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Total positivity of some polynomial matrices that enumerate labeled trees and forests II. Rooted labeled trees and partial functional digraphs



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APPLIED MATHEMATICS

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ABSTRACT

We study three combinatorial models for the lower-triangular matrix with entries $t_{n,k} = \binom{n}{k}n^{n-k}$: two involving rooted trees on the vertex set [n + 1], and one involving partial functional digraphs on the vertex set [n]. We show that this matrix is totally positive and that the sequence of its row-generating polynomials is coefficientwise Hankel-totally positive. We then generalize to polynomials $t_{n,k}(y,z)$ that count improper and proper edges, and further to polynomials $t_{n,k}(y,\phi)$ in infinitely many indeterminates that give a weight y to each improper edge and a weight $m! \phi_m$ for each vertex with m proper children. We show that if the weight sequence ϕ is Toeplitz-totally positive, then the two foregoing totalpositivity results continue to hold. Our proofs use production matrices and exponential Riordan arrays.

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Exponential Riordan array Production matrix Toeplitz matrix Hankel matrix Totally positive matrix Total positivity Toeplitz-total positivity Hankel-total positivity Stieltjes moment problem

1. Introduction and statement of results

It is well known [31,45] that the number of rooted trees on the vertex set $[n + 1] \stackrel{\text{def}}{=} \{1, \ldots, n+1\}$ is $t_n = (n+1)^n$; and it is also known (though perhaps less well so) [5,6,42] that the number of rooted trees on the vertex set [n + 1] in which exactly k children of the root are lower-numbered than the root is

$$t_{n,k} = \binom{n}{k} n^{n-k} . aga{1.1}$$

The first few $t_{n,k}$ and t_n are

$n \setminus k$	0	1	2	3	4	5	6	7	8	$(n+1)^n$
0	1									1
1	1	1								2
2	4	4	1							9
3	27	27	9	1						64
4	256	256	96	16	1					625
5	3125	3125	1250	250	25	1				7776
6	46656	46656	19440	4320	540	36	1			117649
7	823543	823543	352947	84035	12005	1029	49	1		2097152
8	16777216	16777216	7340032	1835008	286720	28672	1792	64	1	43046721

[32, A071207 and A000169].

There is a second combinatorial interpretation of the numbers $t_{n,k}$, also in terms of rooted trees: namely, $t_{n,k}$ is the number of rooted trees on the vertex set [n+1] in which some specified vertex *i* has *k* children.¹

The second proof was found independently by Ira Gessel (private communication).

 $^{^{1}\,}$ This fact ought to be well known, but to our surprise we have been unable to find any published reference. Let us therefore give two proofs:

First proof. Let \mathcal{T}_n^{\bullet} denote the set of rooted trees on the vertex set [n], and let deg_T(i) denote the number of children of the vertex i in the rooted tree T. Rooted trees $T \in \mathcal{T}_{n+1}^{\bullet}$ are associated bijectively to Prüfer sequences $(s_1, \ldots, s_n) \in [n+1]^n$, in which each index $i \in [n+1]$ appears deg_T(i) times [45, pp. 25–26]. There are $\binom{n}{k}n^{n-k}$ sequences in which the index i appears exactly k times. Second proof. There are $f_{n,k} = \binom{n}{k}kn^{n-k-1}k$ -component forests of rooted trees on n labeled vertices (see the references cited in [43, footnote 1]). By adding a new vertex 0 and connecting it to the roots of

Second proof. There are $f_{n,k} = {n \choose k} k n^{n-k-1} k$ -component forests of rooted trees on n labeled vertices (see the references cited in [43, footnote 1]). By adding a new vertex 0 and connecting it to the roots of all the trees, we see that $f_{n,k}$ is also the number of unrooted trees on n+1 labeled vertices in which some specified vertex (here vertex 0) has degree k. Now choose a root: if this root is 0, then vertex 0 has k - 1 children. It follows that the number of rooted trees on n+1 labeled vertices on n+1 labeled vertices in which some specified vertex 0 has k - 1 children. It follows that the number of rooted trees on n+1 labeled vertices in which some specified vertex has k children is $f_{n,k} + nf_{n,k+1} = {n \choose k} n^{n-k}$.

And finally, there is a third combinatorial interpretation of the numbers $t_{n,k}$ [10] that is even simpler than the preceding two. Recall first that a *functional digraph* is a directed graph in which every vertex has out-degree 1; the terminology comes from the fact that such digraphs are in obvious bijection with functions f from the vertex set to itself [namely, ij is an edge if and only if f(i) = j]. Let us now define a **partial functional digraph** to be a directed graph in which every vertex has out-degree 0 or 1; and let us write **PFD**_{n,k} for the set of partial functional digraphs on the vertex set [n] in which exactly k vertices have out-degree 0. (So **PFD**_{n,0} is the set of functional digraphs.) A digraph in **PFD**_{n,k} has n - k edges. It is easy to see that $|\mathbf{PFD}_{n,k}| = t_{n,k}$: there are $\binom{n}{k}$ choices for the out-degree-0 vertices, and n^{n-k} choices for the edges emanating from the remaining vertices.

We will use all three combinatorial models at various points in this paper.

The unit-lower-triangular matrix $(t_{n,k})_{n,k\geq 0}$ has the exponential generating function

$$\sum_{n=0}^{\infty} \sum_{k=0}^{n} t_{n,k} \frac{t^n}{n!} x^k = \frac{e^{xT(t)}}{1 - T(t)}$$
(1.2)

where

$$T(t) \stackrel{\text{def}}{=} \sum_{n=1}^{\infty} n^{n-1} \frac{t^n}{n!}$$
(1.3)

is the tree function [9].² An equivalent statement is that the unit-lower-triangular matrix $(t_{n,k})_{n,k\geq 0}$ is the exponential Riordan array [1,11,13,38] $\mathcal{R}[F,G]$ with $F(t) = \sum_{n=0}^{\infty} n^n t^n / n! = 1/[1 - T(t)]$ and G(t) = T(t); we will discuss this connection in Section 4.1.

The principal purpose of this paper is to prove the total positivity of some matrices related to (and generalizing) t_n and $t_{n,k}$. Recall first that a finite or infinite matrix of real numbers is called *totally positive* (TP) if all its minors are nonnegative, and *strictly totally positive* (STP) if all its minors are strictly positive.³ Background information on totally positive matrices can be found in [16,18,26,34]; they have applications to many areas of pure and applied mathematics. See [43, footnote 4] for many references.

Our first result is the following:

Theorem 1.1.

(a) The unit-lower-triangular matrix $T = (t_{n,k})_{n,k\geq 0}$ is totally positive.

² In the analysis literature, expressions involving the tree function are often written in terms of the Lambert W function W(t) = -T(-t), which is the inverse function to $w \mapsto we^w$ [9,25].

³ Warning: Many authors (e.g. [16-19]) use the terms "totally nonnegative" and "totally positive" for what we have termed "totally positive" and "strictly totally positive", respectively. So it is very important, when seeing any claim about "totally positive" matrices, to ascertain which sense of "totally positive" is being used! (This is especially important because many theorems in this subject require *strict* total positivity for their validity.) We follow the terminology of Karlin [26] and Pinkus [34].

(b) The Hankel matrix $H_{\infty}(\mathbf{t}^{(0)}) = (t_{n+n',0})_{n,n'\geq 0}$ is totally positive.

It is known [19,34] that a Hankel matrix of real numbers is totally positive if and only if the underlying sequence is a Stieltjes moment sequence, i.e. the moments of a positive measure on $[0, \infty)$. And it is also known that $(n^n)_{n\geq 0}$ is a Stieltjes moment sequence.⁴ So Theorem 1.1(b) is equivalent to this known result. But our proof here is combinatorial and linear-algebraic, not analytic.

However, this is only the beginning of the story, because our main interest [40,41,44] is not with sequences and matrices of real numbers, but rather with sequences and matrices of *polynomials* (with integer or real coefficients) in one or more indeterminates \mathbf{x} : in applications they will typically be generating polynomials that enumerate some combinatorial objects with respect to one or more statistics. We equip the polynomial ring $\mathbb{R}[\mathbf{x}]$ with the coefficientwise partial order: that is, we say that P is nonnegative (and write $P \succeq 0$) in case P is a polynomial with nonnegative coefficients. We then say that a matrix with entries in $\mathbb{R}[\mathbf{x}]$ is **coefficientwise totally positive** if all its minors are polynomials with nonnegative coefficients; and we say that a sequence $\mathbf{a} = (a_n)_{n\geq 0}$ with entries in $\mathbb{R}[\mathbf{x}]$ is **coefficientwise Hankel-totally positive** if its associated infinite Hankel matrix $H_{\infty}(\mathbf{a}) = (a_{n+n'})_{n,n'\geq 0}$ is coefficientwise totally positive.

Returning now to the matrix $T = (t_{n,k})_{n,k\geq 0}$, let us define its **row-generating poly**nomials in the usual way:

$$T_n(x) = \sum_{k=0}^n t_{n,k} x^k .$$
 (1.4)

From the definition (1.1) we obtain the explicit formula

$$T_n(x) = (x+n)^n . (1.5)$$

Our second result is then:

Theorem 1.2. The polynomial sequence $\mathbf{T} = (T_n(x))_{n \ge 0}$ is coefficientwise Hankel-totally positive.

$$\frac{n^n}{n!} = \frac{1}{\pi} \int_0^{\pi} \left(\frac{\sin\nu}{\nu} e^{\nu \cot\nu} \right)^n d\nu$$

⁴ The integral representation [3] [25, Corollary 2.4]

shows that $n^n/n!$ is a Stieltjes moment sequence. Moreover, $n! = \int_0^\infty x^n e^{-x} dx$ is a Stieltjes moment sequence. Since the entrywise product of two Stieltjes moment sequences is easily seen to be a Stieltjes moment sequence, it follows that n^n is a Stieltjes moment sequence. But we do not know any simple formula (i.e. one involving only a single integral over a real variable) for its Stieltjes integral representation.

Theorem 1.2 strengthens Theorem 1.1(b), and reduces to it when x = 0. The proof of Theorem 1.2 will be based on studying the **binomial row-generating matrix** $\mathsf{T}B_x$, where B_x is the weighted binomial matrix

$$(B_x)_{ij} = \binom{i}{j} x^{i-j} . aga{1.6}$$

The important fact is that, for any matrix A, the zeroth column of the binomial rowgenerating matrix AB_x consists of the row-generating polynomials of A.

But this is not the end of the story, because we want to generalize these polynomials by adding further variables. Given a rooted tree T and two vertices i, j of T, we say that j is a *descendant* of i if the unique path from the root of T to j passes through i. (Note in particular that every vertex is a descendant of itself.) Now suppose that the vertex set of T is totally ordered (for us it will be [n + 1]), and let e = ij be an edge of T, ordered so that j is a descendant of i. We say that the edge e = ij is **improper** if there exists a descendant of j (possibly j itself) that is lower-numbered than i; otherwise we say that e = ij is **proper**. We denote by imprope(T) [resp. prope(T)] the number of improper (resp. proper) edges in the tree T.

We now introduce these statistics into our second combinatorial model. Let $\mathcal{T}_n^{\langle i;k\rangle}$ denote the set of rooted trees on the vertex set [n] in which the vertex *i* has *k* children. For the identity $|\mathcal{T}_{n+1}^{\langle i;k\rangle}| = t_{n,k}$, we can use any $i \in [n+1]$; but for the following we specifically want to take i = 1. With this choice we observe that the *k* edges from the vertex 1 to its children are automatically proper. We therefore define

$$t_{n,k}(y,z) = \sum_{T \in \mathcal{T}_{n+1}^{\langle 1;k \rangle}} y^{\operatorname{imprope}(T)} z^{\operatorname{prope}(T)-k} .$$
(1.7)

Clearly $t_{n,k}(y,z)$ is a homogeneous polynomial of degree n-k with nonnegative integer coefficients; it is a polynomial refinement of $t_{n,k}$ in the sense that $t_{n,k}(1,1) = t_{n,k}$. (Of course, it was redundant to introduce the two variables y and z instead of just one of them; we did it because it makes the formulae more symmetric.) The first few polynomials $t_{n,k}(y,1)$ are

$n \setminus k$	0	1	2	3	4
0	1				
1	y	1			
2	$y + 3y^2$ 2y + 10y ² + 15y ³	1 + 3y	1		
3	$2y + 10y^2 + 15y^3$	$2 + 10y + 15y^2$	3 + 6y	1	
4	$6y + 40y^2 + 105y^3 + 105y^4$	$6 + 40y + 105y^2 + 105y^3$	$11 + 40y + 45y^2$	6 + 10y	1

The coefficient matrix of the zeroth-column polynomials $t_{n,0}(y,1)$ is [32, A239098/A075856]. This table also suggests the following result, for which we will give a bijective proof:

Proposition 1.3. For $n \ge 1$, $t_{n,0}(y, z) = y t_{n,1}(y, z)$.

In Section 4.2 we will show that the unit-lower-triangular matrix $\mathsf{T}(y, z) = (t_{n,k}(y, z))_{n,k\geq 0}$ is an exponential Riordan array $\mathcal{R}[F, G]$, and we will compute F(t) and G(t).

We now generalize (1.4) by defining the row-generating polynomials

$$T_n(x, y, z) = \sum_{k=0}^n t_{n,k}(y, z) x^k$$
(1.8)

or in other words

$$T_n(x, y, z) = \sum_{T \in \mathcal{T}_{n+1}^{\bullet}} x^{\deg_T(1)} y^{\operatorname{imprope}(T)} z^{\operatorname{prope}(T) - \deg_T(1)}$$
(1.9)

where $\deg_T(1)$ is the number of children of the vertex 1 in the rooted tree T. Note that $T_n(x, y, z)$ is a homogeneous polynomial of degree n in x, y, z, with nonnegative integer coefficients; it reduces to $T_n(x)$ when y = z = 1. Our third result is then:

Theorem 1.4.

