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We build, from the collection of all groups of unitriangular matrices, Hopf monoids in Joyal's category of species. Such structure is carried by the collection of class function spaces on those groups and also by the collection of superclass function spaces in the sense of Diaconis and Isaacs. Superclasses of unitriangular matrices admit a simple description from which we deduce a combinatorial model for the Hopf monoid of superclass functions in terms of the Hadamard product of the Hopf monoids of linear orders and of set partitions. This implies a recent result relating the Hopf algebra of superclass functions on unitriangular matrices to symmetric functions in noncommuting variables. We determine the algebraic structure of the Hopf monoid: it is a free monoid in species with the canonical Hopf structure. As an application, we derive certain estimates on the number of conjugacy classes of unitriangular matrices.

Introduction

A Hopf monoid (in Joyal's category of species) is an algebraic structure akin to that of a Hopf algebra. Combinatorial structures that compose and decompose give rise to Hopf monoids. These objects are the subject of [Aguiar and Mahajan 2010, Part II]. The few basic notions and examples needed for our purposes are reviewed in Section 1, including the Hopf monoids of linear orders, set partitions, and simple graphs and the Hadamard product of Hopf monoids.

The main goal of this paper is to construct a Hopf monoid out of the groups of unitriangular matrices with entries in a finite field and to do this in a transparent manner. The structure exists on the collection of function spaces on these groups and also on the collections of class function and superclass function spaces. It is induced by two simple operations on this collection of groups: the passage from a

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matrix to its principal minors gives rise to the product, and direct sum of matrices gives rise to the coproduct.

Class functions are defined for arbitrary groups. An abstract notion and theory of superclass functions (and supercharacters) for arbitrary groups exists [Diaconis and Isaacs 2008]. While a given group may admit several such theories, there is a canonical choice of superclasses for a special class of groups known as algebra groups. These notions are briefly discussed in Section 4.1. Unitriangular groups are the prototype of such groups, and we employ the corresponding notion of superclasses in Section 4.2. The study of unitriangular superclasses and supercharacters was initiated in [André 1995a; 1995b], making use of the method of Kirillov [1995], and by more elementary means in [Yan 2001].

Preliminaries on unitriangular matrices are discussed in Section 2. The Hopf monoids f(U) of functions and cf(U) of class functions are constructed in Section 3. The nature of the construction is fairly general; in particular, the same procedure yields the Hopf monoid scf(U) of superclass functions in Section 4.2.

Unitriangular matrices over \mathbb{F}_2 may be identified with simple graphs, and direct sums and the passage to principal minors correspond to simple operations on graphs. This yields a combinatorial model for f(U) in terms of the Hadamard product of the Hopf monoids of linear orders and of graphs, as discussed in Section 3.6. The conjugacy classes on the unitriangular groups exhibit great complexity and considerable attention has been devoted to their study [Goodwin 2006; Higman 1960; Kirillov 1995; Vera-López et al. 2008]. We do not attempt an explicit combinatorial description of the Hopf monoid cf(U). On the other hand, superclasses are wellunderstood (Section 4.3), and such a combinatorial description exists for scf(U). In Section 4.5, we obtain a combinatorial model in terms of the Hadamard product of the Hopf monoids of linear orders and of set partitions. This has as a consequence the main result of [Aguiar et al. 2012], as we explain in Section 6.2.

Employing the combinatorial models, we derive structure theorems for the Hopf monoids f(U) and scf(U) in Section 5. Our main results state that both are free monoids with the canonical Hopf structure (in which the generators are primitive).

Applications are presented in Section 6. With the aid of Lagrange's theorem for Hopf monoids, one may derive estimates on the number of conjugacy classes of unitriangular matrices in the form of certain recursive inequalities. We obtain this application in Section 6.1, where we also formulate a refinement of Higman's conjecture on the polynomiality of these numbers. Other applications involving the Hopf algebra of superclass functions of [Aguiar et al. 2012] are given in Section 6.2.

We employ two fields: the *base* field \Bbbk and the field of *matrix entries* \mathbb{F} . We consider algebras and groups of matrices with entries in \mathbb{F} ; all other vector spaces are over \Bbbk . The field of matrix entries is often assumed to be finite and sometimes to be \mathbb{F}_2 .

1. Hopf monoids

We review the basics on Hopf monoids and recall three examples built from linear orders, set partitions, and simple graphs, respectively. We also consider the Hadamard product of Hopf monoids. In later sections, Hopf monoids are built from functions on unitriangular matrices. The constructions of this section will allow us to provide combinatorial models for them.

1.1. Species and Hopf monoids. For the precise definitions of vector species and Hopf monoid, we refer to [Aguiar and Mahajan 2010, Chapter 8]. The main ingredients are reviewed below.

A vector species p is a collection of vector spaces p[I], one for each finite set I, equivariant with respect to bijections $I \cong J$. A morphism of species $f : p \to q$ is a collection of linear maps $f_I : p[I] \to q[I]$ that commute with bijections.

A *decomposition* of a finite set I is a finite sequence (S_1, \ldots, S_k) of disjoint subsets of I whose union is I. In this situation, we write

$$I = S_1 \sqcup \cdots \sqcup S_k.$$

A *Hopf monoid* consists of a vector species h equipped with two collections μ and Δ of linear maps

$$h[S_1] \otimes h[S_2] \xrightarrow{\mu_{S_1,S_2}} h[I] \text{ and } h[I] \xrightarrow{\Delta_{S_1,S_2}} h[S_1] \otimes h[S_2].$$

There is one map in each collection for each finite set *I* and each decomposition $I = S_1 \sqcup S_2$. This data is subject to a number of axioms, of which the main ones follow.

Associativity. For each decomposition $I = S_1 \sqcup S_2 \sqcup S_3$, the diagrams

commute.

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Compatibility. Fix decompositions $S_1 \sqcup S_2 = I = T_1 \sqcup T_2$, and consider the resulting pairwise intersections

 $A := S_1 \cap T_1$, $B := S_1 \cap T_2$, $C := S_2 \cap T_1$, and $D := S_2 \cap T_2$,

as illustrated below:

For any such pair of decompositions, the diagram

$$\begin{split} \boldsymbol{h}[A] \otimes \boldsymbol{h}[B] \otimes \boldsymbol{h}[C] \otimes \boldsymbol{h}[D] & \stackrel{\cong}{\longrightarrow} \boldsymbol{h}[A] \otimes \boldsymbol{h}[C] \otimes \boldsymbol{h}[B] \otimes \boldsymbol{h}[D] \\ & \stackrel{\Delta_{A,B} \otimes \Delta_{C,D}}{\uparrow} & \stackrel{\downarrow}{\bigvee} \mu_{A,C} \otimes \mu_{B,D} & (4) \\ & \boldsymbol{h}[S_1] \otimes \boldsymbol{h}[S_2] \xrightarrow{\mu_{S_1,S_2}} \boldsymbol{h}[I] \xrightarrow{\Delta_{T_1,T_2}} \boldsymbol{h}[T_1] \otimes \boldsymbol{h}[T_2] \end{split}$$

must commute. The top arrow stands for the map that interchanges the middle factors.

In addition, the Hopf monoid **h** is *connected* if $h[\emptyset] = \mathbb{k}$ and the maps

$$h[I] \otimes h[\emptyset] \xrightarrow{\mu_{I,\emptyset}} h[I]$$
 and $h[\emptyset] \otimes h[I] \xrightarrow{\mu_{\emptyset,I}} h[I]$

are the canonical identifications.

The collection μ is the *product*, and the collection Δ is the *coproduct* of the Hopf monoid **h**.

A Hopf monoid is (co)commutative if the left (right) diagram below commutes for all decompositions $I = S_1 \sqcup S_2$:

$$h[S_1] \otimes h[S_2] \xrightarrow{\cong} h[S_2] \otimes h[S_1] \qquad h[S_1] \otimes h[S_2] \xrightarrow{\cong} h[S_2] \otimes h[S_1]$$

$$\mu_{S_1,S_2} \qquad \mu_{S_2,S_1} \qquad \Delta_{S_1,S_2} \qquad h[I] \qquad (5)$$

The top arrows stand for the map that interchanges the factors.

A morphism of Hopf monoids $f : h \to k$ is a morphism of species that commutes with μ and Δ .

1.2. *The Hopf monoid of linear orders.* For any finite set *I*, L[I] is the set of all linear orders on *I*. For instance, if $I = \{a, b, c\}$,

$$L[I] = \{abc, bac, acb, bca, cab, cba\}.$$

Let L[I] denote the vector space with basis L[I]. The collection L is a vector species.

Let $I = S_1 \sqcup S_2$. Given linear orders ℓ_i on S_i , i = 1, 2, their concatenation $\ell_1 \cdot \ell_2$ is a linear order on I. This is the list consisting of the elements of S_1 as ordered by ℓ_1 followed by those of S_2 as ordered by ℓ_2 . Given a linear order ℓ on I and $S \subseteq I$, the restriction $\ell|_S$ (the list consisting of the elements of S written in the order in which they appear in ℓ) is a linear order on S. These operations give rise to maps

$$\begin{array}{ccc}
L[S_1] \times L[S_2] \to L[I], \\
(\ell_1, \ell_2) \mapsto \ell_1 \cdot \ell_2
\end{array} \quad \text{and} \quad \begin{array}{ccc}
L[I] \to L[S_1] \times L[S_2], \\
\ell \mapsto (\ell|_{S_1}, \ell|_{S_2}).
\end{array}$$
(6)

Extending by linearity, we obtain linear maps

$$\mu_{S_1,S_2}: L[S_1] \otimes L[S_2] \rightarrow L[I]$$
 and $\Delta_{S_1,S_2}: L[I] \rightarrow L[S_1] \otimes L[S_2]$

that turn L into a Hopf monoid. For instance, given linear orders ℓ_i on S_i , i = 1, 2, the commutativity of (4) boils down to the fact that the concatenation of $\ell_1|_A$ and $\ell_2|_C$ agrees with the restriction to T_1 of $\ell_1 \cdot \ell_2$. The Hopf monoid L is cocommutative but not commutative. For more details, see [Aguiar and Mahajan 2010, Section 8.5].

1.3. *The Hopf monoid of set partitions.* A *partition* of a finite set *I* is a collection *X* of disjoint nonempty subsets whose union is *I*. The subsets are the *blocks* of *X*.

Given a partition X of I and $S \subseteq I$, the restriction $X|_S$ is the partition of S whose blocks are the nonempty intersections of the blocks of X with S. Let $I = S_1 \sqcup S_2$. Given partitions X_i of S_i , i = 1, 2, their union is the partition $X_1 \sqcup X_2$ of I whose blocks are the blocks of X_1 and the blocks of X_2 . A quasishuffle of X_1 and X_2 is any partition of I whose restriction to S_i is X_i , i = 1, 2.

