

A general bijective algorithm for trees

(enumeration of trees/partition/species/Lagrange inversion)

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ABSTRACT Trees are combinatorial structures that arise naturally in diverse applications. They occur in branching decision structures, taxonomy, computer languages, combinatorial optimization, parsing of sentences, and cluster expansions of statistical mechanics. Intuitively, a tree is a collection of branches connected at nodes. Formally, it can be defined as a connected graph without cycles. Schröder trees, introduced in this paper, are a class of trees for which the set of subtrees at any vertex is endowed with the structure of ordered partitions. An ordered partition is a partition of a set in which the blocks are linearly ordered. Labeled rooted trees and labeled planed trees are both special classes of Schröder trees. The main result gives a bijection between Schröder trees and forests of small trees—namely, rooted trees of height one. Using this bijection, it is easy to encode a Schröder tree by a sequence of integers. Several classical algorithms for trees, including a combinatorial proof of the Lagrange inversion formula, are immediate consequences of this bijection.

1. Introduction

I introduce the concept of *Schröder trees*, which are defined as labeled rooted trees for which the set of subtrees of any vertex is endowed with the structure of ordered partitions. An ordered partition is a partition of a set in which the blocks are linearly ordered. This is a generalization of both labeled rooted trees and labeled plane trees. The term *Schröder tree* was suggested by G.-C. Rota (personal communication), for Schröder was the first to consider plane trees. In the language of species (1), we may say that a Schröder tree is a rooted tree enriched by the species of ordered partitions. A rooted tree of height one will be called a *small tree*. It is essentially a set of more than one element with a distinguished element. A small tree with only one leaf is called a *match*.

We find a bijection between Schröder trees and forests of small trees. Using this bijection, it is straightforward to encode a Schröder tree by a sequence. Many classical results on enumeration of trees are immediate consequences of this bijection. Moreover, the bijection is even valid for Schröder trees enriched by a species on the blocks and small trees enriched by the same species. Especially, the Lagrange inversion formula can be stated explicitly in terms of Schröder trees and the cancellation involving Lagrange inversion turns out to be a sign change in constructing a Schröder tree out of several smaller Schröder trees. Thus, the notion of Schröder trees seems to have answered a question of Rota (personal communication) about what is the intrinsic connection among partitions, rooted trees, and the Lagrange inversion formula, especially, what is the combinatorial nature of the cancellation involving the Lagrange inversion.

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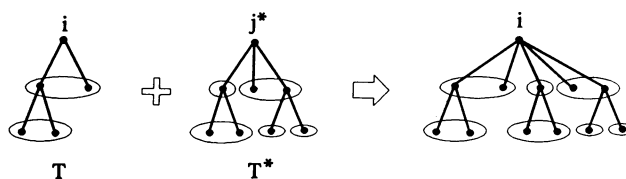
2. A Bijection for Schröder Trees

All the trees considered in this paper are assumed to be labeled trees, unless otherwise stated. For a vertex v in a rooted tree, the number of vertices covered by v is called the *degree* or *outdegree* of v . If v is not a leaf, we shall call the set of vertices covered by v the *fiber* of v . Conversely, if a vertex u is covered by v , we shall call v the *root* of u . In a Schröder tree T , the total number of blocks of partitions on all the fibers is called the number of blocks of T . A vertex in a rooted tree will be called an *internal vertex* if it is not a leaf. The following theorem shows that a Schröder tree on more than one vertex with k blocks can be uniquely decomposed into k small trees. The bijection will be given in the proof.