- (a) The unit-lower-triangular polynomial matrix $\mathsf{T}(y, z) = (t_{n,k}(y, z))_{n,k\geq 0}$ is coefficientwise totally positive (jointly in y, z).
- (b) The polynomial sequence $\mathbf{T} = (T_n(x, y, z))_{n \ge 0}$ is coefficientwise Hankel-totally positive (jointly in x, y, z).

Theorem 1.4 strengthens Theorems 1.1(a) and 1.2, and reduces to them when y = z = 1. The proof of Theorem 1.4(b) will be based on studying the binomial row-generating matrix $T(y, z)B_x$, using the representation of T(y, z) as an exponential Riordan array.

Finally, let us consider our third combinatorial model, which is based on partial functional digraphs. Recall that a *functional digraph* (resp. *partial functional digraph*) is a directed graph in which every vertex has out-degree 1 (resp. 0 or 1). Each weakly connected component of a functional digraph consists of a directed cycle (possibly of length 1, i.e. a loop) together with a collection of (possibly trivial) directed trees rooted at the vertices of the cycle (with edges pointing towards the root). The weakly connected components of a partial functional digraph are trees rooted at the out-degree-0 vertices (with edges pointing towards the root) together with components of the same form as in a functional digraph. We say that a vertex of a partial functional digraph is **recurrent** (or **cyclic**) if it lies on one of the cycles; otherwise we call it **transient** (or **acyclic**). If *j* and *k* are vertices of a digraph, we say that *k* is a **predecessor** of *j* if there exists a directed path from k to j (in particular, every vertex is a predecessor of itself).⁵ Note that "predecessor" in a digraph generalizes the notion of "descendant" in a rooted tree, if we make the convention that all edges in the tree are oriented towards the root. Indeed, if j is a transient vertex in a partial functional digraph, then the predecessors of j are precisely the descendants of j in the rooted tree (rooted at either a recurrent vertex or an out-degree-0 vertex) to which j belongs. On the other hand, if j is a recurrent vertex, then the predecessors of j are all the vertices in the weakly connected component containing j.

Now consider a partial functional digraph on a totally ordered vertex set (which for us will be [n]). We say that an edge \overrightarrow{ji} (pointing from j to i) is **improper** if there exists a predecessor of j (possibly j itself) that is $\leq i$; otherwise we say that the edge \overrightarrow{ji} is **proper**. When j is a transient vertex, this coincides with the notion of improper/proper edge in a rooted tree. When j is a recurrent vertex, the edge \overrightarrow{ji} is always improper, because one of the predecessors of j is i. (This includes the case i = j: a loop is always an improper edge.) We denote by imprope(G) [resp. prope(G)] the number of improper (resp. proper) edges in the partial functional digraph G. We then define the generating polynomial

$$\widetilde{t}_{n,k}(y,z) = \sum_{G \in \mathbf{PFD}_{n,k}} y^{\mathrm{imprope}(G)} z^{\mathrm{prope}(G)} .$$
(1.10)

Since $G \in \mathbf{PFD}_{n,k}$ has n-k edges, $\tilde{t}_{n,k}(y,z)$ is a homogeneous polynomial of degree n-k with nonnegative integer coefficients. By bijection between our second and third combinatorial models, we will prove:

Proposition 1.5. $t_{n,k}(y,z) = \tilde{t}_{n,k}(y,z).$

The row-generating polynomials (1.8)/(1.9) thus have the alternate combinatorial interpretation

$$T_n(x, y, z) = \sum_{G \in \mathbf{PFD}_n} x^{\deg 0(G)} y^{\operatorname{imprope}(G)} z^{\operatorname{prope}(G)}$$
(1.11)

where $\deg 0(G)$ is the number of out-degree-0 vertices in G.

We also have an interpretation of the polynomials $t_{n,k}(y,z)$ in our first combinatorial model (rooted trees in which the root has k lower-numbered children); but since this interpretation is rather complicated, we refer the reader to the Appendix of arXiv:2302.03999v1.

But this is *still* not the end of the story, because we can add even more variables into our second combinatorial model — in fact, an infinite set. Given a rooted tree T on a

⁵ In a functional digraph, Dumont and Ramamonjisoa [15, p. 11] use the term "ascendance", and the notation A(j), to denote the set of all predecessors of j.

totally ordered vertex set and vertices $i, j \in T$ such that j is a child of i, we say that j is a **proper child** of i if the edge e = ij is proper (that is, j and all its descendants are higher-numbered than i). Now let $\phi = (\phi_m)_{m\geq 0}$ be indeterminates, and let $t_{n,k}(y,\phi)$ be the generating polynomial for rooted trees $T \in \mathcal{T}_{n+1}^{\langle 1;k \rangle}$ with a weight y for each improper edge and a weight $\hat{\phi}_m \stackrel{\text{def}}{=} m! \phi_m$ for each vertex $i \neq 1$ that has m proper children:

$$t_{n,k}(y,\phi) = \sum_{T \in \mathcal{T}_{n+1}^{(1;k)}} y^{\operatorname{imprope}(T)} \prod_{i=2}^{n+1} \widehat{\phi}_{\operatorname{pdeg}_T(i)}$$
(1.12)

where $\operatorname{pdeg}_{T}(i)$ denotes the number of *proper* children of the vertex *i* in the rooted tree *T*. We will see later why it is convenient to introduce the factors *m*! in this definition. Observe also that the variables *z* are now redundant and therefore omitted, because they would simply scale $\phi_m \to z^m \phi_m$. And note finally that, in conformity with (1.7), we have chosen to suppress the weight $\hat{\phi}_k$ that would otherwise be associated to the vertex 1. We call the polynomials $t_{n,k}(y,\phi)$ the **generic rooted-tree polynomials**, and the lower-triangular matrix $\mathsf{T}(y,\phi) = (t_{n,k}(y,\phi))_{n,k\geq 0}$ the **generic rooted-tree matrix**. Here $\phi = (\phi_m)_{m\geq 0}$ are in the first instance indeterminates, so that $t_{n,k}(y,\phi)$ belongs to the polynomial ring $\mathbb{Z}[y,\phi]$; but we can then, if we wish, substitute specific values for ϕ in any commutative ring *R*, leading to values $t_{n,k}(y,\phi) \in R[y]$. (Similar substitutions can of course also be made for *y*.) When doing this we will use the same notation $t_{n,k}(y,\phi)$, as the desired interpretation for ϕ should be clear from the context. The polynomial $t_{n,k}(y,\phi)$ is homogeneous of degree *n* in ϕ ; it is also quasi-homogeneous of degree n - k in *y* and ϕ when ϕ_m is assigned weight *m* and *y* is assigned weight 1. By specializing $t_{n,k}(y,\phi)$ to $\phi_m = z^m/m!$ and hence $\hat{\phi}_m = z^m$, we recover $t_{n,k}(y,z)$.

We remark that the matrix $\mathsf{T}(y, \phi)$, unlike $\mathsf{T}(y, z)$, is not *unit*-lower-triangular: rather, it has diagonal entries $t_{n,n}(y, \phi) = \phi_0^n$, corresponding to the tree in which 1 is the root and has all the vertices $2, \ldots, n+1$ as children. More generally, the polynomial $t_{n,k}(y, \phi)$ is divisible by ϕ_0^k , since the vertex 1 always has at least k leaf descendants. So we could define a unit-lower-triangular matrix $\mathsf{T}^\flat(y, \phi) = (t_{n,k}^\flat(y, \phi))_{n,k\geq 0}$ by $t_{n,k}^\flat(y, \phi) =$ $t_{n,k}(y, \phi)/\phi_0^k$. (Alternatively, we could simply choose to normalize to $\phi_0 = 1$.)

In Section 4.3 we will show that $\mathsf{T}(y, \phi)$ is an exponential Riordan array $\mathcal{R}[F, G]$, and we will compute F(t) and G(t).

Also, generalizing Proposition 1.3, we will prove:

Proposition 1.6. For $n \ge 1$, $t_{n,0}(y, \phi) = y t_{n,1}(y, \phi)$.

We can also define the corresponding polynomials $\tilde{t}_{n,k}(y, \phi)$ in the partial-functionaldigraph model, as follows: If G is a partial functional digraph on a totally ordered vertex set, and *i* is a vertex of G, we define the **proper in-degree** of *i*, $\operatorname{pindeg}_G(i)$, to be the number of proper edges \overrightarrow{ji} in G. We then define X. Chen, A.D. Sokal / Advances in Applied Mathematics 157 (2024) 102703

$$\widetilde{t}_{n,k}(y,\phi) = \sum_{G \in \mathbf{PFD}_{n,k}} y^{\mathrm{imprope}(G)} \prod_{i=1}^{n} \widehat{\phi}_{\mathrm{pindeg}_{G}(i)} .$$
(1.13)

Then, generalizing Proposition 1.5, we will prove:

Proposition 1.7. $t_{n,k}(y, \phi) = \tilde{t}_{n,k}(y, \phi).$

Now define the row-generating polynomials

$$T_n(x, y, \phi) = \sum_{k=0}^n t_{n,k}(y, \phi) x^k$$
(1.14)

or in other words

$$T_n(x, y, \phi) = \sum_{T \in \mathcal{T}_{n+1}^{\bullet}} x^{\deg_T(1)} y^{\operatorname{imprope}(T)} \prod_{i=2}^{n+1} \widehat{\phi}_{\operatorname{pdeg}_T(i)} .$$
(1.15)

The main result of this paper is then the following:

Theorem 1.8. Fix $1 \le r \le \infty$. Let R be a partially ordered commutative ring, and let $\phi = (\phi_m)_{m \ge 0}$ be a sequence in R that is Toeplitz-totally positive of order r. Then:

- (a) The lower-triangular polynomial matrix $\mathsf{T}(y, \phi) = (t_{n,k}(y, \phi))_{n,k\geq 0}$ is coefficientwise totally positive of order r (in y).
- (b) The polynomial sequence $\mathbf{T} = (T_n(x, y, \phi))_{n \ge 0}$ is coefficientwise Hankel-totally positive of order r (jointly in x, y).

(The concept of Toeplitz-total positivity in a partially ordered commutative ring will be explained in detail in Section 2.1. Total positivity of order r means that the minors of size $\leq r$ are nonnegative.) Specializing Theorem 1.8 to $r = \infty$, $R = \mathbb{Q}$ and $\phi_m = z^m/m!$ (which is indeed Toeplitz-totally positive: see (2.1) below), we recover Theorem 1.4. The method of proof of Theorem 1.8 will, in fact, be the same as that of Theorem 1.4, suitably generalized.

We now give an overview of the contents of this paper. The main tool in our proofs will be the theory of production matrices [12,13] as applied to total positivity [44], combined with the theory of exponential Riordan arrays [1,11,13,38]. Therefore, in Section 2 we review some facts about total positivity, production matrices and exponential Riordan arrays that will play a central role in our arguments. This development culminates in Corollary 2.18; it is the fundamental theoretical result that underlies all our proofs. In Section 3 we give bijective proofs of Propositions 1.3, 1.5, 1.6 and 1.7. In Section 4 we show that the matrices T , $\mathsf{T}(y, z)$ and $\mathsf{T}(y, \phi)$ are exponential Riordan arrays $\mathcal{R}[F, G]$, and we compute their generating functions F and G. In Section 5 we combine the results of Sections 2 and 4 to complete the proofs of Theorems 1.1, 1.2, 1.4 and 1.8. This paper is a sequel to our paper [43] on the total positivity of matrices that enumerate forests of rooted labeled trees. The methods here are basically the same as in this previous paper, but generalized nontrivially to handle exponential Riordan arrays $\mathcal{R}[F,G]$ with $F \neq 1$. Zhu [47,48] has employed closely related methods. See also Gilmore [21] for some total-positivity results for q-generalizations of tree and forest matrices, using very different methods.

A fuller version of the present paper can be found at arXiv:2302.03999v1: it contains proofs of some known results, which were included there to make the paper self-contained but which are omitted here to save space; it contains alternate proofs of Propositions 4.1 and 5.4; and it also contains an Appendix providing an interpretation of the polynomials $t_{n,k}(y, z)$ in our first combinatorial model.

2. Preliminaries

Here we review some definitions and results from [33,43,44] that will be needed in the sequel. We also include a brief review of exponential Riordan arrays [1,11,13,38] and Lagrange inversion [20]. Omitted proofs can be found in [43] and at arXiv:2302.03999v1.

The treatment of exponential Riordan arrays in Section 2.4 contains one novelty: namely, the rewriting of the production matrix in terms of new series Φ and Ψ (see (2.14) ff. and Proposition 2.14). This is the key step that leads to Corollary 2.18.

2.1. Partially ordered commutative rings and total positivity

In this paper all rings will be assumed to have an identity element 1 and to be nontrivial $(1 \neq 0)$.

A partially ordered commutative ring is a pair (R, \mathcal{P}) where R is a commutative ring and \mathcal{P} is a subset of R satisfying

(a) $0, 1 \in \mathcal{P}$.