Let $\Pi[I]$ denote the set of partitions of I and $\Pi[I]$ the vector space with basis $\Pi[I]$. A Hopf monoid structure on Π is defined and studied in [Aguiar and Mahajan 2010, Section 12.6]. Among its various linear bases, we are interested in the basis $\{m_X\}$ on which the operations are as follows. The product

$$\mu_{S_1,S_2}: \mathbf{\Pi}[S_1] \otimes \mathbf{\Pi}[S_2] \to \mathbf{\Pi}[I]$$

is given by

$$\mu_{S_1,S_2}(m_{X_1} \otimes m_{X_2}) = \sum_{\substack{X: \ X \mid S_1 = X_1 \\ X \mid S_2 = X_2}} m_X.$$
(7)

The coproduct

$$\Delta_{S_1,S_2}: \mathbf{\Pi}[I] \to \mathbf{\Pi}[S_1] \otimes \mathbf{\Pi}[S_2]$$

is given by

$$\Delta_{S_1,S_2}(m_X) = \begin{cases} m_{X|_{S_1}} \otimes m_{X|_{S_2}} & \text{if } S_1 \text{ is the union of some blocks of } X, \\ 0 & \text{otherwise.} \end{cases}$$
(8)

Note that the following conditions are equivalent for a partition X of I:

- S_1 is the union of some blocks of X.
- S_2 is the union of some blocks of X.
- $X = X|_{S_1} \sqcup X|_{S_2}.$

These operations turn the species Π into a Hopf monoid that is both commutative and cocommutative.

1.4. The Hopf monoid of simple graphs. A (simple) graph g on a finite set I is a relation on I that is symmetric and irreflexive. The elements of I are the vertices of g There is an edge between two vertices when they are related by g.

Given a graph g on I and $S \subseteq I$, the restriction $g|_S$ is the graph on S whose edges are the edges of g between elements of S. Let $I = S_1 \sqcup S_2$. Given graphs g_i of S_i , i = 1, 2, their union is the graph $g_1 \sqcup g_2$ of I whose edges are those of g_1 and those of g_2 . A quasishuffle of g_1 and g_2 is any graph on I whose restriction to S_i is g_i , i = 1, 2.

Let G[1] denote the set of graphs on I and G[1] the vector space with basis G[1]. A Hopf monoid structure on G is defined and studied in [Aguiar and Mahajan 2010, Section 13.2]. We are interested in the basis $\{m_g\}$ on which the operations are as follows. The product

$$\mu_{S_1,S_2}: \boldsymbol{G}[S_1] \otimes \boldsymbol{G}[S_2] \to \boldsymbol{G}[I]$$

is given by

$$\mu_{S_1,S_2}(m_{g_1} \otimes m_{g_2}) = \sum_{\substack{g: g \mid S_1 = g_1 \\ g \mid S_2 = g_2}} m_g.$$
(9)

The coproduct

$$\Delta_{S_1,S_2}: \boldsymbol{G}[I] \to \boldsymbol{G}[S_1] \otimes \boldsymbol{G}[S_2]$$

is given by

$$\Delta_{S_1,S_2}(m_g) = \begin{cases} m_{g|_{S_1}} \otimes m_{g|_{S_2}} & \text{if no edge of } g \text{ connects } S_1 \text{ to } S_2, \\ 0 & \text{otherwise.} \end{cases}$$
(10)

Note that no edge of g connects S_1 to S_2 if and only if $g = g|_{S_1} \sqcup g|_{S_2}$.

These operations turn the species G into a Hopf monoid that is both commutative and cocommutative.

Remark 1. The dual of a species p is the collection p^* of dual vector spaces: $p^*[I] = p[I]^*$. A species p is said to be finite-dimensional if each space p[I] is finite-dimensional. Dualizing the operations of a finite-dimensional Hopf monoid h, one obtains a Hopf monoid h^* . The Hopf monoid h is called self-dual if $h \cong h^*$. In general, such isomorphism is not unique.

Over a field of characteristic 0, a Hopf monoid that is connected, commutative, and cocommutative is always self-dual. This is a consequence of the Cartier–Milnor–Moore theorem. (The isomorphism with the dual is not canonical.)

In particular, the Hopf monoids Π and G are self-dual. In [Aguiar and Mahajan 2010], the preceding descriptions of these Hopf monoids are stated in terms of their duals Π^* and G^* . A different description of Π is given in [Aguiar and Mahajan 2010, Section 12.6.2]. To reconcile the two, one should use the explicit isomorphism $\Pi \cong \Pi^*$ given in [Aguiar and Mahajan 2010, Proposition 12.48].

1.5. *The Hadamard product.* Given species p and q, their *Hadamard product* is the species $p \times q$ defined by

$$(\boldsymbol{p} \times \boldsymbol{q})[I] = \boldsymbol{p}[I] \otimes \boldsymbol{q}[I].$$

If **h** and **k** are Hopf monoids, then so is $h \times k$ with the following operations. Let $I = S_1 \sqcup S_2$. The product is

and the coproduct is defined dually. If h and k are (co)commutative, then so is $h \times k$. For more details, see [Aguiar and Mahajan 2010, Section 8.13].

2. Unitriangular matrices

This section sets up the basic notation pertaining to unitriangular matrices and discusses two simple but important constructions: direct sum of matrices and the passage from a matrix to its principal minors. The Hopf monoid constructions of later sections are based on them. The key results are Lemmas 2 and 3. The former is the reason why we must use unitriangular matrices: for arbitrary matrices, the passage to principal minors is not multiplicative. The latter will be responsible (in later sections) for the necessary compatibility between the product and coproduct of the Hopf monoids.

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Let \mathbb{F} be a field, *I* a finite set, and ℓ a linear order on *I*. Let M(*I*) denote the algebra of matrices

$$A = (a_{ij})_{i,j \in I}, \quad a_{ij} \in \mathbb{F} \text{ for all } i, j \in I.$$

The general linear group GL(I) consists of the invertible matrices in M(I), and the subgroup $U(I, \ell)$ consists of the *upper* ℓ -*unitriangular* matrices

$$U = (u_{ij})_{i,j \in I}, \quad u_{ii} = 1 \text{ for all } i \in I \text{ and } u_{ij} = 0 \text{ whenever } i >_{\ell} j.$$

If ℓ' is another linear order on *I*, then $U(I, \ell)$ and $U(I, \ell')$ are conjugate subgroups of GL(I). However, we want to keep track of all groups in this collection and of the manner in which they interact.

2.1. Direct sum of matrices. Suppose $I = S_1 \sqcup S_2$ is a decomposition. Given $A = (a_{ij}) \in M(S_1)$ and $B = (b_{ij}) \in M(S_2)$, their direct sum is

$$A \oplus B = (c_{ij}) \in \mathbf{M}(I),$$

the matrix with entries

$$c_{ij} = \begin{cases} a_{ij} & \text{if both } i, j \in S_1, \\ b_{ij} & \text{if both } i, j \in S_2, \\ 0 & \text{otherwise.} \end{cases}$$

Let $\ell \in L[I]$. The direct sum of an $\ell|_{S_1}$ -unitriangular and an $\ell|_{S_2}$ -unitriangular matrix is ℓ -unitriangular. The morphism of algebras

$$M(S_1) \times M(S_2) \to M(I), \quad (A, B) \mapsto A \oplus B$$

thus restricts to a morphism of groups

$$\sigma_{S_1, S_2} : \mathrm{U}(S_1, \ell|_{S_1}) \times \mathrm{U}(S_2, \ell|_{S_2}) \to \mathrm{U}(I, \ell).$$
(11)

(The dependence of σ_{S_1,S_2} on ℓ is left implicit.)

Direct sum of matrices is associative; thus, for any decomposition $I = S_1 \sqcup S_2 \sqcup S_3$, the diagram

$$U(S_{1}, \ell|_{S_{1}}) \times U(S_{2}, \ell|_{S_{2}}) \times U(S_{3}, \ell|_{S_{3}}) \xrightarrow{\sigma_{S_{1}, S_{2}} \times \operatorname{id}} U(S_{1} \sqcup S_{2}, \ell|_{S_{1} \sqcup S_{2}}) \times U(S_{3}, \ell|_{S_{3}})$$

$$\downarrow^{\sigma_{S_{1} \sqcup S_{2}, S_{3}}} \bigvee^{\sigma_{S_{1} \sqcup S_{2}, S_{3}}} U(S_{1} \sqcup S_{2}, \ell|_{S_{1} \sqcup S_{2}}) \times U(S_{3}, \ell|_{S_{3}}) \xrightarrow{\sigma_{S_{1}, S_{2} \sqcup S_{3}}} U(S_{1} \sqcup S_{2}, \ell|_{S_{1} \sqcup S_{2}}) \times U(S_{3}, \ell|_{S_{3}})$$

$$\downarrow^{\sigma_{S_{1} \sqcup S_{2}, S_{3}}} U(I, \ell)$$

commutes. Note also that, with these definitions, $A \oplus B$ and $B \oplus A$ are the same matrix. Thus, the following diagram commutes:

$$U(S_1, \ell|_{S_1}) \times U(S_2, \ell|_{S_2}) \xrightarrow{\cong} U(S_2, \ell|_{S_2}) \times U(S_1, \ell|_{S_1})$$

$$(13)$$

$$U(S_1 \sqcup S_2, \ell)$$

2.2. *Principal minors.* Given $A = (a_{ij}) \in M(I)$, the *principal minor* indexed by $S \subseteq I$ is the matrix

$$A_S = (a_{ij})_{i,j \in S}.$$

In general, A_S is not invertible even if A is. In addition, the assignment $A \mapsto A_S$ does not preserve multiplications. On the other hand, if U is ℓ -unitriangular, then U_S is $\ell|_S$ -unitriangular. In regard to multiplicativity, we have the following basic fact.

We say that *S* is an ℓ -segment if $i, k \in S$ and $i <_{\ell} j <_{\ell} k$ imply that also $j \in S$.

Let $E_{ij} \in M(I)$ denote the *elementary* matrix in which the (i, j) entry is 1 and all other entries are 0.

Lemma 2. Let $\ell \in L[I]$ and $S \subseteq I$. The map

$$U(I, \ell) \to U(S, \ell|_S), \quad U \mapsto U_S$$

is a morphism of groups if and only if S is an ℓ -segment.

Proof. Suppose the map is a morphism of groups. Let $i, j, k \in I$ be such that $i, k \in S$ and $i <_{\ell} j <_{\ell} k$. The matrices

$$\mathrm{Id} + E_{ij}$$
 and $\mathrm{Id} + E_{jk}$

are in $U(I, \ell)$, and

$$(\mathrm{Id} + E_{ij}) \cdot (\mathrm{Id} + E_{jk}) = \mathrm{Id} + E_{ij} + E_{jk} + E_{ik}$$

If $j \notin S$, then the two matrices are in the kernel of the map while their product is mapped to Id + $E_{ik} \neq$ Id. Thus, $j \in S$ and S is an ℓ -segment.

The converse implication follows from the fact that if U and V are ℓ -unitriangular, then the (i, k) entry of UV is

$$\sum_{\leq \ell j \leq \ell k} u_{ij} v_{jk}.$$

Let $I = S_1 \sqcup S_2$ be a decomposition with $\ell_i \in L[S_i]$, i = 1, 2. We define a map

i

$$\pi_{S_1, S_2} : \mathrm{U}(I, \ell_1 \cdot \ell_2) \to \mathrm{U}(S_1, \ell_1) \times \mathrm{U}(S_2, \ell_2) \tag{14}$$

by

$$U \mapsto (U_{S_1}, U_{S_2}).$$

Note that S_1 is an initial segment for $\ell_1 \cdot \ell_2$ and S_2 is a final segment for $\ell_1 \cdot \ell_2$. Thus, π_{S_1,S_2} is a morphism of groups by Lemma 2.

