldots,E_M>$ is freely generated by the $E_i$, and $E_i$ maps to the tree with one node other that the root which is labeled with $E_i$; the diagonal arrow is induced by the fact that the $E_i$ are derivations.

**Example 5.3** An expression such as

$$p = E_3E_2E_1 - E_3E_1E_2 - E_2E_1E_3 + E_1E_2E_3$$

corresponds to 24 trees, 18 of which cancel (each cancellation saves $O(n^3)$ differentiations). The surviving six differentiations are

$$
\sum a^\mu_3 (D_\mu_3 a^\mu_2) (D_\mu_2 a^\mu_1) D_\mu_1 \\
- \sum a^\mu_3 (D_\mu_3 a^\mu_1) (D_\mu_2 a^\mu_1) D_\mu_1 \\
- \sum a^\mu_2 (D_\mu_3 a^\mu_1) (D_\mu_2 a^\mu_1) D_\mu_1 \\
+ \sum a^\mu_3 (D_\mu_3 a^\mu_2) (D_\mu_2 a^\mu_1) D_\mu_1 \\
+ \sum a^\mu_3 a^\mu_2 (D_\mu_3 D_\mu_2 a^\mu_1) D_\mu_1 \\
- \sum a^\mu_3 a^\mu_2 (D_\mu_3 D_\mu_2 a^\mu_1) D_\mu_1
$$
corresponding to the six trees:

This example illustrates the kinds of cancellations of higher order derivations that are captured by trees. It turns out that the Hopf algebra $H$ of trees labeled with derivations is a natural structure for computing symbolically with derivations and higher order derivations. See [6] and [3].

6 H-Module Algebras for Labeled, Ordered Trees

In this section, we consider what happens when $X$ is not $k^n$, but instead a $C^\infty$ manifold. In this case, we can define $R$ to be the $k$-algebra of $k$-valued $C^\infty$ functions on the manifold.

The key observation is that defining natural $H$-module algebras in this context can be done using a connection and labeled ordered trees.

Let $R$ be a commutative $k$-algebra, and let $\mathcal{D}$ be a Lie algebra of derivations of $R$. A connection [13] is a map $\mathcal{D} \times \mathcal{D} \to \mathcal{D}$ sending $(E, F) \in \mathcal{D} \times \mathcal{D}$ to $\nabla_E F \in \mathcal{D}$ satisfying

- $\nabla_{E_1 + E_2} F = \nabla_{E_1} F + \nabla_{E_2} F$
- $\nabla_E (F_1 + F_2) = \nabla_E F_1 + \nabla_E F_2$
- $\nabla_{f \cdot E} F = f \cdot \nabla_E F$
- $\nabla_E (f \cdot F) = f \cdot \nabla_E F + E(f)F$
where $E, F \in \mathcal{D}$, $f \in R$.

We use the connection as follows. If $E, F \in \mathcal{D}$ and $f \in R$, define:

\[
\circ \cdot (r) = E(r) \\
\circ \cdot E \cdot (r) = \nabla_F E(r)
\]

and extend using induction, the definition of tree multiplication, and a consistency requirement for subtrees of larger trees. We show in [7] that construction defines a $H$-module algebra structure on $R$.

The following theorem is from [7]:

**Theorem 6.1** Let $R$ be a commutative $k$-algebra, and let $\nabla_{EF}$ be a connection on the Lie algebra $\mathcal{D}$ of derivations of $R$. Then the construction above gives a $kT(\mathcal{D})$-module structure on $R$. This module structure induces a map $\psi : kT(\mathcal{D}) \rightarrow \text{End}(R)$, so that the following diagram commutes:

\[
k\langle E_1, \ldots, E_M \rangle \rightarrow kT(\mathcal{D})
\]

\[
\downarrow \psi \\
\text{Diff}(R) \subset \text{End}(R)
\]

This theorem can be applied to derive Runge-Kutta numerical algorithms on groups. See [4] and [3].

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