- (b) If $a, b \in \mathcal{P}$, then $a + b \in \mathcal{P}$ and $ab \in \mathcal{P}$.
- (c) $\mathcal{P} \cap (-\mathcal{P}) = \{0\}.$

We call \mathcal{P} the *nonnegative elements* of R, and we define a partial order on R (compatible with the ring structure) by writing $a \leq b$ as a synonym for $b - a \in \mathcal{P}$. Please note that, unlike the practice in real algebraic geometry [4,28,30,35], we do *not* assume here that squares are nonnegative; indeed, this property fails completely for our prototypical example, the ring of polynomials with the coefficientwise order, since $(1-x)^2 = 1 - 2x + x^2 \succeq 0$.

Now let (R, \mathcal{P}) be a partially ordered commutative ring and let $\mathbf{x} = \{x_i\}_{i \in I}$ be a collection of indeterminates. In the polynomial ring $R[\mathbf{x}]$ and the formal-power-series ring $R[[\mathbf{x}]]$, let $\mathcal{P}[\mathbf{x}]$ and $\mathcal{P}[[\mathbf{x}]]$ be the subsets consisting of polynomials (resp. series)

with nonnegative coefficients. Then $(R[\mathbf{x}], \mathcal{P}[\mathbf{x}])$ and $(R[[\mathbf{x}]], \mathcal{P}[[\mathbf{x}]])$ are partially ordered commutative rings; we refer to this as the **coefficientwise order** on $R[\mathbf{x}]$ and $R[[\mathbf{x}]]$.

A (finite or infinite) matrix with entries in a partially ordered commutative ring is called **totally positive** (TP) if all its minors are nonnegative; it is called **totally positive** of order r (TP_r) if all its minors of size $\leq r$ are nonnegative. It follows immediately from the Cauchy–Binet formula that the product of two TP (resp. TP_r) matrices is TP (resp. TP_r).⁶ This fact is so fundamental to the theory of total positivity that we shall henceforth use it without comment.

We say that a sequence $\mathbf{a} = (a_n)_{n\geq 0}$ with entries in a partially ordered commutative ring is **Hankel-totally positive** (resp. **Hankel-totally positive of order** \mathbf{r}) if its associated infinite Hankel matrix $H_{\infty}(\mathbf{a}) = (a_{i+j})_{i,j\geq 0}$ is TP (resp. TP_r). We say that \mathbf{a} is **Toeplitz-totally positive** (resp. **Toeplitz-totally positive of order** \mathbf{r}) if its associated infinite Toeplitz matrix $T_{\infty}(\mathbf{a}) = (a_{i-j})_{i,j\geq 0}$ (where $a_n \stackrel{\text{def}}{=} 0$ for n < 0) is TP (resp. TP_r).⁷

When $R = \mathbb{R}$, Hankel- and Toeplitz-total positivity have simple analytic characterizations. A sequence $(a_n)_{n\geq 0}$ of real numbers is Hankel-totally positive if and only if it is a Stieltjes moment sequence [19, Théorème 9] [34, section 4.6]. And a sequence $(a_n)_{n\geq 0}$ of real numbers is Toeplitz-totally positive if and only if its ordinary generating function can be written as

$$\sum_{n=0}^{\infty} a_n t^n = C e^{\gamma t} t^m \prod_{i=1}^{\infty} \frac{1+\alpha_i t}{1-\beta_i t}$$

$$(2.1)$$

with $m \in \mathbb{N}$, $C, \gamma, \alpha_i, \beta_i \geq 0$, $\sum \alpha_i < \infty$ and $\sum \beta_i < \infty$: this is the celebrated Aissen–Schoenberg–Whitney–Edrei theorem [26, Theorem 5.3, p. 412]. However, in a general partially ordered commutative ring R, the concepts of Hankel- and Toeplitz-total positivity are more subtle.

We will need a few easy facts about the total positivity of special matrices:

Lemma 2.1 (Bidiagonal matrices). Let A be a matrix with entries in a partially ordered commutative ring, with the property that all its nonzero entries belong to two consecutive diagonals. Then A is totally positive if and only if all its entries are nonnegative.

Lemma 2.2 (Toeplitz matrix of powers). Let R be a partially ordered commutative ring, let $x \in R$, and consider the infinite Toeplitz matrix

 $^{^{6}}$ For infinite matrices, we need some condition to ensure that the product is well-defined. For instance, the product AB is well-defined whenever A is row-finite (i.e. has only finitely many nonzero entries in each row) or B is column-finite.

⁷ When $R = \mathbb{R}$, Toeplitz-totally positive sequences are traditionally called *Pólya frequency sequences* (PF), and Toeplitz-totally positive sequences of order r are called *Pólya frequency sequences of order* r (PF_r). See [26, chapter 8] for a detailed treatment.

$$T_x \stackrel{\text{def}}{=} T_{\infty}(x^{\mathbb{N}}) = \begin{bmatrix} 1 & & & \\ x & 1 & & \\ x^2 & x & 1 & \\ x^3 & x^2 & x & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} .$$
(2.2)

Then every minor of T_x is either zero or else a power of x. Hence T_x is $TP \iff T_x$ is $TP_1 \iff x \ge 0$.

In particular, if x is an indeterminate, then T_x is totally positive in the ring $\mathbb{Z}[x]$ equipped with the coefficientwise order.

Lemma 2.3 (Binomial matrix). In the ring \mathbb{Z} , the binomial matrix $B = \binom{n}{k}_{n,k\geq 0}$ is totally positive. More generally, the weighted binomial matrix $B_{x,y} = (x^{n-k}y^k \binom{n}{k})_{n,k\geq 0}$ is totally positive in the ring $\mathbb{Z}[x,y]$ equipped with the coefficientwise order.

Finally, let us observe that the sufficiency half of the Aissen–Schoenberg–Whitney– Edrei theorem holds (with a slight modification to avoid infinite products) in a general partially ordered commutative ring. We give two versions, depending on whether or not it is assumed that the ring R contains the rationals:

Lemma 2.4 (Sufficient condition for Toeplitz-total positivity). Let R be a partially ordered commutative ring, let N be a nonnegative integer, and let $\alpha_1, \ldots, \alpha_N, \beta_1, \ldots, \beta_N$ and C be nonnegative elements in R. Define the sequence $\mathbf{a} = (a_n)_{n\geq 0}$ in R by

$$\sum_{n=0}^{\infty} a_n t^n = C \prod_{i=1}^{N} \frac{1 + \alpha_i t}{1 - \beta_i t} .$$
(2.3)

Then the Toeplitz matrix $T_{\infty}(a)$ is totally positive.

Of course, it is no loss of generality to have the same number N of alphas and betas, since some of the α_i or β_i could be zero.

Lemma 2.5 (Sufficient condition for Toeplitz-total positivity, with rationals). Let R be a partially ordered commutative ring containing the rationals, let N be a nonnegative integer, and let $\alpha_1, \ldots, \alpha_N, \beta_1, \ldots, \beta_N, \gamma$ and C be nonnegative elements in R. Define the sequence $\mathbf{a} = (a_n)_{n\geq 0}$ in R by

$$\sum_{n=0}^{\infty} a_n t^n = C e^{\gamma t} \prod_{i=1}^{N} \frac{1+\alpha_i t}{1-\beta_i t} .$$
 (2.4)

Then the Toeplitz matrix $T_{\infty}(\mathbf{a})$ is totally positive.

2.2. Production matrices

Let $P = (p_{ij})_{i,j\geq 0}$ be an infinite matrix with entries in a commutative ring R. In order that powers of P be well-defined, we shall assume that P is either row-finite (i.e. has only finitely many nonzero entries in each row) or column-finite.

Let us now define an infinite matrix $A = (a_{nk})_{n,k\geq 0}$ by

$$a_{nk} = (P^n)_{0k} (2.5)$$

(in particular, $a_{0k} = \delta_{0k}$). Writing out the matrix multiplications explicitly, we have

$$a_{nk} = \sum_{i_1,\dots,i_{n-1}} p_{0i_1} p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_{n-2} i_{n-1}} p_{i_{n-1}k} , \qquad (2.6)$$

so that a_{nk} is the total weight for all *n*-step walks in \mathbb{N} from $i_0 = 0$ to $i_n = k$, in which the weight of a walk is the product of the weights of its steps, and a step from *i* to *j* gets a weight p_{ij} . Yet another equivalent formulation is to define the entries a_{nk} by the recurrence

$$a_{nk} = \sum_{i=0}^{\infty} a_{n-1,i} p_{ik} \quad \text{for } n \ge 1$$
 (2.7)

with the initial condition $a_{0k} = \delta_{0k}$.

We call P the **production matrix** and A the **output matrix**, and we write $A = \mathcal{O}(P)$. Note that if P is row-finite, then so is $\mathcal{O}(P)$; if P is lower-Hessenberg, then $\mathcal{O}(P)$ is lowertriangular; if P is lower-Hessenberg with invertible superdiagonal entries, then $\mathcal{O}(P)$ is lower-triangular with invertible diagonal entries; and if P is unit-lower-Hessenberg (i.e. lower-Hessenberg with entries 1 on the superdiagonal), then $\mathcal{O}(P)$ is unit-lowertriangular. In all the applications in this paper, P will be lower-Hessenberg.

Now let $\Delta = (\delta_{i+1,j})_{i,j\geq 0}$ be the matrix with 1 on the superdiagonal and 0 elsewhere. Then for any matrix M with rows indexed by \mathbb{N} , the product ΔM is simply M with its zeroth row removed and all other rows shifted upwards. (Some authors use the notation $\overline{M} \stackrel{\text{def}}{=} \Delta M$.) The recurrence (2.7) can then be written as

$$\Delta \mathcal{O}(P) = \mathcal{O}(P) P . \tag{2.8}$$

It follows that if A is a row-finite matrix that has a row-finite inverse A^{-1} and has first row $a_{0k} = \delta_{0k}$, then $P = A^{-1}\Delta A$ is the unique matrix such that $A = \mathcal{O}(P)$. This holds, in particular, if A is lower-triangular with invertible diagonal entries and $a_{00} = 1$; then A^{-1} is lower-triangular and $P = A^{-1}\Delta A$ is lower-Hessenberg. And if A is unit-lowertriangular, then $P = A^{-1}\Delta A$ is unit-lower-Hessenberg.

We shall repeatedly use the following easy fact:

Lemma 2.6 (Production matrix of a product). Let $P = (p_{ij})_{i,j\geq 0}$ be a row-finite matrix (with entries in a commutative ring R), with output matrix $A = \mathcal{O}(P)$; and let $B = (b_{ij})_{i,j\geq 0}$ be a lower-triangular matrix with invertible (in R) diagonal entries. Then

$$AB = b_{00} \mathcal{O}(B^{-1}PB) . (2.9)$$

That is, up to a factor b_{00} , the matrix AB has production matrix $B^{-1}PB$.

2.3. Production matrices and total positivity

Let $P = (p_{ij})_{i,j\geq 0}$ be a matrix with entries in a partially ordered commutative ring R. We will use P as a production matrix; let $A = \mathcal{O}(P)$ be the corresponding output matrix. As before, we assume that P is either row-finite or column-finite.

When P is totally positive, it turns out [44] that the output matrix $\mathcal{O}(P)$ has two total-positivity properties: firstly, it is totally positive; and secondly, its zeroth column is Hankel-totally positive. Here we state these results without proof; full proofs, as well as some historical remarks and examples, can be found in [43] and at arXiv:2302.03999v1.

Theorem 2.7 (Total positivity of the output matrix). Let P be an infinite matrix that is either row-finite or column-finite, with entries in a partially ordered commutative ring R. If P is totally positive of order r, then so is A = O(P).

Theorem 2.8 (Hankel-total positivity of the zeroth column). Let $P = (p_{ij})_{i,j\geq 0}$ be an infinite row-finite or column-finite matrix with entries in a partially ordered commutative ring R, and define the infinite Hankel matrix of the zeroth column of the output matrix $\mathcal{O}(P)$: $H_{\infty}(\mathcal{O}_0(P)) = ((P^{n+n'})_{00})_{n,n'\geq 0}$. If P is totally positive of order r, then so is $H_{\infty}(\mathcal{O}_0(P))$.

One might hope that Theorem 2.8 could be strengthened to show not only Hankel-TP of the zeroth column of the output matrix $A = \mathcal{O}(P)$, but in fact Hankel-TP of the row-generating polynomials $A_n(x)$ for all $x \ge 0$ (at least when $R = \mathbb{R}$) — or even more strongly, coefficientwise Hankel-TP of the row-generating polynomials. Alas, this hope is vain, for these properties do not hold *in general*:

Example 2.9 (Failure of Hankel-TP of the row-generating polynomials). Let $P = \mathbf{e}_{00} + \Delta$ be the upper-bidiagonal matrix with 1 on the superdiagonal and $1, 0, 0, 0, \ldots$ on the diagonal; by Lemma 2.1 it is TP. Then $A = \mathcal{O}(P)$ is the lower-triangular matrix will all entries 1, so that $A_n(x) = \sum_{k=0}^n x^k$. Since $A_0(x) A_2(x) - A_1(x)^2 = -x$, the sequence $(A_n(x))_{n\geq 0}$ is not even log-convex (i.e. Hankel-TP₂) for any real number x > 0.

Nevertheless, in one important special case — namely, exponential Riordan arrays $\mathcal{R}[1,G]$ — the total positivity of the production matrix *does* imply the coefficientwise Hankel-TP of the row-generating polynomials of the output matrix: this was shown [43,

Theorem 2.20]. That result will be generalized here, in Corollary 2.18, to provide a more general *sufficient* (but not necessary) condition for the coefficientwise Hankel-TP of the row-generating polynomials of the output matrix.