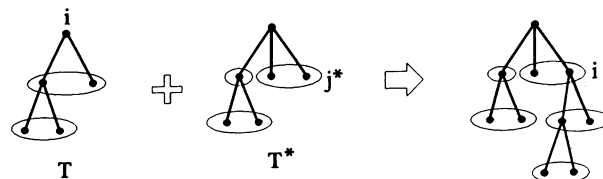
THEOREM 2.1. *There is a bijection between the set of all Schröder trees on n ($n > 1$) vertices with k blocks and the set of forests of k small trees on $n + k - 1$ vertices.*

Proof: I first give the procedure to construct a Schröder tree on $\{1, 2, \dots, n\}$ with k blocks from a forest F of k small trees on $\{1, 2, \dots, n + k - 1\}$. For convenience, we shall mark all the vertices $n + 1, n + 2, \dots, n + k - 1$ by the symbol $*$.

- (1) Find the tree T in F with the smallest root such that there is no marked vertex in T . Let i be the root of T .
- (2) Find the tree T^* in F that contains the smallest marked vertex. Let j^* be this marked vertex.
- (3) If j^* is the root of T^* , then merge T and T^* by identifying i and j^* , keep i as the new vertex, and put the subtrees of T^* at the right-hand side of T . We shall call this operation a *horizontal merge*:



If j^* is a leaf of T^* , then replace j^* with T in T^* . We shall call this operation a *vertical merge*:



- (4) Repeat the above procedure until F becomes a Schröder tree.

At the first step, there are k small trees and $k - 1$ marked vertices; thus there must be a small tree without any marked vertex. After each merge, both the number of trees and the number of marked vertices decrease by 1; this means that we can always find a tree without any marked vertex at any step. It is also clear that a marked vertex is always either a root or

a leaf, so we may eventually get a Schröder tree from the above construction.

The following is the procedure to decompose a Schröder tree into small trees.

- (1) Find the smallest internal vertex i such that all vertices in the leftmost block B in the fiber of i are leaves. Then we may obtain a small tree with root i and leaf set B .
- (2) Remove the block B and relabel the vertex i by $n + 1$. However, the original label i will be reused for later comparisons of vertices.
- (3) Repeat the above procedure and relabel the encountered roots of small trees subsequently by $n + 2, n + 3, \dots, n + k - 1$. \square

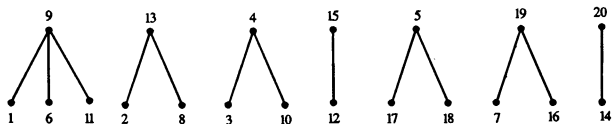
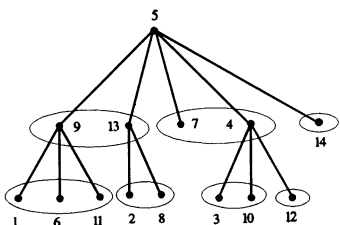
From the above bijection, it is straightforward to obtain the following correspondence between Schröder trees and some sequences on the roots of small trees. Given a sequence $L = a_1 a_2 \dots a_n$ on a set S , the number of distinct elements appearing in L will be called the *multiplicity* of L .

THEOREM 2.2. *There is a bijection between Schröder trees on n ($n > 1$) vertices with k blocks and sequences $a_1 a_2 \dots a_{n-1}$ of multiplicity k on the set $\{1, 2, \dots, n + k - 1\}$.*

Proof: Let F be a forest of k small trees on $\{1, 2, \dots, n + k - 1\}$. Clearly, there is a total of $n - 1$ leaves in F . Let $b_1 b_2 \dots b_{n-1}$ be the increasingly ordered sequence of these $n - 1$ leaves. For any leaf b_i in the forest, let a_i be the root of b_i . Thus, $a_1 a_2 \dots a_{n-1}$ is a sequence of multiplicity k on $\{1, 2, \dots, n + k - 1\}$.

Given a sequence $a_1 a_2 \dots a_{n-1}$ of multiplicity k on $\{1, 2, \dots, n + k - 1\}$, let P be the underlying set and $Q = \{1, 2, \dots, n + k - 1\} \setminus P$. Since P has k elements, Q must have $n - 1$ elements. Let $b_1 b_2 \dots b_{n-1}$ be the increasingly ordered sequence of elements in Q . By letting b_i be a leaf of a_i , we obtain a desired forest of k small trees. \square

Example 2.3: The following are a Schröder tree on 14 vertices, its small tree decomposition, and the corresponding sequence.



