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A theory of general combinatorial differential operators

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Abstract. Let $D = d/dX$. We develop a theory of combinatorial differential operators of the form $\Omega(X, D)$ where $\Omega(X, T)$ is an arbitrary species of structures built on two sorts, X and T, of underlying elements. These operators act on species, $F(X)$, instead of functions. We show how to compose these operators, how to compute their adjoints and their counterparts in the context of underlying symmetric functions and power series. We also analyse how these operators behave when applied to products of species (generalized Leibniz rule) and other combinatorial operations. Special instances of these operators include: combinatorial finite difference operators, $\Phi(X, \Delta)$, corresponding to the species $\Omega(X, T) = \Phi(X, E_+(T))$, where E_+ is the species of non-empty finite sets; pointing operators, $\Lambda(XD)$, which are self-adjoint and correspond to the species $\Omega(X, T) = \Lambda(XT)$; and combinatorial Hammond differential operators, $\Theta(D)$, corresponding to the species $\Omega(X, T) = \Theta(T)$.

Résumé. Soit $D = d/dX$. Nous développons une théorie d'opérateurs différentiels combinatoires de la forme $\Omega(X, D)$ où $\Omega(X, T)$ est une espèce de structures arbitraire construites sur deux sortes, X et T, d'éléments sous-jacents. Ces opérateurs agissent sur des espèces, $F(X)$, plutôt que sur des fonctions. Nous montrons comment composer ces opérateurs, comment calculer leurs adjoints et les opérateurs qui leur correspondent dans le contexte des fonctions symétriques et des séries génératrices. Nous analysons aussi le comportement de ces opérateurs lorsqu'ils sont appliqués au produit d'espèces (règle de Leibniz) ainsi qu'à d'autres opérations combinatoires. Ces opérateurs incluent les opérateurs combinatoires de différences finies, $\Phi(X, \Delta)$, correspondant aux espèces $\Omega(X, T) = \Phi(X, E_+(T))$, où E_+ est l'espèce des ensembles finis non-vides, les opérateurs de pointage, $\Lambda(XD)$, qui sont auto-adjoints et correspondent aux espèces $\Omega(X, T) = \Lambda(XT)$ ainsi que les opérateurs différentiels combinatoires de Hammond, $\Theta(D)$, qui correspondent aux espèces $\Omega(X, T) = \Theta(T)$.

1. Preliminary notions

Informally, a combinatorial *species of structures* is a class of labelled structures which is closed under relabellings along bijections[1]. A structure belonging to a species F is called an F-*structure*. The set of F-structures on a finite underlying set U is assumed to be finite and is denoted by $F[U]$. Hence, $s \in F[U]$ means that s is an F-structure on U. Two F-structures s and t are said *isomorphic* if one can be obtained from the other one by a relabelling induced by a bijection between their underlying sets. More precisely, if $\beta : U \to V$ is such a bijection, the induced relabelling is denoted by $F[\beta] : F[U] \to F[V]$. An isomorphism class of F-structures is called an *unlabelled* F-structure. Two species F and G are equal (isomorphic), and we write $F = G$, if there exists a natural isomorphism (in the sense of theory of category) between them. This means that for each U, there exists a bijection $\alpha_U : F[U] \to G[U]$ such that $G[\beta]\alpha_U = \alpha_V F[\beta]$ for each bijection $\beta : U \to V$.

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[1] Formally, a species of structures is a functor from the category of finite sets and bijections to the category of finite sets and functions, see [**6**].

Several enumerative formal series can be associated to any species F. The most important one is the *cycle index series*, denoted $Z_F(x_1, x_2, x_3, \ldots)$, and is defined by

$$Z_F(x_1, x_2, x_3, \ldots) = \sum_{n \geq 0} \frac{1}{n!} \sum_{\sigma \in \mathbb{S}_n} \mathrm{fix} F[\sigma]\, x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3} \ldots \tag{1.1}$$

where $\mathbb{S}_n$ denotes the symmetric group of order n, $\mathrm{fix}F[\sigma]$ is the number of F-structures on $[n]$ left fixed under the action of the permutation $\sigma \in \mathbb{S}_n$ and σ_i, $i \in \mathbb{N}^*$, is the number of cycles of length i of the permutation $\sigma \in \mathbb{S}_n$. Other classical enumerative formal series, that is, $F(x)$, the *exponential generating series*, and, $\widetilde{F}(x)$, the *tilda generating series* are obtained by specializing the series Z_F,

$$F(x) = Z_F(x, 0, 0, \ldots) \qquad \text{and} \qquad \widetilde{F}(x) = Z_F(x, x^2, x^3, \ldots). \tag{1.2}$$