If $R \subseteq S \subseteq I$, then $(A_S)_R = A_R$. This implies the following commutativity for any decomposition $I = S_1 \sqcup S_2 \sqcup S_3$ and $\ell_i \in L[S_i]$, i = 1, 2, 3:

$$\begin{array}{c}
 U(I, \ell_1 \cdot \ell_2 \cdot \ell_3) \xrightarrow{\pi_{S_1 \sqcup S_2, S_3}} U(S_1 \sqcup S_2, \ell_1 \cdot \ell_2) \times U(S_3, \ell_3) \\ \pi_{S_1, S_2 \sqcup S_3} \downarrow & \downarrow \\
 U(S_1, \ell_1) \times U(S_2 \sqcup S_3, \ell_2 \cdot \ell_3) \xrightarrow{\pi_{S_1 \sqcup S_2, S_3}} U(S_1, \ell_1) \times U(S_2, \ell_2) \times U(S_3, \ell_3)
\end{array}$$
(15)

2.3. *Direct sums and principal minors.* The following key result relates the collection of morphisms σ to the collection π :

Lemma 3. Fix two decompositions $I = S_1 \sqcup S_2 = T_1 \sqcup T_2$, and let A, B, C, and D be the resulting intersections, as in (3). Let ℓ_i be a linear order on S_i , i = 1, 2, and $\ell = \ell_1 \cdot \ell_2$. Then the following diagram commutes:

$$\begin{array}{c|c}
\mathbf{U}(T_{1},\ell|_{T_{1}}) \times \mathbf{U}(T_{2},\ell|_{T_{2}}) \xrightarrow{\pi_{A,C} \times \pi_{B,D}} \mathbf{U}(A,\ell_{1}|_{A}) \times \mathbf{U}(C,\ell_{2}|_{C}) \\ \times \mathbf{U}(B,\ell_{1}|_{B}) \times \mathbf{U}(D,\ell_{2}|_{D}) \\ & \sigma_{T_{1},T_{2}} \\ & \mathbf{U}(I,\ell) \\ & \pi_{S_{1},S_{2}} \\ & \mathbf{U}(S_{1},\ell_{1}) \times \mathbf{U}(S_{2},\ell_{2}) \xleftarrow{\sigma_{A,B} \times \sigma_{C,D}} \mathbf{U}(A,\ell_{1}|_{A}) \times \mathbf{U}(B,\ell_{1}|_{B}) \\ \times \mathbf{U}(C,\ell_{2}|_{C}) \times \mathbf{U}(D,\ell_{2}|_{D}) \end{array}$$

$$(16)$$

Proof. First note that since $\ell|_{T_1} = (\ell_1|_A) \cdot (\ell_2|_C)$, $\pi_{A,C}$ does map as stated in the diagram and similarly for $\pi_{B,D}$. The commutativity of the diagram boils down to the simple fact that

$$(U \oplus V)_{S_1} = U_A \oplus V_B$$

(and a similar statement for S_2 , C, and D). This holds for any $U \in M(T_1)$ and $V \in M(T_2)$.

3. A Hopf monoid of (class) functions

We employ the operations of Section 2 (direct sum of matrices and the passage from a matrix to its principal minors) to build a Hopf monoid structure on the collection of function spaces on unitriangular matrices. The collection of class function spaces gives rise to a Hopf submonoid. With matrix entries in \mathbb{F}_2 , the Hopf monoid of functions may be identified with the Hadamard product of the Hopf monoids of linear orders and of simple graphs.

3.1. *Functions.* Given a set *X*, let f(X) denote the vector space of functions on *X* with values on the base field \Bbbk . The functor

$$f: {sets} \rightarrow {vector spaces}$$

is contravariant. If at least one of two sets X_1 and X_2 is finite, then there is a canonical isomorphism

$$\mathbf{f}(X_1 \times X_2) \cong \mathbf{f}(X_1) \otimes \mathbf{f}(X_2). \tag{17}$$

A function $f \in \mathbf{f}(X_1 \times X_2)$ corresponds to $\sum_i f_i^1 \otimes f_i^2 \in \mathbf{f}(X_1) \otimes \mathbf{f}(X_2)$ if and only if

$$f(x_1, x_2) = \sum_i f_i^1(x_1) f_i^2(x_2)$$
 for all $x_1 \in X_1$ and $x_2 \in X_2$.

Given an element $x \in X$, let $\kappa_x : X \to \Bbbk$ denote its characteristic function:

$$\kappa_x(y) = \begin{cases} 1 & \text{if } y = x, \\ 0 & \text{if not.} \end{cases}$$
(18)

Suppose now that X is finite. As x runs over the elements of X, the functions κ_x form a linear basis of f(X). If $\varphi : X \to X'$ is a function and x' is an element of X', then

$$\kappa_{x'} \circ \varphi = \sum_{\varphi(x)=x'} \kappa_x.$$
⁽¹⁹⁾

Under (17),

$$\kappa_{(x_1,x_2)} \leftrightarrow \kappa_{x_1} \otimes \kappa_{x_2}. \tag{20}$$

3.2. Class functions on groups. Given a group G, let cf(G) denote the vector space of *class functions* on G. These are the functions $f : G \to \mathbb{k}$ that are constant on conjugacy classes of G. If $\varphi : G \to G'$ is a morphism of groups and f is a class function on G', then $f \circ \varphi$ is a class function on G. In this manner,

 $cf: \{groups\} \rightarrow \{vector spaces\}$

is a contravariant functor. If at least one of two groups G_1 and G_2 is finite, then there is a canonical isomorphism

$$\mathbf{cf}(G_1 \times G_2) \cong \mathbf{cf}(G_1) \otimes \mathbf{cf}(G_2) \tag{21}$$

obtained by restriction from the isomorphism (17).

Given a conjugacy class *C* of *G*, let $\kappa_C : G \to \Bbbk$ denote its characteristic function:

$$\kappa_C(x) = \begin{cases} 1 & \text{if } x \in C, \\ 0 & \text{if not.} \end{cases}$$
(22)

Suppose *G* has finitely many conjugacy classes. As *C* runs over the conjugacy classes of *G*, the functions κ_C form a linear basis of cf(G). If *C*' is a conjugacy class of *G*', then

$$\kappa_{C'} \circ \varphi = \sum_{\varphi(C) \subseteq C'} \kappa_C.$$
⁽²³⁾

The conjugacy classes of $G_1 \times G_2$ are of the form $C_1 \times C_2$, where C_i is a conjugacy class of G_i , i = 1, 2. Under (21),

$$\kappa_{C_1 \times C_2} \leftrightarrow \kappa_{C_1} \otimes \kappa_{C_2}. \tag{24}$$

3.3. *Functions on unitriangular matrices.* We assume for the rest of this section that the field \mathbb{F} of matrix entries is finite. Thus, all groups U(*I*, ℓ) of unitriangular matrices are finite.

We define a vector species $\mathbf{f}(U)$ as follows. On a finite set *I*,

$$\mathbf{f}(\mathbf{U})[I] = \bigoplus_{\ell \in \mathbf{L}[I]} \mathbf{f}(\mathbf{U}(I, \ell)).$$

In other words, f(U)[I] is the direct sum of the spaces of functions on all unitriangular groups on *I*. A bijection $\sigma : I \cong J$ induces an isomorphism $U(I, \ell) \cong U(J, \sigma \cdot \ell)$ and therefore an isomorphism $f(U)[I] \cong f(U)[J]$. Thus, f(U) is a species.

Let $I = S_1 \sqcup S_2$ and $\ell_i \in L[S_i]$, i = 1, 2. Applying the functor **f** to the morphism π_{S_1, S_2} in (14) and composing with the isomorphism in (17), we obtain a linear map

$$\mathbf{f}(\mathbf{U}(S_1,\ell_1)) \otimes \mathbf{f}(\mathbf{U}(S_2,\ell_2)) \to \mathbf{f}(\mathbf{U}(I,\ell_1 \cdot \ell_2))$$

Adding over all $\ell_1 \in L[S_1]$ and $\ell_2 \in L[S_2]$, we obtain a linear map

$$\mu_{S_1,S_2} : \mathbf{f}(\mathbf{U})[S_1] \otimes \mathbf{f}(\mathbf{U})[S_2] \to \mathbf{f}(\mathbf{U})[I].$$
(25)

Explicitly, given functions $f : U(S_1, \ell_1) \to \Bbbk$ and $g : U(S_2, \ell_2) \to \Bbbk$,

$$\mu_{S_1,S_2}(f\otimes g): \mathrm{U}(I,\ell_1\cdot\ell_2) \to \Bbbk$$

is the function given by

$$U \mapsto f(U_{S_1})g(U_{S_2}). \tag{26}$$

Similarly, from the map σ_{S_1,S_2} in (11), we obtain the components

$$\mathbf{f}(\mathbf{U}(I,\ell)) \to \mathbf{f}(\mathbf{U}(S_1,\ell|_{S_1})) \otimes \mathbf{f}(\mathbf{U}(S_2,\ell|_{S_2}))$$

(one for each $\ell \in L[I]$) of a linear map

$$\Delta_{S_1,S_2} : \mathbf{f}(\mathbf{U})[I] \to \mathbf{f}(\mathbf{U})[S_1] \otimes \mathbf{f}(\mathbf{U})[S_2].$$
(27)

Explicitly, given a function $f : U(I, \ell) \to \mathbb{k}$, we have $\Delta_{S_1, S_2}(f) = \sum_i f_i^1 \otimes f_i^2$, where

$$f_i^1 : \mathrm{U}(S_1, \ell|_{S_1}) \to \mathbb{k} \text{ and } f_i^2 : \mathrm{U}(S_2, \ell|_{S_2}) \to \mathbb{k}$$

are functions such that

$$f(U_1 \oplus U_2) = \sum_i f_i^{-1}(U_1) f_i^{-2}(U_2)$$

for all $U_1 \in \mathcal{U}(S_1, \ell|_{S_1})$ and $U_2 \in \mathcal{U}(S_2, \ell|_{S_2})$. (28)

Proposition 4. With the operations (25) and (27), the species f(U) is a connected Hopf monoid. It is cocommutative.

Proof. Axioms (1), (2), and (4) follow from (12), (15), and (16) by functoriality. In the same manner, cocommutativity (5) follows from (13). \Box

We describe the operations on the basis of characteristic functions (18). Let $U_i \in U(S_i, \ell_i), i = 1, 2$. It follows from (19) and (20), or from (26), that the product is

$$\mu_{S_1,S_2}(\kappa_{U_1} \otimes \kappa_{U_2}) = \sum_{\pi_{S_1,S_2}(U)=(U_1,U_2)} \kappa_U = \sum_{\substack{U_{S_1}=U_1\\U_{S_2}=U_2}} \kappa_U.$$
(29)

Similarly, the coproduct is

$$\Delta_{S_1,S_2}(\kappa_U) = \sum_{\sigma_{S_1,S_2}(U_1,U_2)=U} \kappa_{U_1} \otimes \kappa_{U_2} = \begin{cases} \kappa_{U_{S_1}} \otimes \kappa_{U_{S_2}} & \text{if } U = U_{S_1} \oplus U_{S_2}, \\ 0 & \text{otherwise.} \end{cases}$$
(30)

3.4. *Constant functions.* Let $\mathbf{1}_{\ell}$ denote the constant function on $U(I, \ell)$ with value 1. Let $I = S_1 \sqcup S_2$. It follows from (26) that

$$\mu_{S_1,S_2}(\mathbf{1}_{\ell_1}\otimes\mathbf{1}_{\ell_2})=\mathbf{1}_{\ell_1\cdot\ell_2}$$

for any $\ell_1 \in L[S_1]$ and $\ell_2 \in L[S_2]$. Similarly, we see from (28) that

$$\Delta_{S_1,S_2}(\mathbf{1}_\ell) = \mathbf{1}_{\ell|S_1} \otimes \mathbf{1}_{\ell|S_2}$$

for any $\ell \in L[I]$. We thus have:

Corollary 5. The collection of maps

$$L[I] \to \mathbf{f}(\mathbf{U})[I], \quad \ell \mapsto \mathbf{1}_{\ell}$$

is an injective morphism of Hopf monoids.