9 13 4 9 19 13 4 9 15 20 19 5 5

3. Rooted Trees

A rooted tree can be regarded as a Schröder tree with every fiber having exactly one block. In the above construction of a Schröder tree T from small trees, there is a fiber of T with more than one block if and only if a horizontal merge occurs. This leads to the following theorem.

THEOREM 3.1. *There is a bijection between rooted trees on n ($n > 1$) vertices with k internal vertices and forests of k small trees on $\{1, 2, \dots, n + k - 1\}$ with unmarked roots, namely every root is not greater than n .*

COROLLARY 3.2. *The number of rooted trees on n vertices with k leaves is $\frac{n!}{k!} S(n - 1, n - k)$, where $S(n, k)$ are the Stirling numbers of the second kind.*

Proof: Let T be any rooted tree on n vertices with k leaves. Consider the small tree decomposition of T ; there are $\binom{n}{n-k}$ ways to choose the $n - k$ unmarked roots of small trees and $(n - k)! S(n - 1, n - k)$ ways to arrange the remaining $n - 1$ elements. \square

COROLLARY 3.3. *Let (d_1, d_2, \dots, d_n) be a sequence of nonnegative integers satisfying $d_1 + d_2 + \dots + d_n = n - 1$. Then the number of rooted trees on $\{v_1, v_2, \dots, v_n\}$ with the outdegree of v_i being d_i is $\binom{n-1}{d_1, d_2, \dots, d_n}$.*

Proof: Let T be a rooted tree with degree sequence (d_1, d_2, \dots, d_n) . For any $d_i > 0$, v_i must be the root of a small tree with d_i leaves in the small tree decomposition of T . Since there is a total of $n - 1$ leaves among all the small trees, the proof is complete by the definition of the multinomial coefficient. \square

The correspondence between Schröder trees and sequences induces a bijection for rooted trees which is similar to the Prüfer correspondence for rooted trees (2, 3).

COROLLARY 3.4. *There is a bijection between the set of rooted trees on n vertices and the set of all sequences of length $n - 1$ on n elements.*

Cayley's formula then follows most naturally from the above corollary. Moreover, Clarke's formula also follows this way.

COROLLARY 3.5 (CLARKE). *The number of rooted trees on $n + 1$ vertices with a specific root and root degree k is $\binom{n-1}{k-1} n^{n-k}$.*

Proof: Suppose T is any rooted tree with a specific root, say v_{n+1} , and root degree k . In the small tree decomposition of T , v_{n+1} is a root of a small tree S with k leaves. Clearly, S must contain the maximum marked vertex, namely $n + 1$ must appear at the end of the sequence representation of T . Thus, we have $\binom{n-1}{k-1}$ ways to choose other $k - 1$ positions to place $n + 1$, and n^{n-k} ways to fill out the remaining $n - k$ positions. \square

4. Plane Trees

Suppose T is a Schröder tree on $n + 1$ vertices. It is clear that T has n blocks if and only if every block of T contains exactly one vertex. Thus, a plane on $n + 1$ vertices can be regarded as a Schröder tree on $n + 1$ vertices with n blocks. By the bijection between Schröder trees and small trees, we obtain a bijection between plane trees on $n + 1$ vertices and forests of n small trees on $2n$ vertices, namely forests of n matches on $2n$ vertices.