Many combinatorial operations can be performed in the framework of the theory of species. The main ones are addition, product, substitution, pointing, cartesian product and derivative. For precise definitions of these operations, see [**2**]. However, in this paper we make an extensive use of the cartesian product and the derivative and we briefly recall their definitions. Let F and G be any species and U a finite set. The *derivative species* $F^{'}$ of a species F is given by $F^{'}[U] = F[U + \{*_U\}]$, where $*_U$ is an element chosen outside of the underlying set U. The *cartesian product* of F and G, denoted $F \times G$, is defined by $(F \times G)[U] = F[U] \times G[U]$.

The behaviour of the cycle index series according to the operations of derivation and of cartesian product is well known; see [**2**]. In particular, we have

$$Z_{F'}(x_1, x_2, x_3, \ldots) = \frac{\partial}{\partial x_1} Z_F(x_1, x_2, x_3, \ldots), \quad Z_{F \times G}(x_1, x_2, x_3, \ldots) = (Z_F \times Z_G)(x_1, x_2, x_3, \ldots), \tag{1.3}$$

where $Z_F \times Z_G$ means the *Hadamard product* of the series Z_F and Z_G.

A *molecular species* M is a species possessing only one isomorphy type. This means that any two M-structures are always isomorphic. Such a species is characterized by the fact that it is indecomposable under the combinatorial sum: M is molecular $\iff$ $(M = F + G \Longrightarrow F = 0$ or $G = 0)$. Any molecular species M can be written under the form of a quotient species $M = X^n/H$, where X^n represents the species of linear orders of length n and $H \leq \mathbb{S}_n$ is a subgroup of the symmetric group of order n. In fact, H is the *stabilizer* of any M-structure. Two molecular species X^n/H and X^m/K are equal (that is, isomorphic as species) if and only if $n = m$ and H and K are conjugate subgroups of $\mathbb{S}_n$. Furthermore, any species F can be uniquely expanded in terms of molecular species as follows:

$$F = \sum_{M \in \mathcal{M}} f_M M,$$

where $\mathcal{M}$ denotes the set of all molecular species and $f_M \in \mathbb{N}$ is the number of subspecies of F isomorphic to M. This expansion is unique and called the *molecular expansion* of the species F.

It is also possible to extend the notion of molecular species to the case of multi-sort species. For instance, for two-sort species, where the two sorts are denoted X and T, each molecular species $M = M(X, T)$ can be written in the form $M(X, T) = X^n T^k/H$, where $H \leq \mathbb{S}_n^X \times \mathbb{S}_k^T$ is the stabilizer of any M-structure and $\mathbb{S}_n^X$ is the symmetric group of order n acting on points of sort X. The exponents n and k are called the *degree* of M in X and T. The cycle index series of a two-sort molecular species $M(X, T) = X^n T^k/H$ is given by the expression

$$Z_M(x_1, x_2, \ldots; t_1, t_2, \ldots) = \frac{1}{|H|} \sum_{h \in H} x_1^{c_1(h)} x_2^{c_2(h)} \ldots t_1^{d_1(h)} t_2^{d_2(h)} \ldots,$$

where $c_i(h)$ (resp. $d_i(h)$), for $i \geq 1$, denotes the number of cycles of length i of the permutation on points of sort X (resp. T) induced by the element $h \in H$ and $|H|$ is the cardinality of H. Note that $\mathbb{S}_n^X \times \mathbb{S}_k^T$ is isomorphic to the Young subgroup $\mathbb{S}_{n,k} \leq \mathbb{S}_{n+k}$ permuting independently $\{1, 2, \ldots, n\}$ and $\{n+1, n+2, \ldots, n+k\}$.

It is important to notice that in the series Z_M above, the monomials in the x_i's always appear before the ones in the t_i's.