3.5. *Class functions on unitriangular matrices.* Let cf(U)[I] be the direct sum of the spaces of class functions on all unitriangular groups on *I*:

$$\mathsf{cf}(\mathsf{U})[I] = \bigoplus_{\ell \in \mathsf{L}[I]} \mathsf{cf}(\mathsf{U}(I, \ell)).$$

This defines a subspecies cf(U) of f(U).

Proceeding in the same manner as in Section 3.3, we obtain linear maps

$$\mathsf{cf}(\mathsf{U})[S_1] \otimes \mathsf{cf}(\mathsf{U})[S_2] \xrightarrow[\Delta S_1, S_2]{} \mathsf{cf}(\mathsf{U})[I]$$

by applying the functor **cf** to the morphisms π_{S_1,S_2} and σ_{S_1,S_2} . This is meaningful since the latter are morphisms of groups (in the case of π_{S_1,S_2} , by Lemma 2).

Proposition 6. With these operations, the species cf(U) is a connected cocommutative Hopf monoid. It is a Hopf submonoid of f(U).

Proof. As in the proof of Proposition 4, the first statement follows by functoriality. The second follows from the naturality of the inclusion of class functions and its compatibility with the isomorphisms in (17) and (21).

We describe the operations on the basis of characteristic functions (22). Let C_i be a conjugacy class of U(S_i , ℓ_i), i = 1, 2. It follows from (23) and (24) that the product is

$$\mu_{S_1, S_2}(\kappa_{C_1} \otimes \kappa_{C_2}) = \sum_{\pi_{S_1, S_2}(C) \subseteq C_1 \times C_2} \kappa_C,$$
(31)

where the sum is over conjugacy classes C in U(I, $\ell_1 \cdot \ell_2$). Similarly, the coproduct is

$$\Delta_{S_1,S_2}(\kappa_C) = \sum_{\sigma_{S_1,S_2}(C_1 \times C_2) \subseteq C} \kappa_{C_1} \otimes \kappa_{C_2}.$$
(32)

Here *C* is a conjugacy class of $U(I, \ell)$, and the sum is over pairs of conjugacy classes C_i of $U(S_i, \ell|_{S_i})$.

Remark 7. Let

 $\mathcal{F}: \{\text{groups}\} \rightarrow \{\text{vector spaces}\}$

be a functor that is contravariant and *bilax monoidal* in the sense of [Aguiar and Mahajan 2010, Section 3.1]. The construction of the Hopf monoids f(U) and cf(U) can be carried out for any such functor \mathcal{F} in place of cf in exactly the same manner. It can also be carried out for a covariant bilax monoidal functor \mathcal{F} in a similar manner.

3.6. *A combinatorial model.* To a unitriangular matrix $U \in U(I, \ell)$, we associate a graph g(U) on I as follows: there is an edge between i and j if i < j in ℓ and $u_{ij} \neq 0$. For example, given nonzero entries $a, b, c \in \mathbb{F}$,

$$\ell = hijk, \quad U = \begin{pmatrix} 1 & 0 & 0 & a \\ 1 & b & c \\ & 1 & 0 \\ & & 1 \end{pmatrix} \implies g(U) = \bullet_{h} \quad \bullet_{i} \quad \bullet_{j} \quad \bullet_{k} \quad (33)$$

Recall the Hopf monoids L and G and the notion of Hadamard product from Section 1. Let

$$\phi: L \times G \to f(U)$$

be the map with components

$$(L \times G)[I] \rightarrow f(U)[I]$$

given as follows. On a basis element $\ell \otimes m_g \in L[I] \otimes G[I] = (L \times G)[I]$, we set

$$\phi(\ell \otimes m_g) = \sum_{\substack{U \in \mathcal{U}(I,\ell) \\ g(U) = g}} \kappa_U \in \mathbf{f}(\mathcal{U}(I,\ell)) \subseteq \mathbf{f}(\mathcal{U})[I]$$
(34)

and extend by linearity. The map relates the *m*-basis of G to the basis of characteristic functions (18) of f(U).

Proposition 8. Let \mathbb{F} be an arbitrary finite field. The map $\phi : L \times G \to f(U)$ is an *injective morphism of Hopf monoids*.

Proof. From the definition of the Hopf monoid operations on a Hadamard product and formulas (6) and (9), it follows that

$$\mu_{S_1,S_2}\big((\ell_1\otimes m_{g_1})\otimes (\ell_2\otimes m_{g_2})\big)=\sum_{\substack{g|_{S_1}=g_1\\g|_{S_2}=g_2}}\ell_1\cdot\ell_2\otimes m_g.$$

Comparing with (29), we see that products are preserved since given $U \in U(I, \ell)$, we have

$$g(U_{S_i}) = g(U)|_{S_i}.$$

The verification for coproducts is similar, employing (6), (10), and (30) and the fact that given $I = S_1 \sqcup S_2$ and $U_i \in U(S_i, \ell|_{S_i})$, we have

$$g(U_1 \oplus U_2) = g(U_1) \sqcup g(U_2).$$

Consider the map $\psi : \mathbf{f}(\mathbf{U}) \to \mathbf{L} \times \mathbf{G}$ given by

$$\psi(\kappa_U) = \ell \otimes m_{g(U)} \tag{35}$$

for any $U \in U(I, \ell)$. Then

$$\psi\phi(\ell\otimes m_g) = (q-1)^{e(g)}\ell\otimes m_g,$$

where q is the cardinality of \mathbb{F} and e(g) is the number of edges in g. Thus, ϕ is injective.

We mention that the map ψ in (35) is a morphism of comonoids but not of monoids in general.

Assume now that the matrix entries are from \mathbb{F}_2 , the field with two elements. In this case, the matrix U is uniquely determined by the linear order ℓ and the graph g(U). Therefore, the map ϕ is invertible with inverse ψ .

Corollary 9. There is an isomorphism of Hopf monoids

$$f(U) \cong L \times G$$

between the Hopf monoid of functions on unitriangular matrices with entries in \mathbb{F}_2 and the Hadamard product of the Hopf monoids of linear orders and simple graphs.

On an arbitrary function $f : U(I, \ell) \to k$, the isomorphism is given by

$$\psi(f) = \ell \otimes \sum_{U \in \mathrm{U}(I,\ell)} f(U) m_{g(U)}.$$

The coefficients of the m-basis elements are the values of f.

4. A Hopf monoid of superclass functions

An abstract notion of *superclass* (and *supercharacter*) has been introduced by Diaconis and Isaacs [2008]. We only need a minimal amount of related concepts that we review in Sections 4.1 and 4.2. For this purpose, we first place ourselves in the setting of algebra groups. In Section 4.2, we construct a Hopf monoid structure on the collection of spaces of superclass functions on the unitriangular groups by the same procedure as that in Section 3. The combinatorics of these superclasses is understood from the thesis of Yan [2001] (reviewed in slightly different terms in Section 4.3), and this allows us to obtain an explicit description for the Hopf monoid of superclass functions with matrix entries in \mathbb{F}_2 to the Hadamard product of the Hopf monoids of linear orders and set partitions. The combinatorial models for functions and for superclass functions are related in Section 4.6.

4.1. Superclass functions on algebra groups. Let n be a *nilpotent* algebra: an associative, nonunital algebra in which every element is nilpotent. Let $\bar{n} = \mathbb{F} \oplus n$ denote the result of adjoining a unit to n. The set

$$G(\mathfrak{n}) = \{1 + n \mid n \in \mathfrak{n}\}$$

is a subgroup of the group of invertible elements of \bar{n} . A group of this form is called an *algebra group*. (This is the terminology employed in [Diaconis and Isaacs 2008] and, in a slightly different context, [André 1999; Isaacs 1995].)

A morphism of nilpotent algebras $\varphi : \mathfrak{m} \to \mathfrak{n}$ has a unique unital extension $\overline{\mathfrak{m}} \to \overline{\mathfrak{n}}$, and this sends $G(\mathfrak{m})$ to $G(\mathfrak{n})$. A morphism of algebra groups is a map of this form.

Warning. When we refer to the algebra group G(n), it is implicitly assumed that the algebra n is given as well.

Following Yan [2001], we define an equivalence relation on $G(\mathfrak{n})$ as follows. Given $x, y \in G(\mathfrak{n})$, we write $x \sim y$ if there exist $g, h \in G(\mathfrak{n})$ such that

$$y - 1 = g(x - 1)h.$$
 (36)

Following now Diaconis and Isaacs [2008], we refer to the equivalence classes of this relation as *superclasses* and to the functions $G(\mathfrak{n}) \to \mathbb{k}$ constant on these classes as *superclass functions*. The set of such functions is denoted $scf(G(\mathfrak{n}))$.

Since

$$gxg^{-1} - 1 = g(x - 1)g^{-1},$$

we have that $x \sim gxg^{-1}$ for any $x, g \in G(\mathfrak{n})$. Thus, each superclass is a union of conjugacy classes, and hence, every superclass function is a class function:

$$\operatorname{scf}(G(\mathfrak{n})) \subseteq \operatorname{cf}(G(\mathfrak{n})).$$
 (37)

A morphism $\varphi : G(\mathfrak{m}) \to G(\mathfrak{n})$ of algebra groups preserves the relation \sim . Therefore, if $f : G(\mathfrak{n}) \to \mathbb{k}$ is a superclass function on $G(\mathfrak{n})$, then $f \circ \varphi$ is a superclass function on $G(\mathfrak{m})$. In this manner,

scf : {algebra groups}
$$\rightarrow$$
 {vector spaces}

is a contravariant functor. In addition, the inclusion (37) is natural with respect to morphisms of algebra groups.

The direct product of two algebra groups is another algebra group. Indeed,

$$G(\mathfrak{n}_1) \times G(\mathfrak{n}_2) \cong G(\mathfrak{n}_1 \oplus \mathfrak{n}_2)$$

and $n_1 \oplus n_2$ is nilpotent. Moreover,

$$(x_1, x_2) \sim (y_1, y_2) \iff (x_1 \sim y_1 \text{ and } x_2 \sim y_2).$$

Therefore, a superclass of the product is a pair of superclasses from the factors, and if at least one of the two groups is finite, there is a canonical isomorphism

$$scf(G(\mathfrak{n}_1) \times G(\mathfrak{n}_2)) \cong scf(G(\mathfrak{n}_1)) \otimes scf(G(\mathfrak{n}_2)).$$

4.2. Superclass functions on unitriangular matrices. Given a finite set I and a linear order ℓ on I, let $\mathfrak{n}(I, \ell)$ denote the subalgebra of M(I) consisting of strictly upper-triangular matrices

$$N = (n_{ij})_{i,j \in I}, \quad n_{ij} = 0$$
 whenever $i \ge_{\ell} j$

Then $\mathfrak{n}(I, \ell)$ is nilpotent and $G(\mathfrak{n}(I, \ell)) = U(I, \ell)$. Thus, the unitriangular groups are algebra groups.

We assume from now on that the field \mathbb{F} is finite.