2.4. Exponential Riordan arrays

Let R be a commutative ring containing the rationals, and let $F(t) = \sum_{n=0}^{\infty} f_n t^n / n!$ and $G(t) = \sum_{n=1}^{\infty} g_n t^n / n!$ be formal power series with coefficients in R; we set $g_0 = 0$. Then the **exponential Riordan array** [1,11,13,38] associated to the pair (F, G) is the infinite lower-triangular matrix $\mathcal{R}[F, G] = (\mathcal{R}[F, G]_{nk})_{n,k\geq 0}$ defined by

$$\mathcal{R}[F,G]_{nk} = \frac{n!}{k!} [t^n] F(t) G(t)^k .$$
(2.10)

That is, the kth column of $\mathcal{R}[F,G]$ has exponential generating function $F(t)G(t)^k/k!$. Equivalently, the bivariate exponential generating function of $\mathcal{R}[F,G]$ is

$$\sum_{n,k=0}^{\infty} \mathcal{R}[F,G]_{nk} \frac{t^n}{n!} x^k = F(t) e^{xG(t)} .$$
(2.11)

The diagonal elements of $\mathcal{R}[F,G]$ are $\mathcal{R}[F,G]_{nn} = f_0 g_1^n$, so the matrix $\mathcal{R}[F,G]$ is invertible in the ring $R_{lt}^{\mathbb{N}\times\mathbb{N}}$ of lower-triangular matrices if and only if f_0 and g_1 are invertible in R.

The following is an easy computation:

Lemma 2.10 (Product of two exponential Riordan arrays). We have

$$\mathcal{R}[F_1, G_1] \mathcal{R}[F_2, G_2] = \mathcal{R}[(F_2 \circ G_1)F_1, G_2 \circ G_1].$$
(2.12)

In particular, if we let $\mathcal{R}[F_2, G_2]$ be the weighted binomial matrix $B_{\xi} = \mathcal{R}[e^{\xi t}, t]$ defined by (1.6), we obtain:

Corollary 2.11 (Binomial row-generating matrix of an exponential Riordan array). We have

$$\mathcal{R}[F,G] B_{\xi} = \mathcal{R}[e^{\xi G}F,G] . \tag{2.13}$$

Similarly, letting $\mathcal{R}[F_1, G_1]$ be the weighted binomial matrix B_{ξ} , we obtain:

Corollary 2.12 (Left binomial transform of an exponential Riordan array). We have

$$B_{\xi} \mathcal{R}[F,G] = \mathcal{R}[e^{\xi t}F,G] . \qquad (2.14)$$

The production matrix of an exponential Riordan array $\mathcal{R}[F,G]$ is as follows: Let $\boldsymbol{a} = (a_n)_{n\geq 0}$ and $\boldsymbol{z} = (z_n)_{n\geq 0}$ be sequences in a commutative ring R, with ordinary generating functions $A(s) = \sum_{n=0}^{\infty} a_n s^n$ and $Z(s) = \sum_{n=0}^{\infty} z_n s^n$. We then define the **exponential AZ matrix** associated to the sequences \boldsymbol{a} and \boldsymbol{z} by

EAZ
$$(\boldsymbol{a}, \boldsymbol{z})_{nk} = \frac{n!}{k!} (z_{n-k} + k a_{n-k+1}),$$
 (2.15)

or equivalently (if R contains the rationals)

$$\operatorname{EAZ}(\boldsymbol{a}, \boldsymbol{z}) = D T_{\infty}(\boldsymbol{z}) D^{-1} + D T_{\infty}(\boldsymbol{a}) D^{-1} \Delta$$
(2.16)

where $D = \text{diag}((n!)_{n>0})$. We also write EAZ(A, Z) as a synonym for EAZ(a, z).

Theorem 2.13 (Production matrices of exponential Riordan arrays). Let L be a lowertriangular matrix (with entries in a commutative ring R containing the rationals) with invertible diagonal entries and $L_{00} = 1$, and let $P = L^{-1}\Delta L$ be its production matrix. Then L is an exponential Riordan array if and only if P is an exponential AZ matrix.

More precisely, $L = \mathcal{R}[F,G]$ if and only if P = EAZ(A,Z), where the generating functions (F(t), G(t)) and (A(s), Z(s)) are connected by

$$G'(t) = A(G(t)), \qquad \frac{F'(t)}{F(t)} = Z(G(t))$$
 (2.17)

or equivalently

$$A(s) = G'(\bar{G}(s)), \qquad Z(s) = \frac{F'(G(s))}{F(\bar{G}(s))}$$
(2.18)

where $\overline{G}(s)$ is the compositional inverse of G(t).

See arXiv: 2302.03999v1 for the proof, which mostly follows [1, pp. 217–218]. We refer to $A(s) = \sum_{n=0}^{\infty} a_n s^n$ and $Z(s) = \sum_{n=0}^{\infty} z_n s^n$ as the **A-series** and **Z-series** associated to the exponential Riordan array $\mathcal{R}[F, G]$.

Remark. The identity $A(s) = G'(\overline{G}(s))$ can equivalently be written as $A(s) = 1/(\overline{G})'(s)$. This is useful in comparing our work with that of Zhu [47,48], who uses the latter formulation.

Let us now show how to rewrite the production matrix (2.16) in a new way, which will be useful in what follows. Define

$$\Psi(s) \stackrel{\text{def}}{=} F(\bar{G}(s)) , \qquad (2.19)$$

so that $F(t) = \Psi(G(t))$ and $\Psi(0) = F(0) = 1$. Then a simple computation using (2.17)/(2.18) shows that

$$Z(s) = \frac{\Psi'(s)}{\Psi(s)} A(s) .$$
 (2.20)

And let us define $\Phi(s) \stackrel{\text{def}}{=} A(s)/\Psi(s)$. Then the pair (Φ, Ψ) is related to the pair (A, Z) by

$$A(s) = \Phi(s) \Psi(s) \tag{2.21a}$$

$$Z(s) = \Phi(s) \Psi'(s) \tag{2.21b}$$

And conversely, given any pair (A, Z) of formal power series (over a commutative ring R containing the rationals) such that A(0) is invertible in R, there is a unique pair (Φ, Ψ) satisfying (2.21) together with the normalization $\Psi(0) = 1$, namely

$$\Psi(s) = \exp\left[\int \frac{Z(s)}{A(s)} \, ds\right] \tag{2.22a}$$

$$\Phi(s) = A(s) \exp\left[-\int \frac{Z(s)}{A(s)} ds\right]$$
(2.22b)

[Here the integral of a formal power series is defined by

$$\int \left(\sum_{n=0}^{\infty} \alpha_n s^n\right) ds \stackrel{\text{def}}{=} \sum_{n=0}^{\infty} \alpha_n \frac{s^{n+1}}{n+1} .$$
(2.23)

It is the unique formal power series with zero constant term whose derivative is the given series.] We refer to $\Phi(s)$ and $\Psi(s)$ as the **\Phi-series** and **\Psi-series** associated to the exponential Riordan array $\mathcal{R}[F, G]$.

Rewriting the production matrix (2.16) in terms of the pair (Φ, Ψ) provides a beautiful — and as we shall see, very useful — factorization. For reasons that shall become clear shortly (see Lemma 2.17 below), it is convenient to study the more general quantity $EAZ(A, Z + \xi A)$:

Proposition 2.14. Let R be a commutative ring containing the rationals, let $\Phi(s) = \sum_{n=0}^{\infty} \phi_n s^n$ and $\Psi(s) = \sum_{n=0}^{\infty} \psi_n s^n$ be formal power series with coefficients in R, and let A(s) and Z(s) be defined by (2.21). Now let ξ be any element of R (or an indeterminate). Then

$$EAZ(A, Z + \xi A) = [D T_{\infty}(\phi) D^{-1}] (\Delta + \xi I) [D T_{\infty}(\psi) D^{-1}]$$
(2.24)

where $D = \operatorname{diag}((n!)_{n\geq 0}).$

To prove Proposition 2.14, we need a lemma. Given a sequence $\psi = (\psi_n)_{n\geq 0}$ in R with ordinary generating function $\Psi(s) = \sum_{n=0}^{\infty} \psi_n s^n$, we define $\psi' = (\psi'_n)_{n\geq 0}$ by $\psi'_n = (n+1)\psi_{n+1}$, so that $\Psi'(s) = \sum_{n=0}^{\infty} \psi'_n s^n$. We then have:

Lemma 2.15. Let ψ and ψ' be as above, and let $D = \text{diag}((n!)_{n>0})$. Then

$$T_{\infty}(\psi') + T_{\infty}(\psi) D^{-1} \Delta D = D^{-1} \Delta D T_{\infty}(\psi) . \qquad (2.25)$$

Proof. All three matrices in (2.25) are lower-Hessenberg, and their (n, k) matrix elements are (for $0 \le k \le n+1$)

$$(n-k+1)\psi_{n-k+1} + k\psi_{n-(k-1)} = (n+1)\psi_{(n+1)-k} . \quad \Box$$
 (2.26)

Remarks.

- 1. The identity (2.25) can also be written as $[D^{-1}\Delta D, T_{\infty}(\psi)] = T_{\infty}(\psi')$, where $[A, B] \stackrel{\text{def}}{=} AB BA$ is the matrix commutator. Thus, $[D^{-1}\Delta D, \cdot]$ is the "differentiation operator" for Toeplitz matrices. Note that $D^{-1}\Delta D$ is the matrix with $1, 2, 3, \ldots$ on the superdiagonal and zeroes elsewhere.
- 2. Lemma 2.15 was found independently by Ding, Mu and Zhu [14, proof of Theorem 2.1]. ■

Proof of Proposition 2.14. From (2.16) we have

$$EAZ(A, Z + \xi A) = D T_{\infty}(z + \xi a) D^{-1} + D T_{\infty}(a) D^{-1} \Delta.$$
 (2.27)

The definitions (2.21) imply

$$T_{\infty}(\boldsymbol{a}) = T_{\infty}(\boldsymbol{\phi}) T_{\infty}(\boldsymbol{\psi}) \tag{2.28a}$$

$$T_{\infty}(\boldsymbol{z} + \boldsymbol{\xi}\boldsymbol{a}) = T_{\infty}(\boldsymbol{\phi}) T_{\infty}(\boldsymbol{\psi}') + \boldsymbol{\xi} T_{\infty}(\boldsymbol{\phi}) T_{\infty}(\boldsymbol{\psi})$$
(2.28b)

Hence

$$\operatorname{EAZ}(A, Z + \xi A) = D \left[T_{\infty}(\phi) T_{\infty}(\psi') + \xi T_{\infty}(\phi) T_{\infty}(\psi) \right] D^{-1} + D T_{\infty}(\phi) T_{\infty}(\psi) D^{-1} \Delta$$
(2.29a)

$$= D T_{\infty}(\boldsymbol{\phi}) \left[\xi T_{\infty}(\boldsymbol{\psi}) + T_{\infty}(\boldsymbol{\psi}') + T_{\infty}(\boldsymbol{\psi}) D^{-1} \Delta D \right] D^{-1}$$
(2.29b)

$$= D T_{\infty}(\phi) \left[\xi T_{\infty}(\psi) + D^{-1} \Delta D T_{\infty}(\psi) \right] D^{-1}$$
(2.29c)

$$= [D T_{\infty}(\phi) D^{-1}] (\Delta + \xi I) [D T_{\infty}(\psi) D^{-1}], \qquad (2.29d)$$

where the next-to-last step used Lemma 2.15. \Box

As an immediate consequence of Proposition 2.14, we have:

Corollary 2.16. Fix $1 \le r \le \infty$. Let R be a partially ordered commutative ring containing the rationals, and let $\phi = (\phi_n)_{n\ge 0}$ and $\psi = (\psi_n)_{n\ge 0}$ be sequences in R that are Toeplitztotally positive of order r. Let ξ be an indeterminate. With the definitions (2.21), the matrix EAZ(A, Z + ξ A) is totally positive of order r in the ring R[ξ] equipped with the coefficientwise order.

Proof. By Lemma 2.1, the matrix $\Delta + \xi I$ is totally positive (of order ∞) in the ring $\mathbb{Z}[\xi]$ equipped with the coefficientwise order. By hypothesis the matrices $T_{\infty}(\phi)$ and $T_{\infty}(\psi)$ are totally positive of order r in the ring R; so Lemma 2.20 implies that also $D T_{\infty}(\phi) D^{-1}$ and $D T_{\infty}(\psi) D^{-1}$ are totally positive of order r in R. The result then follows from Proposition 2.14 and the Cauchy–Binet formula. \Box

Remark. The hypothesis that the ring R contains the rationals can be removed, by using Lemma 2.20 (see Section 2.5) together with the reasoning used in the proof of Theorem 1.8 (see Section 5.3).

It is worth observing that the converse to Corollary 2.16 is false: see Example 2.26 in arXiv:2302.03999v1. So the condition of Corollary 2.16 is sufficient but not necessary for its conclusion.

Finally, a central role will be played in this paper by a simple but remarkable identity for $B_{\xi}^{-1} \text{EAZ}(\boldsymbol{a}, \boldsymbol{z}) B_{\xi}$, where B_{ξ} is the ξ -binomial matrix defined in (1.6) and $\text{EAZ}(\boldsymbol{a}, \boldsymbol{z})$ is the exponential AZ matrix defined in (2.15)/(2.16).