In this paper, we use the following graphical conventions:

1) for any species $F = F(X)$, we find appropriate to represent an F-structure by a drawing of the form of Figure 1 a) where black dots stand for the distinct elements (of sort X) of the underlying set;

2) for a two-sort species $\Omega = \Omega(X,T)$, Figure 1 b) shows the convention used to represent an Ω-structure, where black dots (resp. black squares) are elements of sort X (resp. of sort T);
3) setting $T := 1$ in a species $\Omega(X,T)$, we obtain the species $\Omega(X,1)$ where points of sort T are unlabelled. Notice that white squares represent undistinguishable unlabelled elements of sort T; see Figure 1 c) and the substitution is possible if $\Omega(X,T)$ is "finitary in T". This means that for every finite set U of points of sort X there is no Ω-structure on the pair of sets (U,V) for every sufficiently large finite set V of points of sort T.

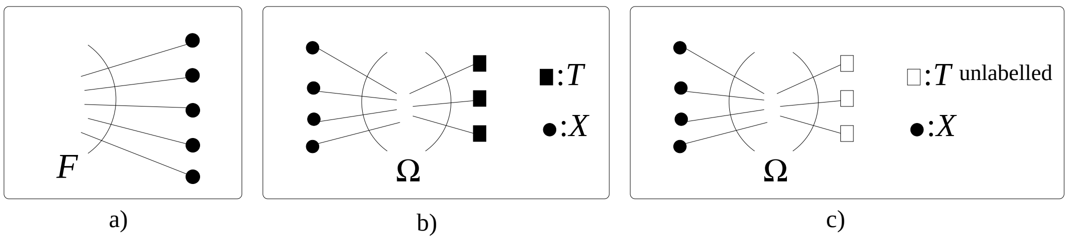


FIGURE 1. a) $F(X)$-structure; b) $\Omega(X,T)$-structure; c) $\Omega(X,1)$-structure

Using these graphical conventions, the structures belonging, for example, to the cartesian product $\Omega_1(X,T) \times \Omega_2(X,T)$ of two-sort species can be represented by Figure 2 a) and a structure belonging ot the species $F^{'}(X)$ can be represented by Figure 2 b).

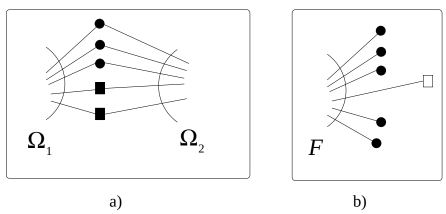


FIGURE 2. a) $\Omega_1(X,T) \times \Omega_2(X,T)$-structure; b) $F^{'}(X)$-structure

Finally, we will make an extensive use in this paper of the so-called *partial cartesian product* according to a sort. Considering two-sort species $\Omega_1(X,T)$ and $\Omega_2(X,T)$, the *partial cartesian product* with respect to the sort T of Ω_1 and Ω_2 is denoted by

$$\Omega_1(X,T) \times_T \Omega_2(X,T) \tag{1.4}$$

and is illustrated by Figure 3. Formally, a $\Omega_1(X,T) \times_T \Omega_2(X,T)$-structure s on a pair (U,V) of sets of sort X and T, respectively, is a pair $s = (s_1, s_2)$ where $s_1 \in \Omega_1[U_1, V]$ and $s_2 \in \Omega_2[U_2, V]$ where $U_1 \cup U_2 = U$ and $U_1 \cap U_2 = \emptyset$. This operation had been first introduced by Gessel and Labelle in [**5**] in the context of Lagrange inversion. It can be checked that $\times_T$ can be written in terms of the ordinary cartesian product as $\Omega_1(X,T)E(Y) \times \Omega_2(Y,T)E(X)\big|_{Y:=X}$.

2. General combinatorial differential operators

2.1. Basic definitions. Let $D = d/dX$ denote the classical combinatorial derivative operator defined by

$$DF(X) = \frac{d}{dX}F(X) = F^{'}(X).$$

We will make use of partial cartesian products and substitutions of the form $T := 1$ to introduce general differential operators of the form $\Omega(X,D)$, where $\Omega(X,T)$ is an arbitrary two-sort species. These operators $\Omega(X,D)$ will transform species into species.