We define, for each finite set I,

$$\operatorname{scf}(\operatorname{U})[I] = \bigoplus_{\ell \in \operatorname{L}[I]} \operatorname{scf}(\operatorname{U}(I, \ell)).$$

This defines a species scf(U). Proceeding in the same manner as in Sections 3.3 and 3.5, we obtain linear maps

$$\mathsf{scf}(\mathsf{U})[S_1] \otimes \mathsf{scf}(\mathsf{U})[S_2] \xrightarrow{\mu_{S_1,S_2}} \mathsf{scf}(\mathsf{U})[I]$$

by applying the functor **scf** to the morphisms π_{S_1,S_2} and σ_{S_1,S_2} . This is meaningful since the latter are morphisms of algebra groups: it was noted in Section 2.1 that σ_{S_1,S_2} is the restriction of a morphism defined on the full matrix algebras while the considerations of Lemma 2 show that π_{S_1,S_2} is the restriction of a morphism defined on the algebra of upper-triangular matrices.

Proposition 10. With these operations, the species scf(U) is a connected cocommutative Hopf monoid. It is a Hopf submonoid of cf(U).

Proof. As in the proof of Proposition 4, the first statement follows by functoriality. The second follows from the naturality of the inclusion (37).

(31) and (32) continue to hold for the (co)product of superclass functions.

The constant function 1_{ℓ} is a superclass function. Thus, the morphism of Hopf monoids of Corollary 5 factors through scf(U) and cf(U):

$$L \hookrightarrow \mathsf{scf}(U) \hookrightarrow \mathsf{cf}(U) \hookrightarrow \mathsf{f}(U).$$

4.3. *Combinatorics of the superclasses.* Yan [2001] showed superclasses are parametrized by certain combinatorial data essentially along the lines presented below.

According to (36), two unitriangular matrices U_1 and U_2 are in the same superclass if and only if U_2 -Id is obtained from U_1 -Id by a sequence of elementary row and column operations. The available operations are from the unitriangular group itself, so the pivot entries cannot be normalized. Thus, each superclass contains a unique matrix U such that U - Id has at most one nonzero entry in each row and each column. We refer to this matrix U as the *canonical representative* of the superclass.

We proceed to encode such representatives in terms of combinatorial data.

We first discuss the combinatorial data. Let ℓ be a linear order on a finite set *I* and *X* a partition of *I*. Let us say that *i*, *j* \in *I* bound an arc if

- *i* precedes j in ℓ ,
- *i* and *j* are in the same block of *X*, say *S*, and
- no other element of S lies between i and j in the order ℓ .

The set of arcs is

$$A(X, \ell) := \{(i, j) \mid i \text{ and } j \text{ bound an arc}\}.$$

Consider also a function

$$\alpha: A(X,\ell) \to \mathbb{F}^{\times}$$

from the set of arcs to the nonzero elements of \mathbb{F} . We say that the pair (X, α) is an *arc diagram* on the linearly ordered set (I, ℓ) . We may visualize an arc diagram:



Here the combinatorial data is

$$\ell = fghijk, \quad X = \{\{f, i, j\}, \{g\}, \{h, k\}\}, \quad \alpha(f, i) = a, \ \alpha(i, j) = b, \ \alpha(h, k) = c.$$

Fix the linear order ℓ . To an arc diagram (X, α) on (I, ℓ) , we associate a matrix $U_{X,\alpha}$ with entries

$$u_{ij} = \begin{cases} \alpha(i, j) & \text{if } (i, j) \in A(X, \ell), \\ 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Clearly, the matrix $U_{X,\alpha}$ is ℓ -unitriangular and $U_{X,\alpha}$ – Id has at most one nonzero entry in each row and each column. In the above example,

$$U_{X,\alpha} = \begin{pmatrix} 1 & 0 & 0 & a & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & c \\ & 1 & d & 0 \\ & & 1 & 0 \\ & & & 1 \end{pmatrix}.$$

Conversely, any canonical representative matrix $U \in U(I, \ell)$ is of the form $U_{X,\alpha}$ for a unique arc diagram (X, α) on (I, ℓ) : the location of the nonzero entries

determines the set of arcs, and the values of the entries determine the function α . The smallest equivalence relation on *I* containing the set of arcs determines the partition *X*.

In conclusion, the canonical representatives, and hence the superclasses, are in bijection with the set of arc diagrams. We let $C_{X,\alpha}$ denote the superclass of $U(I, \ell)$ containing $U_{X,\alpha}$, and we write $\kappa_{X,\alpha}$ for the characteristic function of this class. As (X, α) runs over all arc diagrams on (I, ℓ) , these functions form a basis of the space $scf(U(I, \ell))$.

We describe principal minors and direct sums of the canonical representatives. To this end, fix $\ell \in L[I]$ and recall the notions of union and restriction of set partitions discussed in Section 1.3.

Let $S \subseteq I$ be an arbitrary subset. Given a partition X of I, let $A(X, \ell)|_S$ denote the subset of $A(X, \ell)$ consisting of those arcs (i, j) where both i and j belong to S. We let $\alpha|_S$ denote the restriction of α to $A(X, \ell)|_S$. We have $A(X, \ell)|_S \subseteq A(X|_S, \ell|_S)$, and if S is an ℓ -segment, then

$$A(X, \ell)|_{S} = A(X|_{S}, \ell|_{S}).$$
(38)

In this case, we obtain an arc diagram $(X|_S, \alpha|_S)$ on $(S, \ell|_S)$, and we have

$$(U_{X,\alpha})_S = U_{X|_S,\alpha|_S}.$$
(39)

Suppose now that $I = S_1 \sqcup S_2$ and (X_i, α_i) is an arc diagram on $(S_i, \ell|_{S_i}), i = 1, 2$. Then

$$A(X_1 \sqcup X_2, \ell) = A(X_1, \ell|_{S_1}) \sqcup A(X_2, \ell|_{S_2}).$$
(40)

Let $\alpha_1 \sqcup \alpha_2$ denote the common extension of α_1 and α_2 to this set. Then the pair $(X_1 \sqcup X_2, \alpha_1 \sqcup \alpha_2)$ is then an arc diagram on (I, ℓ) and

$$U_{X_1,\alpha_1} \oplus U_{X_2,\alpha_2} = U_{X_1 \sqcup X_2,\alpha_1 \sqcup \alpha_2}.$$
(41)

4.4. *Combinatorics of the (co)product.* We now describe the product and coproduct of the Hopf monoid scf(U) on the basis { $\kappa_{X,\alpha}$ } of Section 4.3. We employ (31) and (32), which, as discussed in Section 4.2, hold for superclass functions.

Let $I = S_1 \sqcup S_2$ and $\ell_i \in L[S_i]$, i = 1, 2, and consider the product

$$scf(U(S_1, \ell_1)) \times scf(U(S_2, \ell_2)) \rightarrow scf(U(I, \ell_1 \cdot \ell_2))$$

Let (X_i, α_i) be an arc diagram on (I, ℓ_i) , i = 1, 2. According to (31), we have

$$\mu_{S_1,S_2}(\kappa_{X_1,\alpha_1}\otimes\kappa_{X_2,\alpha_2})=\sum_{\pi_{S_1,S_2}(C_{X,\alpha})\subseteq C_{X_1,\alpha_1}\times C_{X_2,\alpha_2}}\kappa_{X,\alpha}$$

a sum over arc diagrams (X, α) on $(I, \ell_1 \cdot \ell_2)$. Since $\pi_{S,T}$ preserves superclasses,

$$\pi_{S_1,S_2}(C_{X,\alpha}) \subseteq C_{X_1,\alpha_1} \times C_{X_2,\alpha_2} \iff \pi_{S_1,S_2}(U_{X,\alpha}) \in C_{X_1,\alpha_1} \times C_{X_2,\alpha_2}$$
$$\iff (U_{X,\alpha})_{S_i} \in C_{X_i,\alpha_i}, \quad i = 1, 2.$$

In view of (39), this is in turn equivalent to

$$X|_{S_i} = X_i$$
 and $\alpha|_{S_i} = \alpha_i$, $i = 1, 2$.

In conclusion,

$$\mu_{S_1,S_2}(\kappa_{X_1,\alpha_1} \otimes \kappa_{X_2,\alpha_2}) = \sum_{\substack{X \mid S_i = X_i \\ \alpha \mid S_i = \alpha_i}} \kappa_{X,\alpha}.$$
(42)

The sum is over all arc diagrams (X, α) on $(I, \ell_1 \cdot \ell_2)$ whose restriction to S_i is (X_i, α_i) for i = 1, 2.

Take now $\ell \in L[I]$, $I = S_1 \sqcup S_2$, and consider the coproduct

$$scf(U(I, \ell)) \rightarrow scf(U(S_1, \ell|_{S_1})) \times scf(U(S_2, \ell|_{S_2}))$$

Let (X, α) be an arc diagram on (I, ℓ) . According to (32), we have

$$\Delta_{S_1,S_2}(\kappa_{X,\alpha}) = \sum_{\sigma_{S_1,S_2}(C_{X_1,\alpha_1} \times C_{X_2,\alpha_2}) \subseteq C_{X,\alpha}} \kappa_{X_1,\alpha_1} \otimes \kappa_{X_2,\alpha_2},$$

a sum over arc diagrams (X_i, α_i) on $(S_i, \ell|_{S_i})$. The superclass $C_{X_1,\alpha_1} \times C_{X_2,\alpha_2}$ contains $(U_{X_1,\alpha_1}, U_{X_2,\alpha_2})$, and hence, its image under σ_{S_1,S_2} contains

$$U_{X_1,\alpha_1} \oplus U_{X_2,\alpha_2} = U_{X_1 \sqcup X_2,\alpha_1 \sqcup \alpha_2}$$

by (41). Therefore,

$$\sigma_{S_1,S_2}(C_{X_1,\alpha_1} \times C_{X_2,\alpha_2}) \subseteq C_{X,\alpha} \iff X_1 \sqcup X_2 = X \text{ and } \alpha_1 \sqcup \alpha_2 = \alpha$$

Note that $X_1 \sqcup X_2 = X$ if and only if S_1 (or equivalently, S_2) is a union of blocks of X. In this case, $X_i = X|_{S_i}$ and $\alpha_i = \alpha|_{S_i}$. In conclusion,

$$\Delta_{S_1, S_2}(\kappa_{X, \alpha}) = \begin{cases} \kappa_{X|_{S_1}, \alpha|_{S_1}} \otimes \kappa_{X|_{S_2}, \alpha|_{S_2}} & \text{if } S_1 \text{ is the union of some blocks of } X, \\ 0 & \text{otherwise.} \end{cases}$$
(43)

4.5. *Decomposition as a Hadamard product.* The apparent similarity between the combinatorial description of the Hopf monoid operations of scf(U) in Section 4.4 and those of the Hopf monoids L and Π in Sections 1.2 and 1.3 can be formalized. Recall the Hadamard product of Hopf monoids from Section 1.5.

Let

$$\phi: L \times \Pi \to \mathsf{scf}(U)$$

be the map with components

$$(L \times \Pi)[I] \rightarrow \mathsf{scf}(U)[I]$$

given as follows. On a basis element $\ell \otimes m_X \in L[I] \otimes \Pi[I] = (L \times \Pi)[I]$, we set

$$\phi(\ell \otimes m_X) = \sum_{\alpha: A(X,\ell) \to \mathbb{F}^{\times}} \kappa_{X,\alpha} \in \mathsf{scf}(\mathcal{U}(I,\ell)) \subseteq \mathsf{scf}(\mathcal{U})[I]$$
(44)

and extend by linearity. The morphism ϕ adds labels to the arcs in all possible ways.