Lemma 2.17 (Identity for $B_{\xi}^{-1} \operatorname{EAZ}(\boldsymbol{a}, \boldsymbol{z}) B_{\xi}$). Let $\boldsymbol{a} = (a_n)_{n \geq 0}$, $\boldsymbol{z} = (z_n)_{n \geq 0}$ and ξ be indeterminates. Then

$$B_{\xi}^{-1} \operatorname{EAZ}(\boldsymbol{a}, \boldsymbol{z}) B_{\xi} = \operatorname{EAZ}(\boldsymbol{a}, \boldsymbol{z} + \xi \boldsymbol{a}) .$$
(2.30)

The special case z = 0 of this lemma was proven in [33, Lemma 3.6]; a simpler proof was given in [43, Lemma 2.16]. Here we have given the easy generalization to include z. Two proofs can be found in arXiv:2302.03999v1: a first proof by direct computation from the definition (2.15)/(2.16), and a second proof using exponential Riordan arrays.

Combining Lemma 2.6 and Theorem 2.8 with Corollary 2.16 and Lemma 2.17, and recalling that the zeroth column of the matrix $\mathcal{R}[F,G]B_x$ consists of the row-generating polynomials of $\mathcal{R}[F,G]$, we obtain:

Corollary 2.18. Fix $1 \le r \le \infty$. Let R be a partially ordered commutative ring containing the rationals, and let $\phi = (\phi_n)_{n\ge 0}$ and $\psi = (\psi_n)_{n\ge 0}$ be sequences in R that are Toeplitz-totally positive of order r. Then the exponential Riordan array $\mathcal{R}[F,G]$ defined by (2.17)/(2.21) has the following two properties:

- (a) The lower-triangular matrix $\mathcal{R}[F,G]$ is totally positive of order r.
- (b) The sequence of row-generating polynomials of $\mathcal{R}[F,G]$ is coefficientwise Hankeltotally positive of order r.

Corollary 2.18 will be the main theoretical tool in this paper.

Remarks.

- 1. The special case $\Psi = 1$ (i.e., F = 1) of Corollary 2.18(b) was proven in [43, Theorem 2.20] and was the fundamental theoretical tool of that paper.
- 2. Another special case of Proposition 2.14 and Corollaries 2.16 and 2.18 was employed recently by Ding, Mu and Zhu [14, proof of Theorem 2.1] to study some far-reaching generalizations of the Eulerian polynomials.
- 3. Example 2.26 in arXiv:2302.03999v1 shows that the condition of Corollary 2.18 is sufficient but not necessary for its two conclusions. ■

Finally, it is worth singling out a subclass of Riordan arrays that will occur in the cases to be studied in the present paper:

Lemma 2.19. Consider an exponential Riordan array $\mathcal{R}[F,G]$ with F(0) = 1 and corresponding series A(s), Z(s), $\Phi(s)$, $\Psi(s)$. Then, for any constant c, the following are equivalent:

- (a) $\mathcal{R}[F,G]_{n,0} = c \mathcal{R}[F,G]_{n,1}$ for all $n \ge 1$.
- (b) $\operatorname{EAZ}(A, Z)_{n,0} = c \operatorname{EAZ}(A, Z)_{n,1}$ for all $n \ge 0$.
- (b') $\operatorname{EAZ}(A, Z) = \operatorname{EAZ}(A, Z) \Delta^{\mathrm{T}} (c \mathbf{e}_{00} + \Delta)$ where \mathbf{e}_{00} denotes the matrix with an entry 1 in position (0, 0) and all other entries zero.
- (c) $\Psi(s) = 1/(1-cs)$.

Proof. (a) \iff (c): (a) holds if and only if F(t) = 1 + cF(t)G(t), or in other words F(t) = 1/[1 - cG(t)], or in other words $\Psi(s) = 1/(1 - cs)$.

(b) \iff (c): By (2.15), (b) holds if and only if $z_n = c(z_{n-1} + a_n)$, or in other words Z(s) = c[sZ(s) + A(s)], or in other words

$$\frac{\Psi'(s)}{\Psi(s)} = \frac{Z(s)}{A(s)} = \frac{c}{1-cs}.$$
(2.31)

Since $\Psi(0) = 1$, this is equivalent to $\Psi(s) = 1/(1 - cs)$.

 $(b') \Longrightarrow (b)$: The zeroth column of the matrix $c \mathbf{e}_{00} + \Delta$ equals c times its first column; so for any matrix M, the zeroth column of the matrix $M(c \mathbf{e}_{00} + \Delta)$ equals c times its first column.

(b) \Longrightarrow (b'): The matrix $\operatorname{EAZ}(A, Z) \Delta^{\mathrm{T}}$ is obtained from $\operatorname{EAZ}(A, Z)$ by removing its zeroth column; it is lower-triangular. And since, by hypothesis, the zeroth column of

 $\operatorname{EAZ}(A, Z)$ is c times its first column, $\operatorname{EAZ}(A, Z)$ can be recovered from $\operatorname{EAZ}(A, Z) \Delta^{\mathrm{T}}$ by right-multiplying by $c \mathbf{e}_{00} + \Delta$. \Box

The case c = 0 (that is, $\Psi = 1$ and hence F = 1) corresponds to the associated subgroup (or Lagrange subgroup) of exponential Riordan arrays; it arose in our earlier work [33,43] on generic Lah and rooted-forest polynomials. Using criterion (a), we can already see that the matrix T defined in (1.1) will correspond to c = 1, while the matrices T(y, z) and $T(y, \phi)$ defined in (1.7)/(1.12) will correspond, according to Propositions 1.3 and 1.6, to c = y. Of course, in order to apply Lemma 2.19 we will first need to prove that these matrices are indeed exponential Riordan arrays: that will be done in Section 4. But we can see now that, once we do this, the Ψ -series will be $\Psi(s) = 1/(1 - cs)$.

2.5. A lemma on diagonal scaling

Given a lower-triangular matrix $A = (a_{nk})_{n,k\geq 0}$ with entries in a commutative ring R, let us define the matrix $A^{\sharp} = (a_{nk}^{\sharp})_{n,k\geq 0}$ by

$$a_{nk}^{\sharp} = \frac{n!}{k!} a_{nk};$$
 (2.32)

this is well-defined since $a_{nk} \neq 0$ only when $n \geq k$, in which case n!/k! is an integer.

If R contains the rationals, we can of course write $A^{\sharp} = DAD^{-1}$ where $D = \text{diag}((n!)_{n\geq 0})$. And if R is a partially ordered commutative ring that contains the rationals and A is TP_r , then we deduce immediately from $A^{\sharp} = DAD^{-1}$ that also A^{\sharp} is TP_r . The following simple lemma [33, Lemma 3.7] shows that this conclusion holds even when R does not contain the rationals:

Lemma 2.20. Let $A = (a_{ij})_{i,j\geq 0}$ be a lower-triangular matrix with entries in a partially ordered commutative ring R, and let $\mathbf{d} = (d_i)_{i\geq 1}$. Define the lower-triangular matrix $A^{\sharp \mathbf{d}} = (a_{ij}^{\sharp \mathbf{d}})_{i,j\geq 0}$ by

$$a_{ij}^{\sharp d} = d_{j+1}d_{j+2}\cdots d_i a_{ij} . (2.33)$$

Then:

- (a) If A is TP_r and **d** are indeterminates, then $A^{\sharp d}$ is TP_r in the ring R[d] equipped with the coefficientwise order.
- (b) If A is TP_r and d are nonnegative elements of R, then $A^{\sharp d}$ is TP_r in the ring R.

The special case $A^{\sharp d} = A^{\sharp}$ corresponds to taking $d_i = i$.

Lemma 2.20 will be important to proving Theorem 1.8 in the case where the ring R does not contain the rationals (see Section 5.3).

2.6. Lagrange inversion

We will use Lagrange inversion in the following form [20]: If $\phi(u)$ is a formal power series with coefficients in a commutative ring R containing the rationals, then there exists a unique formal power series f(t) with zero constant term satisfying

$$f(t) = t \phi(f(t)),$$
 (2.34)

and it is given by

$$[t^{n}] f(t) = \frac{1}{n} [u^{n-1}] \phi(u)^{n} \quad \text{for } n \ge 1 ; \qquad (2.35)$$

and more generally, if H(u) is any formal power series, then

$$[t^n] H(f(t)) = \frac{1}{n} [u^{n-1}] H'(u) \phi(u)^n \quad \text{for } n \ge 1.$$
(2.36)

3. Bijective proofs

In this section we give bijective proofs of Propositions 1.3, 1.5, 1.6 and 1.7. This section can be skipped on a first reading, as it is not needed for proving the main theorems of the paper.

3.1. Proof of Propositions 1.3 and 1.6

Here we will prove Proposition 1.3, which asserts that the polynomials $t_{n,k}(y,z)$ defined in (1.7) satisfy $t_{n,0}(y,z) = y t_{n,1}(y,z)$ for all $n \ge 1$; and more generally Proposition 1.6, which asserts that the polynomials $t_{n,k}(y,\phi)$ defined in (1.12) satisfy $t_{n,0}(y,\phi) = y t_{n,1}(y,\phi)$ for all $n \ge 1$.

We will prove these results by constructing, for each $n \ge 1$, a bijection from the set $\mathcal{T}_{n+1}^{\langle 1;1\rangle}$ of rooted trees on the vertex set [n+1] in which the vertex 1 has exactly one child, to the set $\mathcal{T}_{n+1}^{\langle 1;0\rangle}$ of rooted trees on the vertex set [n+1] in which vertex 1 is a leaf, with the properties that

- (a) the number of improper edges is increased by 1, and
- (b) for each m, the number of vertices with m proper children is preserved, provided that in $T \in \mathcal{T}_{n+1}^{\langle 1;1 \rangle}$ one ignores the vertex 1 (which has one child).

This construction is illustrated in Fig. 1. Since the weight in (1.12) is y for each improper edge and $\hat{\phi}_m = m! \phi_m$ for each vertex $i \neq 1$ with m proper children, this proves $t_{n,0}(y,\phi) = y t_{n,1}(y,\phi)$. Specializing to $\phi_m = z^m/m!$ then yields $t_{n,0}(y,z) = y t_{n,1}(y,z)$.

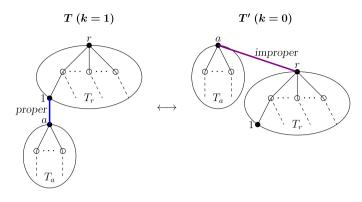


Fig. 1. Bijection between T and T'.

Proof of Proposition 1.6. Fix $n \ge 1$, and let T be a rooted tree on the vertex set [n+1] in which r is the root and the vertex 1 has precisely one child a. Let T_a be the subtree rooted at a, and let T_r the subtree obtained from T by removing T_a and the edge 1a. The vertex 1 is a leaf in T_r .

Now we create a new tree T', rooted at a, as follows: we start with T_a and then graft T_r by making r a child of a. In the tree T', the vertex 1 is a leaf. The map $T \mapsto T'$ map is a bijection, since this construction can be reversed. (The vertex r can be identified in T' as the child of a that has 1 as a descendant.)

Clearly, all the proper (resp. improper) edges in T are still proper (resp. improper) in T', except that:

- (i) The edge 1a in T is proper, which is deleted in T'; and
- (ii) The edge ar in T' is new and improper, since the vertex 1 is a descendant of r.

In particular, the number of vertices with m proper children is the same in T and T', provided that in T one ignores the vertex 1. \Box

3.2. Proof of Propositions 1.5 and 1.7

Now we will prove Proposition 1.5, which asserts the equality of the polynomials $t_{n,k}(y,z)$ defined in (1.7) using rooted trees and the polynomials $\tilde{t}_{n,k}(y,z)$ defined in (1.10) using partial functional digraphs. We will then show that the same argument proves the more general Proposition 1.7, which asserts the equivalence of the polynomials $t_{n,k}(y,\phi)$ defined in (1.12) and the polynomials $\tilde{t}_{n,k}(y,\phi)$ defined in (1.13).

We recall that \mathcal{T}_n^{\bullet} denotes the set of rooted trees on the vertex set [n], while $\mathcal{T}_n^{\langle 1;k\rangle}$ denotes the subset in which the vertex 1 has k children. Similarly, **PFD**_n denotes the set of partial functional digraphs on the vertex set [n], while **PFD**_{n,k} denotes the subset in which there are exactly k vertices of out-degree 0.

To prove Proposition 1.5, we will construct, for each fixed n, a bijection $\phi: \mathcal{T}_{n+1}^{\bullet} \to \mathbf{PFD}_n$ with the following properties:

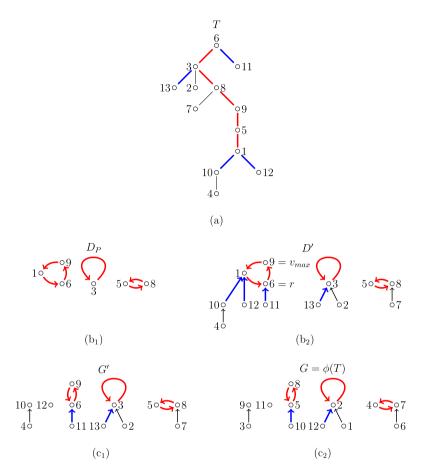


Fig. 2. (a) Tree T in the second model, where $r = v_1 = 6$, $v_{\max} = 9$, $\sigma = 638951 = (169)(3)(58)$, and vertex 1 has two children. The backbone edges are shown in red and are improper; the other improper edges are shown in black; the proper edges are shown in blue. (b_1, b_2) Partial functional digraphs D_P and D'. Improper edges arising from the cycles of the permutation σ are shown in red; the other improper edges are shown in blue. (c_1, c_2) Partial functional digraphs G' and G in the third model, where the two vertices 10 and 12 (resp. 9 and 11) have out-degree 0. Improper edges arising from the cycles of the permutation σ are shown in the figure(s), the reader is referred to the web version of this article.)