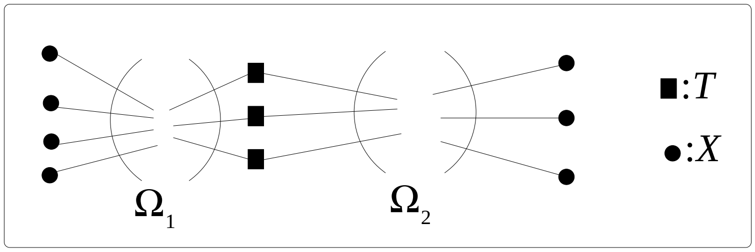


FIGURE 3. Representation of an $\Omega_1(X,T) \times_T \Omega_2(X,T)$-structure

DEFINITION 2.1. (General combinatorial differential operators) Let $\Omega(X,T)$ be a two-sort species and $F(X)$ be a species. If $\Omega(X,T)$ is finitary in T or $F(X)$ is of finite degree in X, then $\Omega(X,D)F(X)$ is the species defined by

$$\Omega(X,D)F(X) := \Omega(X,T) \times_T F(X+T)|_{T:=1}. \tag{2.1}$$

□

Figure 4 a) describes a typical $\Omega(X,D)F(X)$-structure on a set of 9 elements of sort X. For example, let $\Omega(X,T) = A(X,T)$ be the species of rooted trees with internal nodes of sort X and leaves of sort T and $F(X) = C_{10}(X)$ be the species of oriented cycles of length 10, then Figure 4 b) shows a typical $A(X,D)C_{10}(X)$-structure. Taking $\Omega(X,D) = E(L_{\geq 2}(X)D)$ where E and $L_{\geq 2}$ are the species of sets and of lists of length ≥ 2, respectively, then the species of octopuses (see Figure 4 c)) can be written as $\mathrm{Oct}(X) = E(L_{\geq 2}(X)D)C(X)$ where $C(X)$ is the species of oriented cycles.

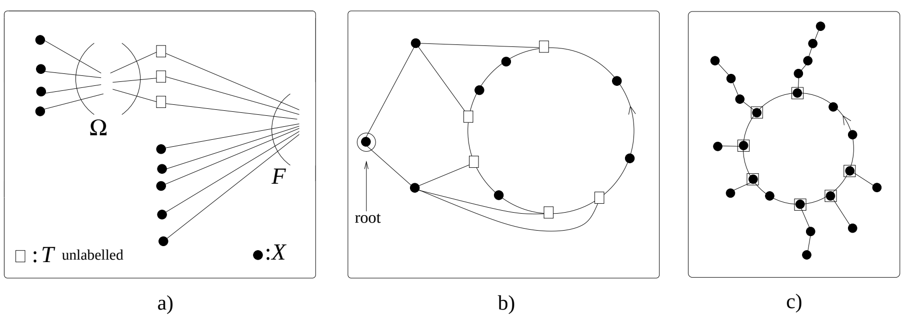


FIGURE 4. a) $\Omega(X,D)F(X)$-structure, b) $A(X,D)C_{10}(X)$-structure and c) an octopus

Note that the restrictions on Ω or F in Definition 2.1 are necessary in order that (2.1) defines a species. For example, for the species $C(X)$ of oriented cycles (of arbitrary lengths), $A(X,D)C(X)$ is not a species since the number of structures would be infinite on any non-empty finite set U. From now, we will always assume that the restrictions in Definition 2.1 are satisfied.

Since every two-sort species $\Omega(X,T)$ can be written as a linear combination $\sum \omega_K \frac{X^n T^k}{K}$ of molecular species, every differential operator $\Omega(X,D)$ is a linear combination of the corresponding *molecular* linear operators of the form $X^n D^k/K,\ K \leq S_{n,k}$. We will denote the action of these operators on species $F(X)$ by

$$\left(\frac{X^n D^k}{K}\right) F(X) = \frac{X^n F^{(k)}(X)}{K}$$

in conformity with the classical notation $X^n D^k F(X) = X^n F^{(k)}(X)$ corresponding to the degenerate case where $K = \{\mathrm{id}\}$. With these notations, we have

THEOREM 2.2. (*Generalized Leibniz rule*) *Let $F(X)$ and $G(X)$ be two species. Then,*

$$\frac{X^n D^k}{K} F(X)G(X) = \sum_{i+j=k} \sum_{L:S_{n,i,j}} \binom{K}{L} \frac{X^n F^{(i)}(X) G^{(j)}(X)}{L} \tag{2.2}$$

*where $L : S_{n,i,j}$ means that L runs through a complete system of representatives of the conjugacy classes of subgroups of $S_{n,i,j}$ and the coefficients $\binom{K}{L}$ are defined by the "addition formula" [**1**],*

$$X^n(T_1+T_2)^k/K = \sum_{i+j=k}\sum_{L:S_{n,i,j}}\binom{K}{L}X^nT_1^iT_2^j/L \tag{2.3}$$