Proposition 11. Let \mathbb{F} be an arbitrary finite field. The map $\phi : L \times \Pi \to \mathsf{scf}(U)$ is an injective morphism of Hopf monoids.

Proof. This follows by comparing definitions, as in the proof of Proposition 8. The relevant equations are (6), (7), and (8) for the operations of $L \times \Pi$ and (42) and (43) for the operations of scf(U).

When the field of matrix entries is \mathbb{F}_2 , the arc labels are uniquely determined. The map ϕ is then invertible with inverse ψ given by

$$\psi(\kappa_{X,\alpha}) = \ell \otimes m_X$$

for any arc diagram (X, α) on a linearly ordered set (I, ℓ) . We thus have:

Corollary 12. There is an isomorphism of Hopf monoids

$$\mathsf{scf}(\mathbf{U}) \cong \boldsymbol{L} \times \boldsymbol{\Pi}$$

between the Hopf monoid of superclass functions on unitriangular matrices with entries in \mathbb{F}_2 and the Hadamard product of the Hopf monoids of linear orders and set partitions.

4.6. *Relating the combinatorial models.* The results of Section 4.5 provide a combinatorial model for the Hopf monoid scf(U). They parallel those of Section 3.6 that do the same for f(U). We now interpret the inclusion $scf(U) \hookrightarrow f(U)$ in these terms.

Let X be a partition on a linearly ordered set (I, ℓ) . We may regard the set of arcs $A(X, \ell)$ as a simple graph on I. Let $G(X, \ell)$ denote the set of simple graphs g on I such that

- g contains the graph $A(X, \ell)$ and
- if *i* < *j* in *l* and *g* \ *A*(*X*, *l*) contains an edge between *i* and *j*, then there exists *k* such that

i < k < j in ℓ and either $(i, k) \in A(X, \ell)$ or $(k, j) \in A(X, \ell)$.

The following illustrates the extra edges (dotted) that may be present in g when an arc (solid) is present in $A(X, \ell)$:



Define a map

 $L \times \Pi \to L \times G$

with components

$$(L \times \Pi)[I] \to (L \times G)[I], \quad \ell \otimes m_X \mapsto \ell \otimes \sum_{g \in G(X,\ell)} m_g.$$

Proposition 13. The map $L \times \Pi \rightarrow L \times G$ is an injective morphism of Hopf monoids. Moreover, the following diagram commutes:



Proof. It is enough to prove the commutativity of the diagram since all other maps in the diagram are injective morphisms. The commutativity boils down to the following fact. Given $X \in \Pi[I], \ell \in L[I]$, and $U \in U(I, \ell)$,

$$U \in C_{X,\alpha}$$
 for some $\alpha : A(X, \ell) \to \mathbb{F}^{\times} \iff g(U) \in G(X, \ell)$.

This expresses the fact that a matrix U belongs to the superclass $C_{X,\alpha}$ if and only if the nonzero entries of U – Id are located either above or to the right of the nonzero entries of the representative $U_{X,\alpha}$.

5. Freeness

We prove that the Hopf monoids f(U) and scf(U) are free and the Hopf structure is isomorphic to the canonical one on a free monoid. We assume that the base field \Bbbk is of characteristic 0, which enables us to apply the results of the Appendix.

5.1. A partial order on arc diagrams. Let (I, ℓ) be a linearly ordered set. Given arc diagrams (X, α) and (Y, β) on (I, ℓ) , we write

$$(X, \alpha) \leq (Y, \beta)$$

if

$$A(X, \ell) \subseteq A(Y, \ell)$$
 and $\beta|_{A(X, \ell)} = \alpha$.

In other words, every arc of X is an arc of Y and with the same label. In particular, the partition Y is coarser than X. On the other hand, the following arc diagrams are incomparable (regardless of the labels) even though the partition on the right is the coarsest one:



The poset of arc diagrams has a unique minimum (the partition into singletons, for which there are no arcs) but several maximal elements. The arc diagrams above are the two maximal elements when $\ell = ijk$ (up to a choice of labels).

A partition X of the linearly ordered set (I, ℓ) is *atomic* if no proper initial ℓ -segment of I is a union of blocks of X. Equivalently, there is no decomposition $I = S_1 \sqcup S_2$ into proper ℓ -segments such that $X = X|_{S_1} \sqcup X|_{S_2}$.



If (X, α) is a maximal element of the poset of arc diagrams, then X is an atomic partition. But if X is atomic, (X, α) need not be maximal (regardless of α).



5.2. *A second basis for* scf(U). We employ the partial order of Section 5.1 to define a new basis $\{\lambda_{X,\alpha}\}$ of scf(U(*I*, ℓ)) by

$$\lambda_{X,\alpha} = \sum_{(X,\alpha) \le (Y,\beta)} \kappa_{Y,\beta}.$$
(45)

The product of the Hopf monoid scf(U) takes a simple form on the λ -basis.

Proposition 14. Let $I = S_1 \sqcup S_2$ and $\ell_i \in L[S_i]$, i = 1, 2. Then

$$\mu_{S_1,S_2}(\lambda_{X_1,\alpha_1} \otimes \lambda_{X_2,\alpha_2}) = \lambda_{X_1 \sqcup X_2,\alpha_1 \sqcup \alpha_2}$$

$$\tag{46}$$

for any arc diagrams (X_i, α_i) on (S_i, ℓ_i) , i = 1, 2.

Proof. We calculate using (42) and (45):

$$\mu_{S_1,S_2}(\lambda_{X_1,\alpha_1} \otimes \lambda_{X_2,\alpha_2}) = \sum_{(X_i,\alpha_i) \le (Y_i,\beta_i)} \mu_{S_1,S_2}(\kappa_{Y_1,\beta_1} \otimes \kappa_{Y_2,\beta_2}) = \sum_{(X_i,\alpha_i) \le (Y|_{S_i},\beta|_{S_i})} \kappa_{Y,\beta}.$$

Now by (38) and (40), we have

$$(X_i, \alpha_i) \leq (Y|_{S_i}, \beta|_{S_i}), i = 1, 2 \iff (X_1 \sqcup X_2, \alpha_1 \sqcup \alpha_2) \leq (Y, \beta).$$

Therefore,

$$\mu_{S_1,S_2}(\lambda_{X_1,\alpha_1} \otimes \lambda_{X_2,\alpha_2}) = \sum_{(X_1 \sqcup X_2,\alpha_1 \sqcup \alpha_2) \le (Y,\beta)} \kappa_{Y,\beta} = \lambda_{X_1 \sqcup X_2,\alpha_1 \sqcup \alpha_2}.$$

The coproduct of the Hopf monoid scf(U) takes the same form on the λ -basis as on the κ -basis.

Proposition 15. Let $I = S_1 \sqcup S_2$ and $\ell \in L[I]$. Then

$$\Delta_{S_1,S_2}(\lambda_{X,\alpha}) = \begin{cases} \lambda_{X|_{S_1},\alpha|_{S_1}} \otimes \lambda_{X|_{S_2},\alpha|_{S_2}} & \text{if } S_1 \text{ is the union of some blocks of } X, \\ 0 & \text{otherwise.} \end{cases}$$
(47)

Proof. Suppose first that S_1 is not the union of blocks of X. Then the same is true for any partition coarser than X, in particular for any partition Y entering in (45). In view of (43), we then have $\Delta_{S_1,S_2}(\lambda_{X,\alpha}) = 0$.

Otherwise, $X = X|_{S_1} \sqcup X|_{S_2}$ and $\alpha = \alpha|_{S_1} \sqcup \alpha|_{S_2}$. Among the arc diagrams (Y, β) entering in (45), only those for which $Y = Y|_{S_1} \sqcup Y|_{S_2}$ contribute to the coproduct, in view of (43). These arc diagrams are of the form $Y = Y_1 \sqcup Y_2$ and $\beta = \beta_1 \sqcup \beta_2$, and by (40), we must have

$$A(X|_{S_i}, \ell|_{S_i}) \subseteq A(Y_i, \ell|_{S_i})$$
 and $\beta_i|_{A(X|_{S_i}, \ell|_{S_i})} = \alpha|_{S_i}, i = 1, 2$

We then have

$$\Delta_{S_1,S_2}(\lambda_{X,\alpha}) = \sum_{\substack{(X,\alpha) \le (Y,\beta) \\ (X|_{S_i},\alpha|_{S_i}) \le (Y_i,\beta_i)}} \Delta(\kappa_{Y,\beta})$$
$$= \sum_{\substack{(X|_{S_i},\alpha|_{S_i}) \le (Y_i,\beta_i)}} \kappa_{Y_1,\beta_1} \otimes \kappa_{Y_2,\beta_2} = \lambda_{X|_{S_1},\alpha|_{S_1}} \otimes \lambda_{X|_{S_2},\alpha|_{S_2}}. \quad \Box$$

Remark 16. The relationship between the λ - and κ -bases of scf(U) is somewhat reminiscent of that between the *p*- and *m*-bases of **Π** [Aguiar and Mahajan 2010, Equation (12.5)]. However, the latter involves a sum over all partitions coarser than a given one. For this reason, the morphism ϕ in (44), which relates the *m*-basis to the κ -basis, does not relate the *p*-basis to the λ -basis in the same manner.

5.3. *Freeness of* scf(U). Let q be a species such that $q[\emptyset] = 0$. A new species $\mathcal{T}(q)$ is defined by $\mathcal{T}(q)[\emptyset] = \Bbbk$ and, on a finite nonempty set I,

$$\mathcal{T}(\boldsymbol{q})[I] = \bigoplus_{\substack{I=I_1 \sqcup \cdots \sqcup I_k \\ k \geq 1, \ I_j \neq \emptyset}} \boldsymbol{q}[I_1] \otimes \cdots \otimes \boldsymbol{q}[I_k].$$

The sum is over all decompositions of I into nonempty subsets. The number k of subsets is therefore bounded above by |I|.

The species $\mathcal{T}(q)$ is a connected monoid with product given by concatenation. To describe this in detail, let $I = S \sqcup T$ and choose decompositions $S = S_1 \sqcup \cdots \sqcup S_k$ and $T = T_1 \sqcup \cdots \sqcup T_l$ and elements $x_i \in q[S_i], i = 1, ..., k$, and $y_j \in q[T_j], j = 1, ..., l$. Write

$$x = x_1 \otimes \cdots \otimes x_i \in \mathcal{T}(\boldsymbol{q})[S]$$
 and $y = y_1 \otimes \cdots \otimes y_i \in \mathcal{T}(\boldsymbol{q})[T].$

The product is

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$$\mu_{S,T}(x \otimes y) = x_1 \otimes \cdots \otimes x_i \otimes y_1 \otimes \cdots \otimes y_j$$

$$\in \boldsymbol{q}[S_1] \otimes \cdots \otimes \boldsymbol{q}[S_k] \otimes \boldsymbol{q}[T_1] \otimes \cdots \otimes \boldsymbol{q}[T_l] \subseteq \mathcal{T}(\boldsymbol{q})[I].$$

The monoid $\mathcal{T}(q)$ is *free* on the species q: a map of species $q \to m$ from q to a monoid m has a unique extension to a morphism of monoids $\mathcal{T}(q) \to m$.

The monoid $\mathcal{T}(q)$ may carry several coproducts that turn it into a connected Hopf monoid. The *canonical* structure is the one for which the elements of q are *primitive*. This means that

$$\Delta_{S,T}(x) = 0$$

for every $x \in q[I]$ and every decomposition $I = S \sqcup T$ into nonempty subsets.

