ON THE MATHEMATICS OF ROOTED TREES

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I am mainly interested in algebraic combinatorics, which consists in discovering the algebraic structures behind various classes of concrete objects, called *combinatorial*. The most obvious example is given by the natural numbers, which can be added or multiplied together. Roughly speaking, combinatorial objects such as trees, graphs, various kinds of diagrams, cacti, partially ordered sets, finite topological spaces, etc., can be considered as "numbers" of a certain kind. The algebra behind them, i.e. the way these objects can be combined together, is in general quite different from the usual addition and multiplication of ordinary numbers.

Rooted trees have been considered for a long time, at least since a famous 160-years old article by A. Cayley [2]. They figure among the most fascinating combinatorial objects. A rooted tree can be defined as a single vertex (the root), or a finite collection of rooted trees, with repetitions allowed, grafted on a common root. This definition must be understood recursively, the same way a natural number is zero or the successor of a natural number. The rooted trees up to five vertices are graphically represented below, with the root at the bottom:

Let T_n be the number of rooted trees with n vertices. The sequence

$$(T_n)_{n\geq 1} = (1, 1, 2, 4, 9, 20, 48, 115, 286, 719, 1842, 4766, \cdots)$$

(number A00081 in the Sloane Online Encyclopedia of Integer Sequences) is well-known: its generating series $T(z) := \sum_{n>1} T_n z^n$ is solution of the functional equation [11]

(1)
$$T(z) = ze^{T(z) + \frac{1}{2}T(z^2) + \frac{1}{3}T(z^3) + \cdots},$$

which leads with some care to the recursive formula:

(2)
$$T_{n+1} = \frac{1}{n} \sum_{k=1}^{n} \left(\sum_{d|k} dT_d \right) T_{n+1-k},$$

and one has asymptotically

(3)
$$T_n \mathop{\sim}_{n \to +\infty} c \omega^n n^{-3/2},$$

where $c = 0.43993237 \cdots$ and $\omega = 2.95576 \cdots$ are Otter's tree constants [10, 9].

Let us now focus on the algebraic aspects: There is a natural bijection B_+ from the set of forests (i.e. collections of trees with repetitions allowed) onto the set of trees, which grafts each tree of the forest on a common root. For example,

$$B_+(\mathbf{V}\bullet)=\mathbf{V}.$$

Two forests can be *multiplied* together, by considering their disjoint union. This product is obviously commutative and associative. This is also possible to "make two forests out of one" by

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applying a so-called comultiplication operator Δ . Technically, for any forest F, the comultiplication $\Delta(F)$ lives in the *tensor product*, i.e. the vector space freely generated by ordered pairs of forests. The multiplication and comultiplication, together with the unit (the empty forest) and the *co-unit*, endow the linear span of forests with the very rich structure of *commutative connected* graded Hopf algebra [1, 5, 12, 4]. This structure plays a prominent role in numerical analysis (Runge-Kutta approximation methods), Quantum Field Theory and Probabiliy (stochastic differential an partial differential equations). The operator B_+ can be interpreted as a Hochschild cocycle for the coalgebra stucture, and is in some sense an initial object among such cocycles on Hopf algebras [8].

Let us now turn to trees themselves: two trees can be multiplied using the *Butcher product*, i.e. by grafting the first tree on the root of the second, for example:

$$I \circ I = V.$$

Contrarily to addition or multiplication of numbers, this product is not commutative nor associative:

$$(\bullet \circ \bullet) \circ \bullet = \bullet, \qquad \bullet \circ (\bullet \circ \bullet) = \mathbf{V}.$$

It however verifies the Non-Associative-Permutative (NAP) relation:

$$s \circ (t \circ u) = t \circ (s \circ u)$$

for any trees s, t, u. The set T of rooted trees is moreover the free NAP set with one generator [6]: for any set E endowed with a binary product * such that a * (b * c) = b * (a * c) for any $a, b, c \in E$, for any choice of element $x \in E$, there is a unique map $\varphi_x : T \to E$ such that $\varphi_x(\bullet) = x$ and $\varphi_x(s \circ t) = \varphi_x(s) * \varphi_x(t)$ for any $s, t \in T$.

A second product, maybe even more interesting, can be defined on rooted trees, at the price of grafting at all vertices instead of sticking to the root. This is only possible in the vector space \mathcal{T} (over some base field **k**) freely generated by trees, namely

$$s \rhd t = \sum_{v \in V(t)} s \rhd_v t,$$

where $s \triangleright_v t$ stands for grafting the tree s on the tree t at the vertex v. For example,

$$arphi arphi arphi = ec arphi + ec arphi$$

The product \triangleright is bilinear. It is neither commutative nor associative:

$$(\bullet \triangleright \bullet) \triangleright \bullet = \bullet, \qquad \bullet \triangleright (\bullet \triangleright \bullet) = \vee + \bullet.$$

It however verifies the pre-Lie relation:

(4)
$$s \triangleright (t \circ u) - (s \triangleright t) \triangleright u = t \triangleright (s \circ u) - (t \triangleright s) \triangleright u$$

for any trees s, t, u. The vector space \mathcal{T} freely spanned by rooted trees is moreover the free pre-Lie algebra with one generator [3]: for any pre-Lie algebra A i.e. any vector space endowed with a bilinear product * satisfying the pre-Lie relation (4), there is a unique linear map $\psi_x : \mathcal{T} \to A$ such that $\psi_x(\bullet) = x$ and $\psi_x(s \triangleright t) = \psi_x(s) * \psi_x(t)$ for any $s, t \in T$.

The current object under investigation with two colleagues at UiB [7] consists in aromatic trees and forests, a natural generalization allowing for loops: an aroma is obtained from a rooted tree by drawing an extra edge between two vertices (distinct or not) and forgetting about the root, an aromatic tree is a collection of trees and aromas with only one tree in it, an aromatic forest is a collection of trees and aromas with some trees (possibly zero) in it. The vector space of aromatic trees carries a structure of *pre-Lie-Rinehart algebra*, which is the algebraic counterpart of the notion of *flat torsion-free Lie algebroid*. We prove that the aromatic forest pre-Lie-Rinehart algebra is the free pre-Lie-Rinehart algebra with one generator. As usual in these matters, we can generalize to several generators by putting decorations on the vertices.

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