□

For example, $n=0$ and $K=\{\mathrm{id}\}$ corresponds to the classical Leibniz rule

$$D^kF(X)G(X) = \sum_{i+j=k}\binom{k}{i}F^{(i)}(X)G^{(j)}(X),$$

while, the molecular operator $E_2(XD)$, where E_2 is the species of 2-sets, corresponds to the formula

$$E_2(XD)(F\cdot G) = (E_2(XD)F)\cdot G + X^2F'\cdot G' + F\cdot(E_2(XD)G)\,.$$

Proposition 2.1. *Let $G(X) := \Omega(X,D)F(X)$, then we have*

$$Z_G(x_1,x_2,x_3,\ldots) = Z_\Omega(x_1,x_2,x_3,\ldots;\frac{\partial}{\partial x_1},2\frac{\partial}{\partial x_2},3\frac{\partial}{\partial x_3},\ldots)Z_F(x_1,x_2,x_3,\ldots). \tag{2.4}$$

□

In Proposition 2.1, the convention of writing all the t_j's to the right of all the x_i's in $Z_\Omega(x_1,x_2,\ldots,t_1,t_2,\ldots)$ must be applied. For example, taking $\Omega(X,D) = E(XD)$, where E is the species of sets, we have $E(XD)F(X) = F(2X)$. In this case, we must take

$$Z_\Omega(x_1,x_2,\ldots,\frac{\partial}{\partial x_1},2\frac{\partial}{\partial x_2},\ldots) = \sum\frac{x_1^{n_1}x_2^{n_2}\ldots(\frac{\partial}{\partial x_1})^{n_1}(\frac{\partial}{\partial x_2})^{n_2}\ldots}{n_1!n_2!\ldots}$$

not

$$\sum\frac{(x_1\frac{\partial}{\partial x_1})^{n_1}(x_2\frac{\partial}{\partial x_2})^{n_2}\ldots}{n_1!n_2!\ldots}.$$

Another example is given by taking a species of the form $\mathcal{P}(X) = X + \mathcal{P}_{\geq 2}(X)$ and considering the operator $\Omega(X,D) = E(\mathcal{P}_{\geq 2}(X)D)$. It is easily seen that

$$E(\mathcal{P}_{\geq 2}(X)D)F(X) = F(\mathcal{P}(X))$$

and formula (2.4) of Proposition 2.1 reduces to the plethystic substitution $Z_{F\circ\mathcal{P}} = Z_F\circ Z_{\mathcal{P}}$ as the reader can check. The operator $\mathcal{P}_{\geq 2}(X)D$ can be called an "eclosion" operator in the terminology of [**8**].

Definition 2.3. (Composition of differential operators) Let $\Omega_1(X,T)$ and $\Omega_2(X,T)$ be two-sort species. Then, we define the composition of $\Omega_1(X,D)$ by $\Omega_2(X,D)$ by the following formula:

$$\Omega_2(X,D)\odot\Omega_1(X,D) = \Omega_3(X,D) \tag{2.5}$$

where

$$\Omega_3(X,T) = \Omega_2(X,T)\odot\Omega_1(X,T) := \Omega_2(X,T+T_0)\times_{T_0}\Omega_1(X+T_0,T)|_{T_0:=1} \tag{2.6}$$

and T_0 is an auxiliary extra sort.

Figure 5 illustrates an $\Omega_3(X,T)$-structure.

The composition $\Omega_2(X,D)\odot\Omega_1(X,D)$ corresponds to the application of $\Omega_1(X,D)$ followed by $\Omega_2(X,D)$. The operation $\odot$ is associative but non-commutative. For example, $(XD)\odot(X^2D) = 2X^2D + X^3D^2$ while $(X^2D)\odot(XD) = X^2D + X^3D^2$.

Proposition 2.2. *Let $\Omega_3(X,T) = \Omega_2(X,T)\odot\Omega_1(X,T)$, then, we have, for any species $F = F(X)$,*

$$\Omega_3(X,D)F(X) = \Omega_2(X,D)\left[\Omega_1(X,D)F(X)\right].$$

Proof. See Figure 6.