More details can be found in [Aguiar and Mahajan 2010, Sections 11.2.1–11.2.2].

Let $D(I, \ell)$ denote the set of arc diagrams (X, α) for which X is an atomic set partition of the linearly ordered set (I, ℓ) . Let $d(I, \ell)$ be the vector space with basis $D(I, \ell)$. Define a species d by

$$\boldsymbol{d}[I] = \bigoplus_{\ell \in \mathrm{L}[I]} \boldsymbol{d}(I, \ell).$$

Consider the map of species $d \rightarrow scf$ with components

$$d[I] \to \mathsf{scf}(U)[I], \quad (X, \alpha) \mapsto \lambda_{X, \alpha}.$$

The map sends the summand $d(I, \ell)$ of d[I] to the summand $scf(U(I, \ell))$ of scf(U)[I]. By freeness, it extends to a morphism of monoids

$$\mathcal{T}(\boldsymbol{d}) \rightarrow \mathbf{scf}(\mathbf{U}).$$

Proposition 17. The map $\mathcal{T}(d) \to \mathsf{scf}(U)$ is an isomorphism of monoids. In particular, the monoid $\mathsf{scf}(U)$ is free.

Proof. Let (X, α) be an arbitrary arc diagram on (I, ℓ) . Let I_1, \ldots, I_k be the minimal ℓ -segments of I, numbered from left to right, such that each I_j is a union of blocks of X. Let $\ell_j = \ell|_{I_j}, X_j = X|_{I_j}$, and $\alpha_j = \alpha|_{I_j}$. Then X_j is an atomic partition of (I_j, ℓ_j) ,

$$X_1 \sqcup \cdots \sqcup X_j = X$$
 and $\alpha_1 \sqcup \cdots \sqcup \alpha_j = \alpha$.

By (46),

$$\mu_{I_1,\ldots,I_k}(\lambda_{X_1,\alpha_1}\otimes\cdots\otimes\lambda_{X_k,\alpha_k})=\lambda_{X,\alpha}.$$

Thus, the morphism $\mathcal{T}(d) \to \mathbf{scf}(U)$ sends the basis element $(X_1, \alpha_1) \otimes \cdots \otimes (X_k, \alpha_k)$ of $d(I_1, \ell_1) \otimes \cdots \otimes d(I_k, \ell_k)$ to the basis element $\lambda_{X,\alpha}$ of $\mathbf{scf}(U(I, \ell))$ and is therefore an isomorphism.

We may state Proposition 17 by saying that the superclass functions $\lambda_{X,\alpha}$ freely generate the monoid **scf**(U) as (X, α) runs over all arc diagrams for which X is an atomic set partition.

The generators, however, need not be primitive. For instance,



which is not 0. Nevertheless, Proposition 23 allows us to conclude the following:

Corollary 18. Let \Bbbk be a field of characteristic 0. There exists an isomorphism of Hopf monoids $scf(U) \cong T(d)$, where the latter is endowed with its canonical Hopf structure.

As discussed in the Appendix, an isomorphism may be constructed with the aid of the first Eulerian idempotent.

Let $\Pi_a(I, \ell)$ be the vector space with basis the set of atomic partitions on (I, ℓ) . When the field of matrix entries is \mathbb{F}_2 , arc diagrams reduce to atomic set partitions and $d(I, \ell)$ identifies with $\Pi_a(I, \ell)$. Combining Corollaries 12 and 18, we obtain an isomorphism of Hopf monoids

$$\boldsymbol{L} \times \boldsymbol{\Pi} \cong \mathcal{T}(\boldsymbol{\Pi}_a), \tag{48}$$

where

$$\mathbf{\Pi}_{a}[I] = \bigoplus_{\ell \in \mathrm{L}[I]} \mathbf{\Pi}_{a}(I, \ell).$$

5.4. A second basis for G and for f(U). Given two unitriangular matrices U and $V \in U(I, \ell)$, let us write $U \leq V$ if

$$u_{ij} = v_{ij}$$
 whenever $u_{ij} \neq 0$.

In other words, some zero entries in U may be nonzero in V; the other entries are the same for both matrices.

We define a new basis $\{\lambda_U\}$ of $\mathbf{f}(\mathbf{U}(I, \ell))$ by

$$\lambda_U = \sum_{U \le V} \kappa_V.$$

Let $I = S_1 \sqcup S_2$, $U \in U(I, \ell)$, and $g_i \in U(S_i, \ell_i)$, i = 1, 2. It is easy to derive the following formulas from (29) and (30):

$$\mu_{S_1,S_2}(\lambda_{U_1} \otimes \lambda_{U_2}) = \lambda_{U_1 \oplus U_2},\tag{49}$$

$$\Delta_{S_1, S_2}(\lambda_U) = \begin{cases} \lambda_{U_{S_1}} \otimes \lambda_{U_{S_2}} & \text{if } U = U_{S_1} \oplus U_{S_2}, \\ 0 & \text{otherwise.} \end{cases}$$
(50)

(49) implies that f(U) is a free monoid with generators λ_U indexed by unitriangular matrices U for which the graph g(U) is connected.

For completeness, one may define a new basis $\{p_g\}$ of G[I] by

$$p_g = \sum_{g \subseteq h} m_h. \tag{51}$$

The sum is over all simple graphs *h* with vertex set *I* and with the same or more edges than *g*. Let $I = S_1 \sqcup S_2$, $g \in G[I]$, and $g_i \in G[S_i]$, i = 1, 2. From (9) and (10), one obtains

$$\mu_{S_1,S_2}(p_{g_1} \otimes p_{g_2}) = p_{g_1 \sqcup g_2},\tag{52}$$

$$\Delta_{S_1,S_2}(p_g) = \begin{cases} p_{g|_{S_1}} \otimes p_{g|_{S_2}} & \text{if no edge of } g \text{ connects } S_1 \text{ to } S_2, \\ 0 & \text{otherwise.} \end{cases}$$
(53)

Equation (52) implies that G is the free commutative monoid on the species of connected graphs. From (44), we deduce that the morphism ϕ of Proposition 8 takes the following form on these bases:

$$\phi(\ell \otimes p_g) = \sum_{\substack{U \in \mathrm{U}(I,\ell) \\ g(U) = g}} \lambda_U.$$

6. Applications

We conclude with some applications and remarks regarding past and future work.

6.1. *Counting conjugacy classes.* Let $k_n(q)$ be the number of conjugacy classes of the group of unitriangular matrices of size *n* with entries in the field with *q* elements. Higman's conjecture states that, for fixed *n*, k_n is a polynomial function of *q*. Much effort has been devoted to the precise determination of these numbers or their asymptotic behavior [Goodwin 2006; Goodwin and Röhrle 2009; Higman 1960; Robinson 1998; Vera-López and Arregi 2003; Vera-López et al. 2008].

We fix q and let n vary. It turns out that the existence of a Hopf monoid structure on class functions imposes certain linear conditions on the sequence $k_n(q)$, as we explain next.

Given a finite-dimensional Hopf monoid h, consider the generating function

$$\mathsf{T}_{\boldsymbol{h}}(x) = \sum_{n \ge 0} \dim_{\mathbb{K}}(\boldsymbol{h}[n]_{\mathsf{S}_n}) x^n.$$
(54)

Here [n] denotes the set $\{1, 2, ..., n\}$ and $h[n]_{S_n}$ is the (quotient) space of coinvariants for the action of the symmetric group (afforded by the species structure of h).

For example, since

$$(L \times \Pi)[n]_{\mathbf{S}_n} = (L[n] \otimes \Pi[n])_{\mathbf{S}_n} \cong \Pi[n],$$

we have

$$\mathsf{T}_{L\times\Pi}(x) = \sum_{n\geq 0} B_n x^n,\tag{55}$$

where B_n is the *n*-th Bell number, the number of partitions of the set [n].

On the other hand, from (48),

$$\mathsf{T}_{L\times\Pi}(x) = \mathsf{T}_{\mathcal{T}(\Pi_a)}(x).$$

It is a general fact that, for a species q with $q[\emptyset] = 0$,

$$\mathsf{T}_{\mathcal{T}(\boldsymbol{q})}(\boldsymbol{x}) = \frac{1}{1 - \mathsf{T}_{\boldsymbol{q}}(\boldsymbol{x})}.$$

(This follows from [Bergeron_F et al. 1998, Theorem 2.b, Section 1.4] for instance). Therefore,

$$\mathsf{T}_{L \times \Pi}(x) = \frac{1}{1 - \sum_{n \ge 1} A_n x^n},$$
(56)

where A_n is the number of atomic partitions of the linearly ordered set [n].

From (55) and (56), we deduce that

$$\sum_{n\geq 0} B_n x^n = \frac{1}{1-\sum_{n\geq 1} A_n x^n},$$

a fact known from [Bergeron and Zabrocki 2009].

Consider now the injections

$$scf(U) \hookrightarrow cf(U)$$
 and $L \times \Pi \hookrightarrow scf(U)$.

Both are morphisms of Hopf monoids (Propositions 10 and 11). *Lagrange's theorem* for Hopf monoids implies in this situation that both quotients

$$\frac{\mathsf{T}_{\mathbf{cf}(\mathsf{U})}(x)}{\mathsf{T}_{\mathbf{scf}(\mathsf{U})}(x)} \quad \text{and} \quad \frac{\mathsf{T}_{\mathbf{scf}(\mathsf{U})}(x)}{\mathsf{T}_{L \times \Pi}(x)}$$

belong to $\mathbb{N}[[x]]$, that is, have nonnegative (integer) coefficients [Aguiar and Lauve 2012, Corollary 13]. In particular,

$$\frac{\mathsf{T}_{\mathsf{cf}(\mathsf{U})}(x)}{\mathsf{T}_{L\times\Pi}(x)} \in \mathbb{N}[[x]]$$

as well.

We have

$$\mathsf{cf}(\mathsf{U})[n]_{\mathsf{S}_n} = \left(\bigoplus_{\ell \in \mathsf{L}[n]} \mathsf{cf}(\mathsf{U}([n], \ell))\right)_{\mathsf{S}_n} \cong \mathsf{cf}(\mathsf{U}([n])).$$

Therefore,

$$\Gamma_{\mathbf{cf}(\mathbf{U})}(x) = \sum_{n \ge 0} k_n(q) x^n.$$

By combining the above, we deduce

$$\left(\sum_{n\geq 0}k_n(q)x^n\right)\left(1-\sum_{n\geq 1}A_nx^n\right)\in\mathbb{N}[[x]],$$

whence the following result:

Corollary 19. The following linear inequalities are satisfied for every $n \in \mathbb{N}$ and every prime power q:

$$k_n(q) \ge \sum_{i=0}^{n-1} A_{n-i} k_i(q).$$
 (57)

For instance, for n = 8, the inequality is

$$k_6(q) \ge 92 + 22k_1(q) + 6k_2(q) + 2k_3(q) + k_4(q) + k_5(q).$$

Inequality (57) is stronger than merely stating that there are more conjugacy classes than superclasses. For instance, for q = 2 and n = 6, the right-hand side of the inequality is 213 (provided we use the correct values for $k_i(2)$ for $i \le 5$) while there are only $B_6 = 203$ superclasses. The first few values of the sequence $k_n(2)$ appear in [OEIS Foundation 2010] as A007976; in particular, $k_6(2) = 275$.

The numbers $k_n(q)$ are known for $n \le 13$ from work of Vera-López and Arregi [1992; 1995; 2003]; see also [Vera-López et al. 2008]. (There is an incorrect sign in the value given for $k_7(q)$ in [Vera-López and Arregi 1995, page 923]: the lowest term should be -7q.)