COROLLARY 4.1. *There is a bijection between plane trees on $n + 1$ vertices and forests of n matches on $2n$ vertices.*

If we order the n matches vertically, we may get a permutation on $2n$ elements. Hence, the number of labeled plane trees on $n + 1$ vertices is $(2n)!/n!$. Dividing this number by $(n + 1)!$, we then obtain the number of unlabeled plane trees on $n + 1$ vertices. This is the well-known Catalan number

$$C_n = \frac{1}{n+1} \binom{2n}{n}.$$

By the correspondence between Schröder trees and sequences, we see that a plane tree on $n + 1$ vertices can be encoded by a sequence $a_1 a_2 \cdots a_n$ of multiplicity n on $2n$ elements. Clearly, no element could appear more than once in such sequences. Thus we have the following corollary.

COROLLARY 4.2. *There is a bijection between plane trees on $n + 1$ vertices and permutations of length n on $2n$ elements.*

The above bijection seems to be the simplest interpretation of Catalan numbers. Moreover, we may have the following refinement (4).

COROLLARY 4.3 (NARAYANA). *The number of unlabeled plane trees on $n + 1$ vertices with k leaves equals*

$$T_{n+1,k} = \frac{1}{n+1} \binom{n+1}{k} \binom{n-1}{n-k}.$$

Proof: Let T be any plane tree on $\{1, 2, \dots, n + 1\}$. By the above bijection between plane trees on $n + 1$ vertices and forests of matches on a total of $2n$ vertices, it is clear that T is a plane tree with k leaves if and only if there are exactly k unmarked vertices among the leaves in the corresponding forest of T . Thus, we have $\binom{n+1}{k}$ ways to choose the k unmarked leaves, and $\binom{n-1}{n-k}$ ways to choose the remaining $n - k$ marked leaves. Once the leaves are chosen, there are $n!$ ways to arrange the roots. Dividing the total number of choices by $(n + 1)!$, we may obtain the desired formula for unlabeled plane trees. \square

By turning every match in the forest decomposed from a plane tree upside down, we obtain an involution on the set of all plane trees on n vertices, which maps a leaf to an internal vertex and vice versa.

Note that our basic bijection for Schröder trees is automatically valid for Schröder trees with every block endowed with the structure of linear orders or even other combinatorial structures. Therefore, a plane tree can be uniquely decomposed into small plane trees.

COROLLARY 4.4. *There is a bijection between the set of plane trees on n ($n > 1$) vertices with k internal vertices and the set of forests of k small plane trees on $n + k - 1$ vertices with unmarked roots.*

The Narayana number also follows from the above corollary. If we consider k -ary plane trees (i.e., plane trees with every fiber having k vertices) on $kn + 1$ vertices, we may have the following bijection.

COROLLARY 4.5. *There is a bijection between the set of k -ary plane trees on $kn + 1$ vertices and the set of forests of n small k -ary plane trees with unmarked roots.*

In the above corollary, there are $kn + 1$ unmarked vertices, so we may have $\binom{kn+1}{n}$ ways to choose the n roots in the forest. After these n roots are chosen, we may order them in an increasing order. Therefore, any order of the kn leaves determines the forest. Hence the number of k -ary labeled plane trees on $kn + 1$ vertices is

$$\binom{kn+1}{n} (kn)!$$

So we have the following formula for the number of unlabeled k -ary plane trees on $kn + 1$ vertices (2, 5):

$$\frac{1}{kn+1} \binom{kn+1}{n}.$$

In general, given any degree sequence (d_1, d_2, \dots, d_n) satisfying $d_1 + d_2 + \dots + d_n = n - 1$, there are always $(n - 1)!$ labeled plane trees having this degree sequence. This relation connects the enumeration of plane trees to the enumeration of certain degree sequences. Although it could also follow from Corollary 3.3, it did not seem to be paid enough attention in the study of enumeration of plane trees. For example, from this point of view it would be obvious to obtain the number of unlabeled plane trees with a given degree type (6, 7).