■

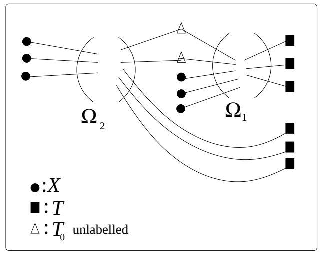


FIGURE 5. $\Omega_2(X, T+T_0) \times_{T_0} \Omega_1(X+T_0, T)|_{T_0:=1}$-structure

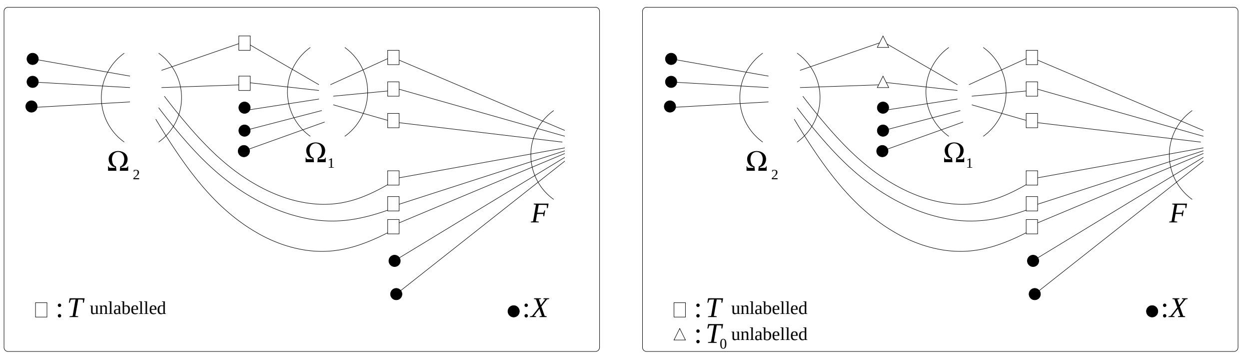


FIGURE 6. a) $\Omega_2(X, D)\,[\Omega_1(X, D)F(X)]$ and b) $[\Omega_2(X, T) \odot \Omega_1(X, T)]\,F(X)$

THEOREM 2.4. *Let* $\Omega_2(X, T) = \frac{X^a T^k}{A}$ *and* $\Omega_1(X, T) = \frac{X^b T^\ell}{B}$ *be two molecular species on two sorts where* $A \leq \mathbb{S}_{a,k}$ *and* $B \leq \mathbb{S}_{b,\ell}$. *Then, for the species* $\Omega(X, T) = \Omega_2(X, T) \odot \Omega_1(X, T)$, *we have,*

$$Z_\Omega = \sum_{n_1, n_2, \ldots} \frac{\left((\frac{\partial}{\partial t_1})^{n_1}(2\frac{\partial}{\partial t_2})^{n_2} \ldots Z_{\frac{X^a T^k}{A}}\right)\left((\frac{\partial}{\partial x_1})^{n_1}(2\frac{\partial}{\partial x_2})^{n_2} \ldots Z_{\frac{X^b T^\ell}{B}}\right)}{1^{n_1} n_1! 2^{n_2} n_2! \ldots}. \tag{2.7}$$

Proof. We have

$$Z_{\frac{X^a(T_0+T)^k}{A}} = \mathrm{e}^{t_{01}\frac{\partial}{\partial t_1} + \frac{t_{02}}{2}\frac{2\partial}{\partial t_2} + \frac{t_{03}}{3}\frac{3\partial}{\partial t_3} + \cdots} Z_{\frac{X^a T^k}{A}}(x_1, x_2, \ldots; t_1, t_2, \ldots) \tag{2.8}$$

$$= \sum_{n_1, n_2, \ldots} \frac{t_{01}^{n_1} t_{02}^{n_2} \ldots (\frac{\partial}{\partial t_1})^{n_1}(2\frac{\partial}{\partial t_2})^{n_2} \ldots}{1^{n_1} n_1! 2^{n_2} n_2! \ldots} Z_{\frac{X^a T^k}{A}}(x_1, x_2, \ldots; t_1, t_2, \ldots) \tag{2.9}$$

In a similar way,

$$Z_{\frac{(X+T_0)^b T^\ell}{B}} = \sum_{n_1, n_2, \ldots} \frac{t_{01}^{n_1} t_{02}^{n_2} \ldots (\frac{\partial}{\partial x_1})^{n_1}(2\frac{\partial}{\partial x_2})^{n_2} \ldots}{1^{n_1} n_1! 2^{n_2} n_2! \ldots} Z_{\frac{X^b T^\ell}{B}}(x_1, x_2, \ldots; t_1, t_2, \ldots). \tag{2.10}$$

The result follows using the cartesian product according to the sort T_0 and letting $t_{0i} := 1$, $i = 1, 2, 3, \ldots$.