We may derive additional information on these numbers from the injective morphism of Hopf monoids (Proposition 6)

$$cf(U) \hookrightarrow f(U).$$

Define a sequence of integers $c_n(q)$, $n \ge 1$, by means of

$$\sum_{n \ge 0} k_n(q) x^n = \frac{1}{1 - \sum_{n \ge 1} c_n(q) x^n}.$$
(58)

Arguing as above, we obtain the following result:

Corollary 20. The following linear inequalities are satisfied for every $n \in \mathbb{N}$ and every prime power q:

$$q^{\binom{n}{2}} \ge \sum_{i=1}^{n} q^{\binom{n-i}{2}} c_i(q).$$
(59)

Through (58), these inequalities impose further constraints on the numbers $k_n(q)$. The first few values of the sequence $c_n(q)$ are as follows with t = q - 1:

$$c_{1}(q) = 1,$$

$$c_{2}(q) = t,$$

$$c_{3}(q) = t^{2} + t,$$

$$c_{4}(q) = 2t^{3} + 4t^{2} + t,$$

$$c_{5}(q) = 5t^{4} + 14t^{3} + 9t^{2} + t,$$

$$c_{6}(q) = t^{6} + 18t^{5} + 55t^{4} + 54t^{3} + 16t^{2} + t.$$

Conjecture 21. There exist polynomials $p_n(t) \in \mathbb{N}[t]$ such that $c_n(q) = p_n(q-1)$ for every prime power q and every $n \ge 1$.

Using the formulas given by Vera-López et al. [2008, Corollaries 10–11] for computing $k_n(q)$, we have verified the conjecture for $n \le 13$.

Polynomiality of $k_n(q)$ is equivalent to that of $c_n(q)$. On the other hand, the nonnegativity of c_n as a polynomial of t implies that of k_n but not conversely. Thus, Conjecture 21 is a strong form of Higman's.

It is possible to show, using the methods of [Aguiar and Mahajan 2012], that the monoid cf(U) is free. This implies that the integers $c_n(q)$ are nonnegative for every $n \ge 1$ and prime power q.

6.2. From Hopf monoids to Hopf algebras. It is possible to associate a number of graded Hopf algebras to a given Hopf monoid h. This is the subject of [Aguiar and Mahajan 2010, Part III]. In particular, there are two graded Hopf algebras $\mathcal{K}(h)$ and $\overline{\mathcal{R}}(h)$ related by a canonical surjective morphism

$$\mathfrak{K}(\boldsymbol{h}) \twoheadrightarrow \overline{\mathfrak{K}}(\boldsymbol{h}).$$

The underlying spaces of these Hopf algebras are

$$\mathscr{K}(\boldsymbol{h}) = \bigoplus_{n \ge 0} \boldsymbol{h}[n] \text{ and } \overline{\mathscr{K}}(\boldsymbol{h}) = \bigoplus_{n \ge 0} \boldsymbol{h}[n]_{S_n},$$

where $h[n]_{S_n}$ is as in (54). The product and coproduct of these Hopf algebras is built from those of the Hopf monoid h together with certain canonical transformations. The latter involve certain combinatorial procedures known as *shifting* and *standardization*. For more details, we refer to [Aguiar and Mahajan 2010, Chapter 15].

For example, one has that

$$\overline{\mathcal{R}}(\boldsymbol{L}) = \Bbbk[\boldsymbol{x}]$$

is the polynomial algebra on one primitive generator while $\Re(L)$ is the Hopf algebra introduced by Patras and Reutenauer [2004].

According to [Aguiar and Mahajan 2010, Section 17.4], $\overline{\mathcal{R}}(\Pi)$ is the ubiquitous Hopf algebra of *symmetric functions* while $\mathcal{K}(\Pi)$ is the Hopf algebra of *symmetric functions in noncommuting variables*, an object studied in various references including [Aguiar and Mahajan 2006, Section 6.2; Bergeron et al. 2006; Bergeron and Zabrocki 2009; Rosas and Sagan 2006].

For any Hopf monoid *h*, one has [Aguiar and Mahajan 2010, Theorem 15.13]

$$\mathscr{K}(\boldsymbol{L} \times \boldsymbol{h}) \cong \mathscr{K}(\boldsymbol{h})$$

Combining with Corollary 12, we obtain that, when the field of coefficients is \mathbb{F}_2 ,

$$\overline{\mathcal{H}}(\mathsf{scf}(\mathsf{U})) \cong \overline{\mathcal{H}}(\boldsymbol{L} \times \boldsymbol{\Pi}) \cong \mathcal{H}(\boldsymbol{\Pi}).$$

In other words, the Hopf algebra constructed from superclass functions on unitriangular matrices (with entries in \mathbb{F}_2) via the functor $\overline{\mathcal{R}}$ is isomorphic to the Hopf algebra of symmetric functions in noncommuting variables. This is the main result of [Aguiar et al. 2012].

The freeness of the Hopf algebra $\mathcal{H}(\Pi)$, a fact known from [Harčenko 1978; Wolf 1936], is a consequence of Proposition 17.

We mention that one may arrive at Corollary 19 by employing the Hopf algebra $\overline{\mathcal{H}}(cf(U))$ (rather than the Hopf monoid cf(U)) and appealing to Lagrange's theorem for graded connected Hopf algebras.

6.3. *Supercharacters and beyond.* The notion of superclass on a unitriangular group comes with a companion notion of *supercharacter* and a full-fledged theory relating them. This is due to the pioneering work of André [1995a; 1995b] and later Yan [2001]. Much of this theory extends to algebra groups [André 1999; Diaconis and Isaacs 2008; Diaconis and Thiem 2009]. More recently, a connection with classical work on Schur rings has been understood [Hendrickson 2010].

In regards to the object of present interest, the Hopf monoid scf(U), this implies the existence of a second canonical linear basis consisting of supercharacters. The work of André and Yan provides a *character formula*, which yields the change of basis between superclass functions and supercharacters. We plan to study the Hopf monoid structure of scf(U) on the supercharacter basis in future work.

Appendix: On free Hopf algebras and Hopf monoids

A free algebra may carry several Hopf algebra structures. It always carries a canonical one in which the generators are primitive. It turns out that under certain conditions, any Hopf structure on a free algebra is isomorphic to the canonical one. We provide such a result below. An analogous result holds for Hopf monoids in vector species. This is applied in the paper in Section 5.

We assume that the base field \Bbbk is of characteristic 0.

We employ the *first Eulerian idempotent* [Gerstenhaber and Schack 1991; Loday 1998, Section 4.5.2; Reutenauer 1993, Section 8.4]. For any connected Hopf algebra H, the identity map id : $H \rightarrow H$ is locally unipotent with respect to the convolution product of End(H). Therefore,

$$e := \log(\mathrm{id}) = \sum_{k \ge 1} \frac{(-1)^{k+1}}{k} (\mathrm{id} - \iota \epsilon)^{*k}$$
(60)

is a well-defined linear endomorphism of H. Here

 $\iota : \Bbbk \to H \quad \text{and} \quad \epsilon : H \to \Bbbk$

denote the unit and counit maps of H, respectively, and the powers are with respect to the convolution product. It is an important fact that if H is in addition cocommutative, then e(x) is a primitive element of H for any $x \in H$. In fact, the operator e is in this case a projection onto the space of primitive elements [Patras 1994; Schmitt 1994, pages 314–318].

Let T(V) denote the free algebra on a vector space V:

$$T(V) = \bigoplus_{n \ge 0} V^{\otimes n}$$

The product is concatenation of tensors. We say in this case that V freely generates.

The unique morphisms of algebras

$$\Delta: T(V) \to T(V) \otimes T(V)$$
 and $\epsilon: T(V) \to \Bbbk$

given for all $v \in V$ by

$$\Delta(v) = 1 \otimes v + v \otimes 1 \quad \text{and} \quad \epsilon(v) = 0$$

turn T(V) into a connected, cocommutative Hopf algebra. This is the *canonical* Hopf structure on T(V).

Proposition 22. Let \Bbbk be a field of characteristic 0. Let H be a connected cocommutative Hopf algebra over \Bbbk . Suppose $H \cong T(W)$ as algebras in such a way that the image of W lies in the kernel of the ϵ . Then there exists a (possibly different) isomorphism of Hopf algebras $H \cong T(W)$, where the latter is endowed with its canonical Hopf structure.

Proof. We may assume H = T(W) as algebras for some subspace W of ker(ϵ). Since H is connected and k is of characteristic 0, the Eulerian idempotent e is defined. Let V = e(W). We show below that $V \cong W$ and that V freely generates H. Since H is cocommutative, V consists of primitive elements, and therefore, $H \cong T(V)$ as Hopf algebras. This completes the proof.

Let

$$H_+ = \bigoplus_{n \ge 1} W^{\otimes n}.$$

Since ϵ is a morphism of algebras, $H_+ \subseteq \ker(\epsilon)$, and since both spaces are of codimension 1, they must agree: $H_+ = \ker(\epsilon)$.

Define $\Delta_+: H_+ \to H_+ \otimes H_+$ by

$$\Delta_+(x) = \Delta(x) - 1 \otimes x - x \otimes 1.$$

By counitality,

$$(\epsilon \otimes \mathrm{id})\Delta_+ = 0 = (\mathrm{id} \otimes \epsilon)\Delta_+$$

Therefore, $\Delta_+(H_+) \subseteq \ker(\epsilon) \otimes \ker(\epsilon) = H_+ \otimes H_+$, and hence,

 $\Delta^{(k-1)}_+(H_+)\subseteq H_+^{\otimes k}$

for all $k \ge 1$. In addition, since H = T(W) as algebras,

$$\mu^{(k-1)}(H_+^{\otimes k}) \subseteq \sum_{n \ge 2} W^{\otimes n}$$

for all $k \ge 2$.

Take $w \in W$. Then

$$e(w) = \sum_{k \ge 1} \frac{(-1)^{k+1}}{k} (\mathrm{id} - \iota \epsilon)^{*k} (w) = w + \sum_{k \ge 2} \frac{(-1)^{k+1}}{k} \mu^{(k-1)} \Delta_+^{(k-1)} (w)$$
$$\equiv w + \sum_{n \ge 2} W^{\otimes n}.$$

By triangularity, $e: W \to V$ is invertible, and hence, V generates H.

Now take $w_1, w_2 \in W$. It follows from the above that

$$\boldsymbol{e}(w_1)\boldsymbol{e}(w_2) \equiv w_1w_2 + \sum_{n\geq 3} W^{\otimes n},$$

and a similar triangular relation holds for higher products. Hence, V generates H freely. \Box

The Eulerian idempotent is defined for connected Hopf monoids in species by the same formula as (60). Let p be a species such that $p[\emptyset] = 0$. The free monoid $\mathcal{T}(p)$ and its canonical Hopf structure is discussed in [Aguiar and Mahajan 2010, Section 11.2]. The arguments in Proposition 22 may easily be adapted to this setting to yield the following result:

Proposition 23. Let \Bbbk be a field of characteristic 0. Let h be a connected cocommutative Hopf monoid in vector species over \Bbbk . Suppose $h \cong \mathcal{T}(p)$ as monoids for some species p such that $p[\varnothing] = 0$. Then there exists a (possibly different) isomorphism of Hopf monoids $h \cong \mathcal{T}(p)$, where the latter is endowed with its canonical Hopf structure.

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