- (a) ϕ maps $\mathcal{T}_{n+1}^{\langle 1;k\rangle}$ onto $\mathbf{PFD}_{n,k}$.
- (b) ϕ preserves the number of improper edges.
- (c) $\phi|_{\mathcal{T}_{n+1}^{(1;k)}}$ reduces the number of proper edges by k.

We observe that (c) is an immediate consequence of (a) and (b), since trees in $\mathcal{T}_{n+1}^{\bullet}$ have n edges, while digraphs in $\mathbf{PFD}_{n,k}$ have n-k edges.

Proof of Proposition 1.5. (The reader may wish to follow, along with this proof, the example shown in Fig. 2.)

Let T be a rooted tree on the vertex set [n + 1] in which the vertex 1 has k children. Note that the k edges from vertex 1 to its children are all proper. Now let $P = v_1 \cdots v_{\ell+1}$ $(\ell \ge 0)$ be the unique path in T from the root $v_1 = r$ to the vertex $v_{\ell+1} = 1$; we call it the "backbone". (Here $\ell = 0$ corresponds to the case in which vertex 1 is the root.) Removing from T the edges of the path P, we obtain a collection of (possibly trivial) trees $T_1, \ldots, T_{\ell+1}$ rooted at the vertices $v_1, \ldots, v_{\ell+1}$.

Now regard P as a permutation σ (written in word form) of its elements written in increasing order.⁸ In particular, $\sigma(1) = r$ and $\sigma(v_{\max}) = 1$ where $v_{\max} = \max(v_1, \ldots, v_{\ell+1})$. Let D_P be the digraph whose vertex set is $\{v_1, \ldots, v_{\ell+1}\}$, with edges ij whenever $j = \sigma(i)$. Then D_P consists of disjoint directed cycles (possibly of length 1); it is the representation in cycle form of the permutation σ .

Now let D' be the digraph obtained from D_P by attaching the trees $T_1, \ldots, T_{\ell+1}$ to D_P (identifying vertices with the same label) and directing all edges of those trees towards the root. Then D' is a functional digraph on the vertex set [n+1]. Furthermore, the map $T \mapsto D'$ is a bijection, since all the above steps can be reversed.

Now let G' be the digraph obtained from D' by deleting the vertex 1 and the k tree edges incident on vertex 1, and contracting the edges $\overrightarrow{v_{\max}1}$ and $\overrightarrow{1r}$ into a single edge $\overrightarrow{v_{\max}r}$. Then G' is a digraph on the vertex set $\{2, \ldots, n+1\}$ in which every vertex has outdegree 1 except for the k children of vertex 1 in T, which have out-degree 0. Relabeling all vertices $i \to i - 1$, we obtain a partial functional digraph $G = \phi(T) \in \mathbf{PFD}_{n,k}$.

The step from D' to G can also be reversed: given a partial functional digraph $G = \mathbf{PFD}_{n,k}$, we relabel the vertices $i \to i+1$ and then insert the vertex 1 immediately after the largest cyclic vertex of G (if any; otherwise 1 becomes a loop in D'); all the vertices of out-degree 0 in G are made to point to the vertex 1 in D'.

It follows that the map $\phi: T \mapsto G$ is a bijection from $\mathcal{T}_{n+1}^{\bullet}$ to \mathbf{PFD}_n that maps $\mathcal{T}_{n+1}^{\langle 1;k \rangle}$ onto $\mathbf{PFD}_{n,k}$.

Clearly, in the rooted tree T, all the edges in the path $P = v_1 \cdots v_{\ell+1}$ are improper, since each vertex in P has $v_{\ell+1} = 1$ as its descendant. These ℓ edges correspond, after relabeling, to $\ell + 1$ cyclic edges in the functional digraph D'. These latter edges in turn correspond, after removal of vertex 1 and contraction of its edges, to ℓ cyclic edges in the partial functional digraph G' (and hence also G). Because they are cyclic edges, they are necessarily improper. All the other improper/proper edges in T coincide with improper/proper edges ij in the partial functional digraph G' (and hence G) where i is a transient vertex. \Box

Remark. The first part of this proof (namely, the map $T \mapsto D'$) is the well-known bijection from doubly-rooted trees to functional digraphs on the same vertex set [27, pp. 224–225] [45, p. 26]. In our application we need the second step to remove the

⁸ That is, let $v'_1 < \ldots < v'_{\ell+1}$ be the elements of the set $S = \{v_1, \ldots, v_{\ell+1}\}$ written in increasing order. Then σ is the permutation of S defined by $\sigma(v'_i) = v_i$.

vertex 1 and thereby obtain a map from rooted trees on the vertex set [n+1] to partial functional digraphs on the vertex set [n].

Proof of Proposition 1.7. In the preceding proof, each vertex $i \neq 1$ in the rooted tree T corresponds to a vertex i - 1 in the partial functional digraph $G = \phi(T)$. And for each proper child j of i in T, the proper edge ij in T corresponds to a proper edge $\overline{j-1}i-1$ in G; and those are the only proper edges in G. Therefore, if the vertex $i \neq 1$ in T has m proper children, then the vertex i-1 in G has m proper incoming edges. This proves that $t_{n,k}(y, \phi) = \tilde{t}_{n,k}(y, \phi)$. \Box

4. The matrices $\mathsf{T}, \mathsf{T}(y,z)$ and $\mathsf{T}(y,\phi)$ as exponential Riordan arrays

In this section we show that the matrices T , $\mathsf{T}(y, z)$ and $\mathsf{T}(y, \phi)$ are exponential Riordan arrays $\mathcal{R}[F, G]$, and we compute their generating functions F and G as well as their A-, Z-, Φ - and Ψ -series.

4.1. The matrix \mathbf{T}

Proposition 4.1. Define

$$t_{n,k} = \binom{n}{k} n^{n-k} . aga{4.1}$$

Then the unit-lower-triangular matrix $\mathsf{T} = (t_{n,k})_{n,k\geq 0}$ is the exponential Riordan array $\mathcal{R}[F,G]$ with $F(t) = \sum_{n=0}^{\infty} n^n t^n / n!$ and $G(t) = \sum_{n=1}^{\infty} n^{n-1} t^n / n!$.

Before proving Proposition 4.1, let us use it to compute the A-, Z-, Φ - and Ψ -series:

Corollary 4.2. The exponential Riordan array $T = \mathcal{R}[F, G]$ has

$$A(s) = \frac{e^s}{1-s}, \quad Z(s) = \frac{e^s}{(1-s)^2}$$
(4.2)

and

$$\Phi(s) = e^{s}, \quad \Psi(s) = \frac{1}{1-s}.$$
(4.3)

Proof. We observe that G(t) is the tree function T(t) [9], which satisfies the functional equation $T(t) = te^{T(t)}$. Furthermore, we have F(t) = 1/[1 - T(t)]: this well-known fact can be proven using the Lagrange inversion formula [see (4.4) below specialized

to x = 0] or by various other methods.⁹ We now apply Theorem 2.13 to determine the functions A(s) and Z(s). Implicit differentiation of the functional equation yields $T'(t) = e^{T(t)}/[1 - T(t)]$, which implies that $A(s) = e^s/(1 - s)$. On the other hand, it follows immediately from the relation between F and G that $\Psi(s) = 1/(1 - s)$. This implies that $\Phi(s) = e^s$ and $Z(s) = e^s/(1 - s)^2$. \Box

We have five proofs of Proposition 4.1: a direct algebraic proof using Lagrange inversion and an Abel identity; an inductive algebraic proof, using a different Abel identity; a third algebraic proof using the A- and Z-sequences of an ordinary Riordan array; a combinatorial proof using exponential generating functions based on the interpretation of $t_{n,k}$ as counting partial functional digraphs; and a bijective combinatorial proof based on the interpretation of $t_{n,k}$ as counting rooted labeled trees according to the number of children of the root that are lower-numbered than the root. Here we give only the first proof; the other four proofs can be found in arXiv:2302.0399v1. In Section 4.2 we will give yet another combinatorial proof (also using exponential generating functions), this time based on the interpretation of $t_{n,k}$ as counting rooted labeled trees according to the number of children of a specified vertex i; but this proof will be given in the more general context of the polynomials $t_{n,k}(y, z)$.

First Proof of Proposition 4.1. The tree function T(t) satisfies the functional equation $T(t) = te^{T(t)}$. We use Lagrange inversion (2.36) with $\phi(u) = e^u$ and $H(u) = e^{xu}/(1-u)$: this gives

$$[t^{n}] \frac{e^{xT(t)}}{1-T(t)} = \frac{1}{n} [u^{n-1}] \left(\frac{x}{1-u} + \frac{1}{(1-u)^{2}}\right) e^{(x+n)u}$$
(4.4a)

$$= \frac{1}{n} \sum_{k=0}^{n-1} (x+k+1) \frac{(x+n)^{n-1-k}}{(n-1-k)!}$$
(4.4b)

$$= \frac{1}{n!} \sum_{k=0}^{n-1} \binom{n-1}{k} k! (x+k+1) \frac{(x+n)^{n-1-k}}{(n-1-k)!}$$
(4.4c)

$$=\frac{(x+n)^n}{n!},\qquad(4.4d)$$

where the last step used an Abel identity [37, p. 21, eq. (25) with $n \to n-1$ and $x \to x+1$]. In view of (1.5), this proves (1.2), which by (2.11) proves that $\mathsf{T} = \mathcal{R}[F, G]$. \Box

⁹ Algebraic proof. $F(t) = 1 + tT'(t) = 1 + \frac{te^{T(t)}}{1 - T(t)} = 1 + \frac{T(t)}{1 - T(t)} = \frac{1}{1 - T(t)}$, where the first equality used the power series defining F(t) and T(t), the second equality used the identity $T'(t) = \frac{e^{T(t)}}{1 - T(t)}$ arising from implicit differentiation of the functional equation, and the third equality used the functional equation. Combinatorial proof. This follows from the identity of combinatorial species: endofunctions = permutations \circ rooted trees [2, pp. 41, 43]. See also [45, Exercise 5.32(b)] for a related combinatorial proof.

4.2. The matrix T(y,z)

We now prove that the matrix $\mathsf{T}(y, z) = (t_{n,k}(y, z))_{n,k\geq 0}$ is an exponential Riordan array $\mathcal{R}[F, G]$, and we compute F and G. Most of this computation was done a quartercentury ago by Dumont and Ramamonjisoa [15]: their arguments handled the case k = 0, and we extend those arguments slightly to handle the case of general k. Our presentation follows the notation of [43].

Let \mathcal{T}_n^{\bullet} denote the set of rooted trees on the vertex set [n]; let $\mathcal{T}_n^{[i]}$ denote the subset of \mathcal{T}_n^{\bullet} in which the root vertex is i; and let $\mathcal{T}_n^{\langle i;k \rangle}$ denote the subset of \mathcal{T}_n^{\bullet} in which the vertex i has k children. Given a tree $T \in \mathcal{T}_n^{\bullet}$, we write imprope(T) for the number of improper edges of T. Now define the generating polynomials

$$R_n(y,z) = \sum_{T \in \mathcal{T}_n^{\bullet}} y^{\operatorname{imprope}(T)} z^{n-1-\operatorname{imprope}(T)}$$

$$(4.5)$$

$$S_n(y,z) = \sum_{T \in \mathcal{T}_{n+1}^{[1]}} y^{\operatorname{imprope}(T)} z^{n-\operatorname{imprope}(T)}$$

$$(4.6)$$

$$A_{n,k}(y,z) = t_{n,k}(y,z) = \sum_{T \in \mathcal{T}_{n+1}^{(1;k)}} y^{\text{imprope}(T)} z^{n-k-\text{imprope}(T)}$$
(4.7)

in which each improper (resp. proper) edge gets a weight y (resp. z) except that in $A_{n,k}$ the k proper edges connecting the vertex 1 to its children are unweighted. And then define the exponential generating functions

$$\mathcal{R}(t;y,z) = \sum_{n=1}^{\infty} R_n(y,z) \, \frac{t^n}{n!} \tag{4.8}$$

$$\mathcal{S}(t;y,z) = \sum_{n=0}^{\infty} S_n(y,z) \, \frac{t^n}{n!} \tag{4.9}$$

$$\mathcal{A}_{k}(t;y,z) = \sum_{n=0}^{\infty} A_{n,k}(y,z) \, \frac{t^{n}}{n!} \tag{4.10}$$

We will then prove the following key result, which is a slight extension of [15, Proposition 7] to handle the case $k \neq 0$:

Proposition 4.3. The series \mathcal{R} , \mathcal{S} and \mathcal{A}_k satisfy the following identities:

(a)
$$\mathcal{S}(t; y, z) = \exp \left[z \mathcal{R}(t; y, z) \right]$$

(b) $\mathcal{A}_k(t; y, z) = \frac{\mathcal{R}(t; y, z)^k / k!}{1 - y \mathcal{R}(t; y, z)}$

(c)
$$\frac{d}{dt}\mathcal{R}(t;y,z) = \mathcal{A}_0(t;y,z)\mathcal{S}(t;y,z)$$

and hence

(d)
$$\frac{d}{dt}\mathcal{R}(t;y,z) = \frac{\exp\left[z\mathcal{R}(t;y,z)\right]}{1-y\mathcal{R}(t;y,z)}$$

Solving the differential equation of Proposition 4.3(d) with the initial condition $\mathcal{R}(0; y, z) = 0$, we obtain:

Corollary 4.4. The series $\mathcal{R}(t; y, z)$ satisfies the functional equation

$$y - z + yz\mathcal{R} = (y - z + z^2t)e^{z\mathcal{R}}$$

$$(4.11)$$

 \sim

and hence has the solution

$$\mathcal{R}(t;y,z) = \frac{1}{z} \left[T\left(\left(1 - \frac{z}{y} + \frac{z^2}{y}t\right) e^{-\left(1 - \frac{z}{y}\right)} \right) - \left(1 - \frac{z}{y}\right) \right]$$
(4.12)

where T(t) is the tree function (1.3).