■

Using another time the linearity of the molecular expansion, we easily obtain:

COROLLARY 2.1. Let $\Omega_2(X, T)$ and $\Omega_1(X, T)$ be any two-sort species. Then, we have

$$Z_{\Omega_2 \odot \Omega_1} = \sum_{n_1, n_2, \ldots} \frac{\left((\frac{\partial}{\partial t_1})^{n_1}(2\frac{\partial}{\partial t_2})^{n_2} \ldots Z_{\Omega_2}\right)\left((\frac{\partial}{\partial x_1})^{n_1}(2\frac{\partial}{\partial x_2})^{n_2} \ldots Z_{\Omega_1}\right)}{1^{n_1} n_1! 2^{n_2} n_2! \ldots}. \tag{2.11}$$

□

2.2. Bilinear form and adjoint operators. In [**6**], Joyal introduced a bilinear form, denoted $<\,,>$, in the realm of species in the following way: given two species $F = F(X)$ and $G = G(X)$, $< F(X), G(X) >$ is defined by

$$< F(X), G(X) > = \; F(X) \times_X G(X)|_{X:=1} \; = \; \text{number of unlabelled } F \times G-\text{structures}, \tag{2.12}$$

provided it is finite (see Figure 7 a)). It is well known (see [**5, 6**]) that, for any species $H(X)$,

$$< H(D)F(X), G(X) > = < F(X), H(X)G(X) >,$$

which means that multiplication by $H(X)$ is a right adjoint to $H(D)$.

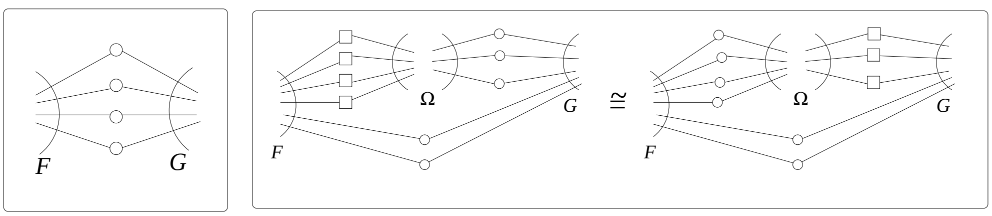
We have the following more general result:

Proposition 2.3. *Let $\Omega(X,T)$ be a two-sort species. Then,*

$$< \Omega(X,D)F(X), G(X) > = < F(X), \Omega(D,X)G(X) > .$$

That is $(\Omega(X,D))^* := \Omega(D,X)$ is the adjoint *operator of $\Omega(X,D)$.*

Proof. See Figure 7 b). ■



a) b)

Figure 7. a) $< F(X), G(X) >$ and b) $< \Omega(X,D)F(X)), G(X) > = < F(X), \Omega(D,X)G(X) >$

Proposition 2.4. *Let $\Omega_1(X,T)$ and $\Omega_2(X,T)$ be two sort-species. Then, we have*

$$\left(\Omega_2(X,D) \odot \Omega_1(X,D)\right)^* = \Omega_1^*(X,D) \odot \Omega_2^*(X,D) = \Omega_1(D,X) \odot \Omega_2(D,X). \tag{2.13}$$

□

3. Special cases

3.1. Combinatorial Hammond differential operators. The special case $\Omega(X,T) = \Theta(T)$ corresponds to the classical Hammond combinatorial differential operator defined by (see [**4, 6**])

$$\Theta(D)F(X) = (E(X)\Theta(T)) \times (F(X+T))\Big|_{T:=1} := \Theta(T) \times_T F(X+T)\Big|_{T:=1}. \tag{3.1}$$

Figure 8 shows a typical $\Theta(D)F(X)$-structure. Note that, contrarily to the general case, the composition

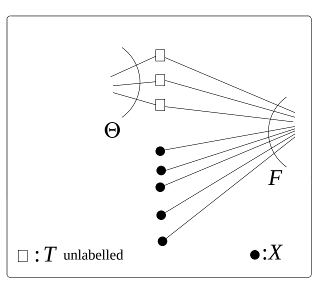


Figure 8. A typical $\Theta(D)F(X)$-structure

$\Theta(D) \odot \Psi(D)$ of Hammond operators is commutative since it corresponds to ordinary multiplication:

$$\Theta(D) \odot \Psi(D) = (\Theta \cdot \Psi)(D). \tag{3.2}$$

EXAMPLE 3.1. The following relations can be easily established by appropriate drawings and details are left to the reader.