COROLLARY 4.6 (ERDÉLYI-ETHERINGTON). *Let $1^{n_0} 2^{n_1} \cdots m^{n_m}$ be a partition of $n - 1$, i.e., $n_1 + 2n_2 + \dots + mn_m = n - 1$, and $n_0 = n - (n_1 + n_2 + \dots + n_m)$. Then the number of unlabeled plane trees having n_i vertices with degree i equals*

$$\frac{(n_0 + n_1 + \dots + n_m - 1)!}{n_0! n_1! \cdots n_m!}.$$

Proof: Consider the number of degree sequences (d_1, d_2, \dots, d_n) with n_i numbers being i . This number is the same as the number of ways to distribute $n - 1$ identical balls into n distinguishable boxes such that there are n_i boxes having exactly i balls, which equals $\binom{n}{n_0, n_1, \dots, n_m}$. Multiplying this number by $(n - 1)!$, we get the number of labeled plane trees with the given degree type, then dividing by $n!$, it becomes the desired number for unlabeled plane trees. \square

The same observation also leads to a quick solution to a problem of Klarner (5). He considered the number $U_{n+1,k}$ of unlabeled plane trees on $n + 1$ vertices in which every vertex has outdegree not greater than k , but he did not find an explicit formula for $U_{n+1,k}$. Let $V_{n+1,k}$ be the corresponding number for labeled plane trees. Clearly, we have the relation $V_{n+1,k} = (n + 1)! U_{n+1,k}$. It is easy to see that the number of degree sequences $(d_1, d_2, \dots, d_{n+1})$ satisfying $0 \leq d_i \leq k$ is the coefficient of x^n in

$$(1 + x + \dots + x^k)^{n+1} = \frac{(1 - x^{k+1})^{n+1}}{(1 - x)^{n+1}} = \left(\sum_{i \geq 0} (-1)^i \binom{n+1}{i} x^{(k+1)i} \right) \left(\sum_{j \geq 0} \binom{n+j}{j} x^j \right).$$

It follows that

$$U_{n+1,k} = \frac{1}{n+1} \sum_{(k+1)i+j=n} (-1)^i \binom{n+1}{i} \binom{n+j}{j}.$$

The decomposition of rooted trees into small trees naturally extends to enriched trees by a general species. Let M be a species. Then the number of M -enriched trees on n vertices with degree sequence (d_1, d_2, \dots, d_n) is

$$\binom{n-1}{d_1, d_2, \dots, d_n} \cdot |M[d_1]| \cdot |M[d_2]| \cdots |M[d_n]|.$$

This gives the following formula for the number of M -enriched trees on n vertices (1).

COROLLARY 4.7. *Let M be a species and*

$$M(x) = \sum_{n \geq 0} |M[n]| \frac{x^n}{n!}$$

be the generating function of M . Then the number of M -enriched trees on n vertices equals the coefficient of $\frac{x^{n-1}}{(n-1)!}$ in $M^n(x)$.

Since we know that the generating function for the number of ordered partitions is $(2 - e^x)^{-1}$, by the above corollary, we have the following formula for the number of Schröder trees on n vertices:

$$\frac{1}{2^n} \sum_{k \geq 0} \binom{n+k-1}{k} \frac{k^{n-1}}{2^k}.$$

As another example of enriched trees, we consider rooted trees in which every fiber is endowed with a cyclic permutation, and we call them *cyclic trees*. The bijection for Corollary 3.2 essentially shows that the number of cyclic trees on n vertices is

$$\sum_{k=1}^{n-1} (n)_k |s(n-1, k)|, \tag{4.1}$$

where $s(n, k)$ are the Stirling numbers of the first kind. Since the generating function for cyclic permutations is $1 + \log \frac{1}{1-x}$, the above formula also follows from Corollary 4.7 and the following well-known identity:

$$\frac{\left(\log \frac{1}{1-x}\right)^k}{k!} = \sum_{i \geq k} |s(i, k)| \frac{x^i}{i!}.$$