Comparing Proposition 4.3(b) with the definition (2.10) of exponential Riordan arrays, we conclude:

Corollary 4.5. The matrix T(y, z) is the exponential Riordan array $\mathcal{R}[F, G]$ where

$$F(t) = \frac{1}{1 - y\mathcal{R}(t; y, z)}, \quad G(t) = \mathcal{R}(t; y, z)$$
(4.13)

and $\mathcal{R}(t; y, z)$ is given by (4.12).

And comparing Proposition 4.3(b,d) with the definitions (2.17)/(2.19)/(2.21) of the A-series, Z-series, Φ -series and Ψ -series of an exponential Riordan array, we conclude:

Corollary 4.6. The exponential Riordan array T(y, z) has

$$A(s) = \frac{e^{zs}}{1 - ys}, \quad Z(s) = \frac{ye^{zs}}{(1 - ys)^2}$$
(4.14)

and

$$\Phi(s) = e^{zs}, \quad \Psi(s) = \frac{1}{1 - ys}.$$
(4.15)

The proof of Proposition 4.3 follows the elegant argument of Jiang Zeng that was presented in [15, section 7], and extends it in part (b) to handle $k \neq 0$:

Proof of Proposition 4.3. (a) Consider a tree $T \in \mathcal{T}_{n+1}^{[1]}$, and suppose that the root vertex 1 has $k \geq 0$ children. All k edges emanating from the root vertex are proper and thus get a weight z each. Deleting these edges and the vertex 1, one obtains an *unordered* partition of $\{2, \ldots, n+1\}$ into blocks B_1, \ldots, B_k and a rooted tree T_j on each block B_j . Standard enumerative arguments then yield the relation (a) for the exponential generating functions.

(b) Consider a tree $T \in \mathcal{T}_{n+1}^{\langle 1;k \rangle}$ with root r, and let r_1, \ldots, r_{l+1} $(l \ge 0)$ be the path in T from the root $r_1 = r$ to the vertex $r_{l+1} = 1$. (Here l = 0 corresponds to the case in which the vertex 1 is the root.) All l edges of this path are improper, and all k edges from the vertex 1 to its children are proper (and unweighted). Deleting these edges and the vertex 1, one obtains a partition of $\{2, \ldots, n+1\}$ into an *ordered* collection of blocks B_1, \ldots, B_l and an *unordered* collection of blocks B'_1, \ldots, B'_k , together with a rooted tree on each block. Standard enumerative arguments then yield the relation (b) for the exponential generating functions.

(c) In a tree $T \in \mathcal{T}_n^{\bullet}$, focus on the vertex 1 (which might be the root, a leaf, both or neither). Let T' be the subtree rooted at 1, and let T'' be the tree obtained from T by deleting all the vertices of T' except the vertex 1 (it thus has the vertex 1 as a leaf). The vertex set [n] is then partitioned as $\{1\} \cup V' \cup V''$, where $\{1\} \cup V'$ is the vertex set of T' and $\{1\} \cup V''$ is the vertex set of T''; and T is obtained by joining T' and T'' at the common vertex 1. Standard enumerative arguments then yield the relation (c) for the exponential generating functions. \Box

Remarks.

- 1. Dumont and Ramamonjisoa also gave [15, sections 2–5] a second (and very interesting) proof of the k = 0 case of Proposition 4.3, based on a context-free grammar [7] and its associated differential operator.
- 2. We leave it as an open problem to find a direct combinatorial proof of the functional equation (4.11), without using the differential equation of Proposition 4.3(d).
- 3. The polynomials $R_n(y, z)$ enumerate rooted trees according to the number of improper and proper edges; they are homogenized versions of the celebrated **Ramanujan polynomials** [8,15,22–24,29,36,39,43,46] [32, A054589].
- 4. The polynomials R_n and $A_{n,0}$ also arise [24] as derivative polynomials for the tree function: in the notation of [24] we have $R_n(y,1) = G_n(y-1)$ and $A_{n,0}(y,1) = y F_n(y-1)$ for $n \ge 1$. The formula (4.12) is then equivalent to [24, Theorem 4.2, equation for G_n].

4.3. The matrix $T(y,\phi)$

We now show how Proposition 4.3 can be generalized to incorporate the additional indeterminates $\boldsymbol{\phi} = (\phi_m)_{m \geq 0}$. We define \mathcal{T}_n^{\bullet} , $\mathcal{T}_n^{[i]}$ and $\mathcal{T}_n^{\langle i;k \rangle}$ as before, and then define the obvious generalizations of (4.5)–(4.7):

$$R_n(y,\phi) = \sum_{T \in \mathcal{T}_n^{\bullet}} y^{\operatorname{imprope}(T)} \prod_{i=1}^{n+1} \widehat{\phi}_{\operatorname{pdeg}_T(i)}$$
(4.16)

$$S_n(y,\phi) = \sum_{T \in \mathcal{T}_{n+1}^{[1]}} y^{\operatorname{imprope}(T)} \prod_{i=1}^{n+1} \widehat{\phi}_{\operatorname{pdeg}_T(i)}$$
(4.17)

$$A_{n,k}(y,\phi) = t_{n,k}(y,\phi) = \sum_{T \in \mathcal{T}_{n+1}^{(1;k)}} y^{\text{imprope}(T)} \prod_{i=2}^{n+1} \widehat{\phi}_{\text{pdeg}_{T}(i)}$$
(4.18)

where $\operatorname{pdeg}_{T}(i)$ denotes the number of proper children of the vertex *i* in the rooted tree T, and $\widehat{\phi}_{m} = m! \phi_{m}$. (Note that in R_{n} and S_{n} we give weights to all the vertices, while in $A_{n,k}$ we do *not* give any weight to the vertex 1.¹⁰) We then define the exponential generating functions

$$\mathcal{R}(t;y,\phi) = \sum_{n=1}^{\infty} R_n(y,\phi) \, \frac{t^n}{n!} \tag{4.19}$$

$$\mathcal{S}(t;y,\phi) = \sum_{n=0}^{\infty} S_n(y,\phi) \, \frac{t^n}{n!} \tag{4.20}$$

$$\mathcal{A}_k(t; y, \phi) = \sum_{n=0}^{\infty} A_{n,k}(y, \phi) \, \frac{t^n}{n!} \tag{4.21}$$

Let us also define the generating function

$$\Phi(s) \stackrel{\text{def}}{=} \sum_{m=0}^{\infty} \phi_m s^m = \sum_{m=0}^{\infty} \widehat{\phi}_m \frac{s^m}{m!} .$$
(4.22)

We then have:

Proposition 4.7. The series \mathcal{R} , \mathcal{S} and \mathcal{A}_k defined in (4.19)–(4.21) satisfy the following identities:

(a)
$$S(t; y, \phi) = \Phi(\mathcal{R}(t; y, \phi))$$

(b) $\mathcal{A}_k(t; y, \phi) = \frac{\mathcal{R}(t; y, z)^k / k!}{1 - y \mathcal{R}(t; y, \phi)}$
(c) $\frac{d}{dt} \mathcal{R}(t; y, \phi) = \mathcal{A}_0(t; y, \phi) S(t; y, \phi)$

and hence

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¹⁰ This differs from the convention used in [43, eq. (3.24)], where $A_n = A_{n,0}$ included a factor $\phi_0 = \hat{\phi}_0$ associated to the leaf vertex 1.

(d)
$$\frac{d}{dt}\mathcal{R}(t;y,\phi) = \frac{\Phi(\mathcal{R}(t;y,\phi))}{1-y\mathcal{R}(t;y,\phi)}$$

Proof. The proof is identical to that of Proposition 4.3, with the following modifications: (a) Consider a tree $T \in \mathcal{T}_{n+1}^{[1]}$ in which the root vertex 1 has k children. Since all k

edges emanating from the root vertex are proper, we get here a factor $\hat{\phi}_k/k!$ in place of the $z^k/k!$ that was seen in Proposition 4.3. Therefore, the function e^{zs} in Proposition 4.3 is replaced here by the generating function $\Phi(s)$.

(b) No change is needed.

(c) No change is needed. (The tree T'' has vertex 1 as a leaf, but in $A_{n,0}$ the vertex 1 is anyway unweighted.) \Box

Comparing Proposition 4.7(b) with the definition (2.10) of exponential Riordan arrays, we conclude:

Corollary 4.8. The matrix $\mathsf{T}(y, \phi)$ is the exponential Riordan array $\mathcal{R}[F, G]$ where

$$F(t) = \frac{1}{1 - y\mathcal{R}(t; y, \phi)}, \quad G(t) = \mathcal{R}(t; y, \phi)$$

$$(4.23)$$

and $\mathcal{R}(t; y, \phi)$ is the solution of the differential equation of Proposition 4.7(d) with initial condition $\mathcal{R}(0; y, \phi) = 0$.

We observe that (4.23) is identical in form to (4.13); only \mathcal{R} is different.

Comparing Proposition 4.7(b,d) with the definitions (2.17)/(2.19)/(2.21) of the Aseries, Z-series, Φ -series and Ψ -series of an exponential Riordan array, we conclude:

Corollary 4.9. The exponential Riordan array $\mathsf{T}(y, \phi)$ has

$$A(s) = \frac{\Phi(s)}{1 - ys}, \quad Z(s) = \frac{y \Phi(s)}{(1 - ys)^2}$$
(4.24)

and

$$\Psi(s) = \frac{1}{1 - ys} \tag{4.25}$$

where $\Phi(s)$ is given by (4.22).

We see that $\Psi(s)$ is the same here as in (4.15); only Φ is different. Proposition 4.7 and Corollaries 4.8–4.9 reduce to Proposition 4.3 and Corollaries 4.5–4.6 if we take $\phi_m = z^m/m!$ and hence $\hat{\phi}_m = z^m$, $\Phi(s) = e^{zs}$.

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5. Proof of Theorems 1.1, 1.2, 1.4 and 1.8

In this section we will prove Theorems 1.1, 1.2, 1.4 and 1.8. The proofs are now very easy: we combine the general theory of total positivity in exponential Riordan arrays developed in Section 2 (culminating in Corollary 2.18) with the specific computations of Φ - and Ψ -series carried out in Section 4.

It suffices of course to prove Theorem 1.8, since Theorems 1.1, 1.2 and 1.4 are contained in it as special cases: take $\phi_m = z^m/m!$ to get Theorem 1.4; then take y = z = 1 to get Theorems 1.1 and 1.2. However, we find it instructive to work our way up, starting with Theorems 1.1 and 1.2 and then gradually adding extra parameters.

5.1. The matrix \mathbf{T}

Proof of Theorems 1.1 and 1.2. In order to employ the theory of exponential Riordan arrays, we work here in the ring \mathbb{Q} , even though the matrix elements actually lie in \mathbb{Z} .

By Corollary 4.2, the exponential Riordan array T has $\Phi(s) = e^s$ and $\Psi(s) = 1/(1-s)$. By Lemma 2.5, the corresponding sequences ϕ and ψ (namely, $\phi_m = 1/m!$ and $\psi_m = 1$) are Toeplitz-totally positive in \mathbb{Q} . Corollary 2.18 then yields Theorems 1.1(a) and 1.2. Theorem 1.1(b) is obtained from Theorem 1.2 by specializing to x = 0. \Box

Since this proof employed the production-matrix method (hidden inside Corollary 2.18), it is worth making explicit what the production matrix is:

Proposition 5.1 (Production matrix for T). The production matrix $P = T^{-1}\Delta T$ is the unit-lower-Hessenberg matrix

$$P = B_1 \Delta D T_1 D^{-1} (5.1)$$

where B_1 is the binomial matrix [i.e. (1.6) at x = 1], T_1 is the lower-triangular matrix of all ones [i.e. (2.2) at x = 1], and $D = \text{diag}((n!)_{n>0})$. More generally, we have

$$B_{\xi}^{-1}P B_{\xi} = B_1 (\Delta + \xi I) DT_1 D^{-1} .$$
(5.2)

Proof. Since $\phi_m = 1/m!$ and $\psi_m = 1$, Proposition 2.14 implies

$$P = DT_{\infty} ((1/m!)_{m \ge 0}) D^{-1} \Delta DT_1 D^{-1} = B_1 \Delta DT_1 D^{-1} , \qquad (5.3)$$

and Lemma 2.17 implies (5.2). \Box

Remarks.

1. The zeroth and first columns of the matrix P are identical: that is, $p_{n,0} = p_{n,1}$. This can be seen from Lemma 2.19 with c = 1, by noting either that $t_{n,0} = t_{n,1}$ for $n \ge 1$

or that $\Psi(s) = 1/(1-s)$. Alternatively, it can be seen directly from (5.1): the zeroth and first columns of the matrix ΔDT_1D^{-1} are identical (namely, they are both equal to 1/(n+1)!); so the zeroth and first columns of $M \Delta DT_1D^{-1}$ are identical, for any row-finite matrix M. (Indeed, this would be the case if $D = \text{diag}((n!)_{n\geq 0})$ were replaced by any diagonal matrix $\text{diag}(d_0, d_1, d_2, \ldots)$ satisfying $d_0 = d_1$.) We will also see that $p_{n,0} = p_{n,1}$ in the explicit formula (5.16).

