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Exhaustive generation of atomic combinatorial differential operators

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ABSTRACT

Labelle and Lamathe introduced in 2009 a generalization of the standard combinatorial differential species operator D, by giving a combinatorial interpretation to $\Omega(X, D)F(X)$, where $\Omega(X, T)$ and $F(X)$ are two-sort and one-sort species respectively. One can show that such operators can be decomposed as sums of products of simpler operators called atomic combinatorial differential operators. In their paper, Labelle and Lamathe presented a list of the first atomic differential operators. In this paper, we describe an algorithm that allows to generate (and enumerate) all of them, subject to available computer resources. We also give a detailed analysis of how to compute the molecular components of $\Omega(X, D)F(X)$.

1. Introduction

Since its introduction by Joyal in 1981 [9], the theory of species of structures has a noticeable influence in a variety of fields including combinatorics, algebraic data types [16], and also for the generation of combinatorial structures, either random [5,3] or exhaustive [12]. Many aspects have been developed and the theory remains an active research domain for which the reader can find a comprehensive account in the monography of Bergeron et al. [2].

One of its fundamental concepts is the notion of derivative of a species. Indeed, for any species F, the combinatorial interpretation of DF is well known: A DF-structure on a set U is simply an F-structure on the set $U \cup \{*\}$ where $*$ is an element not in U. In other words, a DF-structure is an F-structure with a placeholder for one element as Fig. 1a illustrates. Moreover, we have a good grip on the notion of $D^n F$, obtained from n successive applications of D on a species F. We often describe the differential operator D^n as an $L_n(D)$-structure, that is an n-list of operators D (see Fig. 1b).

Joyal further developed this idea of graphical arrangements of the differential operator D by introducing in [10] a more general differential operator. It gives, for any species G, a combinatorial interpretation to a combinatorial operator denoted by $G(D)$. For example, Fig. 2a illustrates the differential operator $\mathcal{C}(D)$ where $\mathcal{C}$ is the species of oriented cycles. But what combinatorial interpretation can one give to a circular arrangement of D's and X's as in Fig. 2b?

Labelle and Lamathe answered this question in [11] (see also [13]) by introducing a generalization of the differential operator $G(D)$. For any two-sort species $\Omega(X, T)$, they defined a differential operator $\Omega(X, D)$, called generalized combinatorial differential operator. In the same manner as for ordinary species, such operators can be decomposed as a sum of products of operators $X^m D^k / K$ called atomic combinatorial differential operators, where K is some suitable subgroup of

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Fig. 1. (a) A DL_6-structure on the set $U = \{1, 2, 3, 4, 5\}$ where L_6 denotes the species of six elements lists. The placeholder element is represented as a white square (□); (b) The differential operator D^n as an $L_n(D)$-structure.

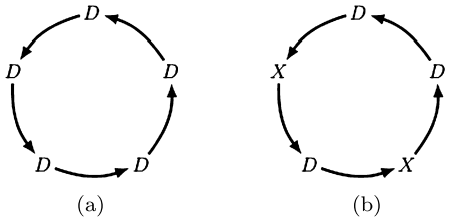

Fig. 2. (a) The general differential operator $\mathcal{C}(D)$ as a $\mathcal{C}(D)$-structure; (b) A circular arrangement of operators D and singletons species X.

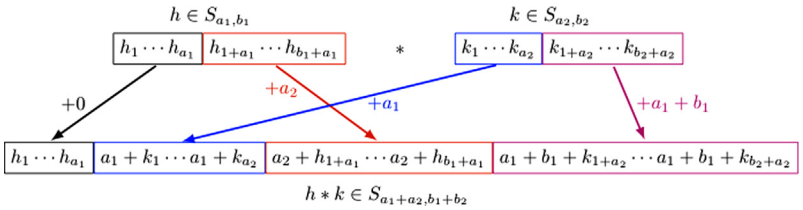

Fig. 3. The definition of the shift performed on h and k to obtain $h * k$ in Definition 2.1.

$S_{m,k}$. They provide a partial list of all such operators for $m + k \leqslant 7$ (see also [4] for molecular species). The main purpose of this paper is to develop an algorithm which extends this list to include all atomic operators for $m + k \leqslant n$, $n \in \mathbb{N}$.

2. Preliminaries

A *species of structures* F is a functor $F : \mathbb{B} \longrightarrow \mathbb{B}$ from the category $\mathbb{B}$ of finite sets with bijections to itself. A number of combinatorial operations are defined on species, namely addition, multiplication, cartesian product, composition and derivation. Those concepts can be extended to sets with k different sorts of elements. To denote one-sort and two-sort species, we use the notation $F(X)$ and $\Omega(X, T)$ for $k = 1$ and $k = 2$.

Molecular and atomic species play a very important role in the study of species. A species M is said to be *molecular* if and only if $M = F + G \Rightarrow F = 0$ or $G = 0$. In the same manner, a molecular species A is said to be *atomic* if and only if $A = FG \Rightarrow F = 1$ or $G = 1$.

One can show that any molecular species $M = M(X)$ is isomorphic to a species X^n/H, where H is a subgroup of S_n. This species is defined by setting for every finite set U

$$\frac{X^n}{H}[U] = \left\{\lambda H \mid \lambda : [n] \xrightarrow{\sim} U \text{ is a bijection}\right\}, \tag{1}$$

where $\lambda H = \{\lambda \circ h \mid h \in H\}$. One can then show that two molecular species X^n/H and X^m/K are isomorphic if and only if $n = m$ and H is conjugate to K in S_n. Similarly, any molecular two-sort species $M = M(X, T)$ is isomorphic to a species $X^m T^k/H$ where H is a subgroup of $S_{m,k}$. Here, $S_{m,k}$ denotes the Young subgroup of S_{m+k} permuting independently $\{1, 2, \ldots, m\}$ and $\{m + 1, m + 2, \ldots, m + k\}$. Note that $S_{m,k} \simeq S_m \times S_k$ (see [15,2] for more details).

For our purpose, we need a few important and useful results about products of two-sort molecular species.

Definition 2.1. Let H and K be subgroups of S_{a_1,b_1} and S_{a_2,b_2} respectively. The subgroup $H * K$ of $S_{a_1+a_2,b_1+b_2}$ is defined by

$$H * K = \{\omega = h * k \mid h \in H \text{ and } k \in K\},$$

where $h * k$ is the permutation obtained by the following shift operation on the four blocks of h and k:

$$\begin{array}{lll}
\text{Block of size } a_1 \longrightarrow & \omega_1 \ldots \omega_{a_1} & = h_1 \ldots h_{a_1} \\
\text{Block of size } a_2 \longrightarrow & \omega_{a_1+1} \ldots \omega_{a_1+a_2} & = a_1 + k_1 \ldots a_1 + k_{a_2} \\
\text{Block of size } b_1 \longrightarrow & \omega_{a_1+a_2+1} \ldots \omega_{a_1+a_2+b_1} & = a_2 + h_{1+a_1} \ldots a_2 + h_{b_1+a_1} \\
\text{Block of size } b_2 \longrightarrow & \omega_{a_1+a_2+b_1+1} \ldots \omega_{a_1+a_2+b_1+b_2} & = a_1 + b_1 + k_{1+a_2} \ldots a_1 + b_1 + k_{b_2+a_2}
\end{array}$$

Fig. 3 illustrates this shift $(*)$ operation.