5. Lagrange Inversion Formula

Let $f(x) = \sum_{n \geq 1} a_n x^n / n!$ be a formal power series with $a_1 \neq 0$ and $g(x) = \sum_{n \geq 1} b_n x^n / n!$ be the functional inverse of $f(x)$, namely the formal power series satisfying $f(g(x)) = g(f(x)) = x$. The Lagrange inversion formula states that

$$b_n = \text{the coefficient of } \frac{x^{n-1}}{(n-1)!} \text{ in } \left(\frac{x}{f(x)}\right)^n. \tag{5.1}$$

There is an equivalent form for b_n involving the *exponential Bell polynomials* $B_{n,k}(x_1, x_2, \dots, x_n)$. For a partition of a finite set, we assign x_i as the weight of a block of i elements and define the weight of the partition as the product of the weights of all blocks. Then $B_{n,k}(x_1, x_2, \dots, x_n)$ is defined as the sum of weights of all the partitions of $\{1, 2, \dots, n\}$ with k blocks. An equivalent expression for b_n is as follows [see Comtet (8)]:

$$b_n = \sum_{k=1}^{n-1} \frac{(-1)^k}{a_1^{n+k}} B_{n+k-1,k}(0, a_2, a_3, \dots). \tag{5.2}$$

It is well known that the functional composition of two formal power series can be explained by the convolution of the incidence algebra of the partition lattice. The proof of the Lagrange inversion formula then turns out to be the verification of the following identity (1, 9):

$$\sum_{\{B_1, B_2, \dots, B_k\}} b_{i_1} b_{i_2} \dots b_{i_k} a_k = \delta_{n1}, \tag{5.3}$$

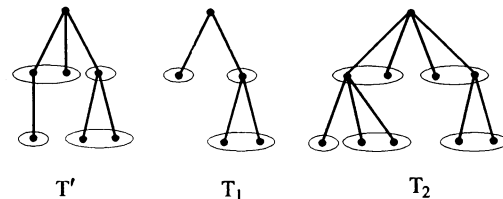
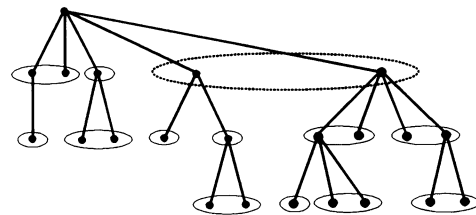
where $\{B_1, B_2, \dots, B_k\}$ runs over all partitions of $\{1, 2, \dots, n\}$ and $i_1 = |B_1|, i_2 = |B_2|, \dots, i_k = |B_k|$. Although there have been several combinatorial proofs of the Lagrange inversion formula, none of them seems to have revealed the combinatorial nature of the cancellation in the above identity. Re-

cently a combinatorial explanation of such cancellation was obtained by Haiman and Schmitt (10) by using a bijection between semilabeled trees and partitions. This bijection was also discovered independently by Erdős and Székely (11). Rota predicted that an ultimately satisfactory combinatorial interpretation should exist (personal communication). It turned out that the cancellation for the Lagrange inversion corresponds to a sign change in constructing a Schröder tree from several smaller Schröder trees. In other words, we obtain an involution on the set of rooted forests of Schröder trees on more than one vertex; here a rooted forest means a forest with a distinguished tree.

THEOREM 5.1. *There is a bijection between Schröder trees on n ($n > 1$) vertices and rooted forests on n vertices with at least two Schröder trees.*

Proof: Let T be a Schröder tree on n vertices. Since $n > 1$, we may assume that $\{v_1, v_2, \dots, v_k\}$ is the last block in the fiber of the root of T . Let T_i be the subtree of T with root v_i for all i and T' be the subtree of T by removing all T_i s from T . Thus, we obtain a forest of Schröder trees on n vertices with T' as the distinguished tree. Clearly, the above construction is reversible. \square

The bijection in the above proof is illustrated below:



For a Schröder tree T with more than one vertex, we shall call the last block in the fiber of the root the *critical block* of T . To express the Lagrange inversion formula in terms of Schröder trees, we need to define the weight of a Schröder tree T . Suppose d_0, d_1, d_2, \dots is a sequence of indeterminates. The *weight* of the root of T is defined to be $1/d_0$, and the *weight* of any block of k vertices is defined to be $-d_k/d_0^{k+1}$; the *weight* of T is then defined to be the product of weights of the root and all blocks, denoted by $w(T)$. For example, the Schröder tree in Example 2.3 has weight $-d_2^2 d_3^2 / d_0^{21}$. Let W_n be the sum of weights of all Schröder trees on n vertices. Clearly, $W_1 = 1/d_0$.

Let T be a Schröder tree on more than one vertex and $B = \{v_1, v_2, \dots, v_{k-1}\}$ be its critical block, and $T', T_1, T_2, \dots, T_{k-1}$ be the decomposition of T into a rooted forest of k Schröder trees as in Theorem 5.1. Since the weight of the block B in T is $-d_{k-1}/d_0^k$ and the weight of any root of T_i is $1/d_0$, it follows that

$$w(T)d_0 = -w(T')w(T_1) \dots w(T_{k-1})d_{k-1}.$$

Thus, we have

$$W_n d_0 = - \sum_{\{B_1, B_2, \dots, B_k\}} W_{i_1} W_{i_2} \dots W_{i_k} k d_{k-1},$$

where $\{B_1, B_2, \dots, B_k\}$ runs over all partitions on $\{1, 2, \dots, n\}$ with more than one block, and $i_1 = |B_1|, \dots, i_k = |B_k|$. The factor k in the above identity comes from the number of ways to distinguish a tree in a forest of k trees. Now set $a_k = kd_{k-1}$, or define the weight of the root of a Schröder tree as $1/a_1$ and the weight of any block of $k - 1$ vertices as $-a_k/(ka_k^2)$. By comparing the above identity and Eq. 5.3, we obtain

THEOREM 5.2. For the above formal power series $f(x)$, its compositional inverse $g(x)$ is given by

$$b_n = \sum_T w(T),$$

where T runs over all Schröder trees on n vertices.

The Lagrange inversion formula in the form of Eq. 5.2 immediately follows from the above theorem and the bijection between Schröder trees and forests of small trees. To prove Eq. 5.1, we need the following formula for the coefficient c_n in the formal power series $h(x) = \sum_{n \geq 0} c_n x^n / n! = (\sum_{n \geq 0} d_n x^n / n!)^{-1}$. It can be proved combinatorially or by using the antipode formula of Schmitt (12) that

$$c_n = \sum_{(B_1, B_2, \dots, B_k)} \frac{(-1)^k}{d_0^{k+1}} d_{i_1} d_{i_2} \cdots d_{i_k},$$

where (B_1, B_2, \dots, B_k) runs over all ordered partitions of $\{1, 2, \dots, n\}$. The above expression of c_n suggests another definition of the weight $w'(T)$ of a Schröder tree T : for a fiber with ordered partition (B_1, B_2, \dots, B_k) , its weight is defined by $(-1)^k d_{i_1} d_{i_2} \cdots d_{i_k} / d_0^{k+1}$, while the weight of a leaf is set to $1/d_0$, and the weight $w'(T)$ is defined as the product of weights of all fibers and leaves. It can be easily seen that this definition of weight is essentially the same as the definition

given before, and these two definitions coincide if we assume $a_1 = 1$. Therefore, the Lagrange inversion in the form of Eq. 5.1 follows from the combinatorial interpretation of Corollary 4.7.

This paper is dedicated to S. S. Chern. It formed part of the author's doctoral thesis, written under the direction of Prof. Gian-Carlo Rota. The author is deeply indebted to Prof. Rota for his inspiring guidance and generous help. Thanks are also due to Prof. Richard Stanley for helpful discussions and to the referees for their valuable suggestions.

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