The equality $p_{n,0} = p_{n,1}$ implies, by Lemma 2.19(b) \iff (b'), the factorization

$$P = P\Delta^{\mathrm{T}} \left(\mathbf{e}_{00} + \Delta \right) \tag{5.4}$$

where \mathbf{e}_{00} denotes the matrix with an entry 1 in position (0,0) and all other entries zero, and $P\Delta^{\mathrm{T}}$ is the lower-triangular matrix obtained from P by deleting its zeroth column.

2. Closely related to the production matrix $P = B_1 \Delta DT_1 D^{-1}$ are

$$\widehat{P} = B_1 D T_1 D^{-1} \Delta \quad \text{and} \quad \widehat{P}' = \Delta B_1 D T_1 D^{-1} . \quad (5.5)$$

It was shown in [43, Section 4.1] that \widehat{P} is the production matrix for the forest matrix $\mathsf{F} = (f_{n,k})_{n,k\geq 0}$ where $f_{n,k} = \binom{n}{k} k n^{n-k-1}$ counts k-component forests of rooted trees on n labeled vertices; and that $\widehat{P}' = \Delta \widehat{P} \Delta^{\mathrm{T}}$ is the production matrix for $\mathsf{F}' = \Delta \mathsf{F} \Delta^{\mathrm{T}} = (f_{n+1,k+1})_{n,k\geq 0}$. All three production matrices correspond to the same A-series $A(s) = e^s/(1-s)$, but with different splittings into Φ and Ψ .

We have more to say about this production matrix P, but in order to avoid disrupting the flow of the argument we defer it to Section 5.4.

5.2. The matrix $\mathbf{T}(y,z)$

Proof of Theorem 1.4. In order to employ the theory of exponential Riordan arrays, we work here in the ring $\mathbb{Q}[y, z]$, even though the matrix elements actually lie in $\mathbb{Z}[y, z]$.

By Corollary 4.6, the exponential Riordan array $\mathsf{T}(y, z)$ has $\Phi(s) = e^{zs}$ and $\Psi(s) = 1/(1-ys)$. By Lemma 2.5, the corresponding sequences ϕ and ψ (namely, $\phi_m = z^m/m!$ and $\psi_m = y^m$) are Toeplitz-totally positive in the ring $\mathbb{Q}[y, z]$ equipped with the coefficientwise order. Corollary 2.18 then yields Theorem 1.4. \Box

Analogously to Proposition 5.1, we have:

Proposition 5.2 (Production matrix for T(y,z)). The production matrix $P(y,z) = T(y,z)^{-1}\Delta T(y,z)$ is the unit-lower-Hessenberg matrix

$$P(y,z) = B_z \Delta DT_y D^{-1} \tag{5.6}$$

where B_z is the weighted binomial matrix (1.6), T_y is the Toeplitz matrix of powers (2.2), and $D = \text{diag}((n!)_{n\geq 0})$. More generally,

$$B_{\xi}^{-1}P(y,z) B_{\xi} = B_z \left(\Delta + \xi I\right) DT_y D^{-1} .$$
(5.7)

Remarks.

1. The zeroth and first columns of the matrix P(y, z) satisfy $p_{n,0} = yp_{n,1}$. This can be seen from Lemma 2.19 with c = y, by noting either that $t_{n,0}(y, z) = yt_{n,1}(y, z)$ for $n \ge 1$ (Proposition 1.3) or that $\Psi(s) = 1/(1 - ys)$. Alternatively, it can be seen directly from (5.1): the zeroth column of the matrix $\Delta DT_y D^{-1}$ is y times the first column (they are, respectively, $y^{n+1}/(n+1)!$ and $y^n/(n+1)!$); so the zeroth column of $M \Delta DT_y D^{-1}$ is y times the first column, for any row-finite matrix M. The equality $p_{n,0} = yp_{n,1}$ implies, by Lemma 2.19(b) \iff (b'), the factorization

$$P(y,z) = P(y,z) \Delta^{\mathrm{T}} (y \mathbf{e}_{00} + \Delta) .$$
 (5.8)

2. Closely related to the production matrix $P(y,z) = B_z \Delta DT_y D^{-1}$ are

$$\widehat{P}(y,z) = B_z DT_y D^{-1} \Delta \quad \text{and} \quad \widehat{P}'(y,z) = \Delta B_z DT_y D^{-1} .$$
(5.9)

It was shown in [43, Section 4.3] that $\widehat{P}(y, z)$ is the production matrix for $\mathsf{F}(y, z) = (f_{n,k}(y,z))_{n,k\geq 0}$ where $f_{n,k}(y,z)$ counts k-component forests of rooted trees on the vertex set [n] with a weight y (resp. z) for each improper (resp. proper) edge. Likewise, $\widehat{P}'(y,z) = \Delta \widehat{P}(y,z)\Delta^{\mathrm{T}}$ is the production matrix for $\mathsf{F}'(y,z) = \Delta \mathsf{F}(y,z)\Delta^{\mathrm{T}} = (f_{n+1,k+1}(y,z))_{n,k\geq 0}$. All three production matrices correspond to the same A-series $A(s) = e^{zs}/(1-ys)$, but with different splittings into Φ and Ψ .

5.3. The matrix $\mathbf{T}(y, \phi)$

The proof is similar to that in the preceding subsections, but a bit of care is needed to handle the case in which the ring R does not contain the rationals.

Proof of Theorem 1.8. We start by letting $\phi = (\phi_m)_{m \ge 0}$ be indeterminates, and working in the ring $\mathbb{Q}[y, \phi]$.

By Corollary 4.9, the exponential Riordan array $\mathsf{T}(y, \phi)$ has $\Phi(s) = \sum_{m=0}^{\infty} \phi_m s^m$ and $\Psi(s) = 1/(1-ys)$, so $\psi_m = y^m$. We therefore have $\mathsf{T}(y, \phi) = \mathcal{O}(P)$ and more generally $\mathsf{T}(y, \phi)B_x = \mathcal{O}(B_x^{-1}PB_x)$, where Proposition 2.14 and Lemma 2.17 tell us that

$$B_x^{-1} P B_x = [D T_{\infty}(\phi) D^{-1}] (\Delta + xI) [D T_{\infty}(\psi) D^{-1}].$$
 (5.10)

We now use the definition (2.32) to rewrite this as

$$B_x^{-1} P B_x = T_{\infty}(\boldsymbol{\phi})^{\sharp} \left(\Delta + xI\right) T_{\infty}(\boldsymbol{\psi})^{\sharp} .$$
(5.11)

Having done this, the equality $\mathsf{T}(y, \phi)B_x = \mathcal{O}(B_x^{-1}PB_x)$ is now a valid identity in the ring $\mathbb{Z}[y, \phi]$. We can therefore now substitute elements ϕ in any commutative ring R for the indeterminates ϕ , and the identity still holds.

By hypothesis the sequence ϕ is Toeplitz-totally positive in the ring R. By Lemma 2.4, the sequence ψ is Toeplitz-totally positive in the ring $\mathbb{Z}[y]$ equipped with the coefficientwise order. By Lemma 2.20, the matrices $T_{\infty}(\phi)^{\sharp}$ and $T_{\infty}(\psi)^{\sharp}$ are also totally positive. Therefore $B_x^{-1}PB_x$ is totally positive in the ring R[x, y] equipped with the coefficientwise order. Lemma 2.6 and Theorem 2.8 then yield Theorem 1.8. \Box

Proposition 5.3 (Production matrix for $T(y, \phi)$). The production matrix $P(y, \phi) = T(y, \phi)^{-1} \Delta T(y, \phi)$ is the unit-lower-Hessenberg matrix

$$P(y,\phi) = T_{\infty}(\phi)^{\sharp} \Delta T_{y}^{\sharp}$$
(5.12)

where T_u is the Toeplitz matrix of powers (2.2), and \sharp is defined in (2.32). More generally,

$$B_{\xi}^{-1}P(y,\phi)B_{\xi} = T_{\infty}(\phi)^{\sharp} \left(\Delta + \xi I\right)T_{y}^{\sharp}.$$
(5.13)

Remark.

1. The zeroth and first columns of the matrix $P(y, \phi)$ satisfy $p_{n,0} = yp_{n,1}$, for exactly the same reasons as were observed for P(y, z). This implies the factorization

$$P(y, \boldsymbol{\phi}) = P(y, \boldsymbol{\phi}) \Delta^{\mathrm{T}} \left(y \, \mathbf{e}_{00} + \Delta \right) \,. \tag{5.14}$$

2. Closely related to the production matrix $P(y, \phi) = T_{\infty}(\phi)^{\sharp} \Delta T_{y}^{\sharp}$ are

$$\widehat{P}(y,\phi) = T_{\infty}(\phi)^{\sharp} T_{y}^{\sharp} \Delta \quad \text{and} \quad \widehat{P}'(y,\phi) = \Delta T_{\infty}(\phi)^{\sharp} T_{y}^{\sharp} .$$
(5.15)

It was shown in [43, Section 4.4] that $\hat{P}(y, \phi)$ is the production matrix for $\mathsf{F}(y, \phi) = (f_{n,k}(y, \phi))_{n,k\geq 0}$ where $f_{n,k}(y, \phi)$ counts k-component forests of rooted trees on the vertex set [n] with a weight y for each improper edge and a weight $\hat{\phi}_m \stackrel{\text{def}}{=} m! \phi_m$ for each vertex with m proper children. Likewise, $\hat{P}'(y, \phi) = \Delta \hat{P}(y, \phi) \Delta^{\mathrm{T}}$ is the production matrix for $\mathsf{F}'(y, \phi) = \Delta \mathsf{F}(y, \phi) \Delta^{\mathrm{T}} = (f_{n+1,k+1}(y, \phi))_{n,k\geq 0}$. All three production matrices correspond to the same A-series $A(s) = \Phi(s)/(1-ys)$, but with different splittings into Φ and Ψ .

5.4. More on the production matrix for T

We now wish to say a bit more about the production matrix P for the tree matrix T. We begin by giving an explicit formula: **Proposition 5.4.** The production matrix $P = T^{-1}\Delta T$ is the unit-lower-Hessenberg matrix with entries

$$p_{n,k} = n \binom{n}{k} S_{n-k} + \binom{n+1}{k}$$
(5.16a)

$$=\frac{n!}{k!(n-k+1)!}(nS_{n-k+1}+1)$$
(5.16b)

where S_m denotes the ordered subset number [32, A000522]

$$S_m \stackrel{\text{def}}{=} \sum_{k=0}^m \frac{m!}{k!} \,. \tag{5.17}$$

These matrix elements satisfy in particular $p_{n,0} = p_{n,1} = nS_n + 1$ for all $n \ge 0$.

The formula (5.16) has a very easy proof, based on the theory of exponential Riordan arrays together with our formulae for A(s) and Z(s); we give here this proof. On the other hand, it is also of some interest to see that this production matrix can be derived by "elementary" algebraic methods, without relying on the machinery of exponential Riordan arrays or on any combinatorial interpretation; this second proof can be found in arXiv:2302.03999v1.

First Proof of Proposition 5.4. From $A(s) = e^s/(1-s)$ we have

$$a_n = \sum_{j=0}^n \frac{1}{j!} = \frac{S_n}{n!} .$$
 (5.18)

From $Z(s) = e^s/(1-s)^2$ we have

$$z_n = \sum_{j=0}^n \frac{n+1-j}{j!} = n \sum_{j=0}^n \frac{1}{j!} + \frac{1}{n!} = \frac{nS_n+1}{n!} .$$
 (5.19)

Theorem 2.13 and (2.15) give

$$p_{n,k} = \frac{n!}{k!} \left(z_{n-k} + k \, a_{n-k+1} \right), \tag{5.20}$$

and a little algebra leads to (5.16a,b). It is then easy to see that $p_{n,0} = p_{n,1} = nS_n + 1$. \Box

Remarks.

1. The first few rows of this production matrix are

This matrix P (or its lower-triangular variant $P\Delta^{\rm T}$ in which the zeroth column is deleted) is not currently in [32]. However, the zeroth and first columns are [32, A001339], and the second column $p_{n,2} = nS_n/2$ is [32, A036919].

- 2. As mentioned earlier, it is not an accident that $p_{n,0} = p_{n,1}$: by Lemma 2.19 this reflects the fact that $\Psi(s) = 1/(1-s)$, or equivalently that $t_{n,0} = t_{n,1}$. For the same reason, the production matrices P(y, z) and $P(y, \phi)$ satisfy $p_{n,0} = yp_{n,1}$.
- 3. The ordered subset numbers satisfy the recurrence $S_m = mS_{m-1} + 1$.

Let us now state some further properties of the matrix elements $p_{n,k}$:

Proposition 5.5. Define the matrix $P = (p_{n,k})_{n,k>0}$ by (5.16)/(5.17). Then:

(a) The $p_{n,k}$ are nonnegative integers that satisfy the backward recurrence

$$p_{n,k} = (k+1)p_{n,k+1} + \binom{n}{k-1}$$
(5.22)

with initial condition $p_{n,n+1} = 1$. (b) The $p_{n,k}$ are also given by

$$p_{n,k} = \frac{nS_n - Q_k(n)}{k!} , \qquad (5.23)$$

where

$$Q_k(n) = -1 + \sum_{j=2}^k (j-1)! \binom{n}{j-2}$$
(5.24a)

$$= -1 + \sum_{j=2}^{k} (j-1) n^{j-2}$$
 (5.24b)

are polynomials in n with integer coefficients. In particular, $Q_0(n) = Q_1(n) = -1$ and $Q_2(n) = 0$, so that $p_{n,0} = p_{n,1} = nS_n + 1$ and $p_{n,2} = nS_n/2$.

The proof, plus some further remarks, can be found at arXiv:2302.03999v1.

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