(1) For $\Theta(T) = E_2(T)$, the species of two-element sets, we have

$$E_2(D)(F \cdot G) = (E_2(D)F) \cdot G + F^{'}G^{'} + (E_2(D)G) \cdot F, \tag{3.3}$$

$$E_2(D)(E \circ F) = (E \circ F) \cdot (E_2(D)F + E_2(F^{'})). \tag{3.4}$$

In particular, for the species $F = C$ of oriented cycles and $E \circ C = S$ of permutations, the previous equation takes the form

$$E_2(D)S = S \cdot (E_2(D)F + E_2(L)).$$

(2) *Translation operators.* Taking $\Theta(X) = E(X)$, the species of sets, we obtain the translation operator denoted $E(D)$, whose action is described by

$$E(D)F(X) = F(X+1), \qquad E^n(D)F(X) = F(X+n).$$

(3) When $\Theta(T) = T^n$, $n \geq 0$, then we recover the usual n-th derivatives

$$\Theta(D)F(X) = D^n F(X) = \frac{d^n G(X)}{dX^n}.$$

(4) *Catalan derivative.* Let $\Theta(T) = B(T)$ be the species of binary trees. It is well known that this species satisfies the functional equation $B = 1 + TB^2$. Since $1/B(T) = 1 - TB(T)$ we deduce that

$$B(D)F(X) = G(X) \quad \Longleftrightarrow \quad F(X) = (1 - DB(D))\, G(X).$$

It is important to notice that the species $1 - TB(T)$ is virtual, in this case.

(5) We can generalize the preceding example by taking any species $\mathcal{B} = \mathcal{B}(T)$ with constant term equal to 1 since such a species is invertible under product (in the context of virtual species; see [**2, 7**]), we have

$$\mathcal{B}(D)F(X) = G(X) \Longleftrightarrow F(X) = \frac{1}{\mathcal{B}(D)}G(X).$$

$\square$

3.2. Self-adjoint and pointing operators. Since the adjoint of an operator $\Omega(X, D)$ is $\Omega(D, X)$, self-adjoint operators correspond to symmetric species $\Omega(X, T) = \Omega(T, X)$. For example, the operator X^3D^3/K, where $K =< (123)(456) >\leq S_{3,3}$ is self-adjoint and $\Phi(X + D)$ is self-adjoint for any species $\Phi(X)$.

An important class of self-adjoint operators is the Λ-pointing operators defined by $\Lambda(XD)$, where $\Lambda = \Lambda(T)$ is an arbitrary species. Figure 9 a) shows a typical $\Lambda(XD)F(X)$-structure. The special case $\Lambda(T) = T$ corresponds to the classical one-element pointing. The composition of pointing operators is *not* commutative and is given by

$$\Lambda_2(XD) \odot \Lambda_1(XD) = \Omega(X, D),$$

where

$$\Omega(X, T) = \Lambda_2(XT + XT_0) \times_{T_0} \Lambda_1(XT + T_0T)\Big|_{T_0:=1}.$$

Taking $\Lambda(T) = T^2$, we obtain the operator $(XD)^2$ which corresponds to pointing an ordered pair of *distinct* elements in structures (see Figure 9 b)) and $(XD)^2$ corresponds to the species $(XT)^2 = X^2T^2$. On the contrary, for ordinary (*i.e.*, classical) differential operators, we have $(XD)^2 \neq X^2D^2$ because multiplicative notation is used to denote composition of ordinary differential operators. This fact is expressed as $(XD)^{\odot 2} \neq X^2D^2$ in the present context. Indeed,

$$(XD)^{\odot 2} := (XD) \odot (XD) = XD + X^2D^2 \neq (XD)^2 = X^2D^2$$

since we can point the *same* element in two successive pointings (see Figure 9 c)).

Taking $\Lambda(T) = C(T)$, the species of oriented cycles, we obtain the operator $C(XD)$ of cyclic-pointing. An interesting subspecies of $C(XD)F(X)$ has recently been introduced by Bodirsky et al. [**3**]. It consists of all *unbiased* cyclically pointed F-structures. In such structures, the pointed cycle must be one of the

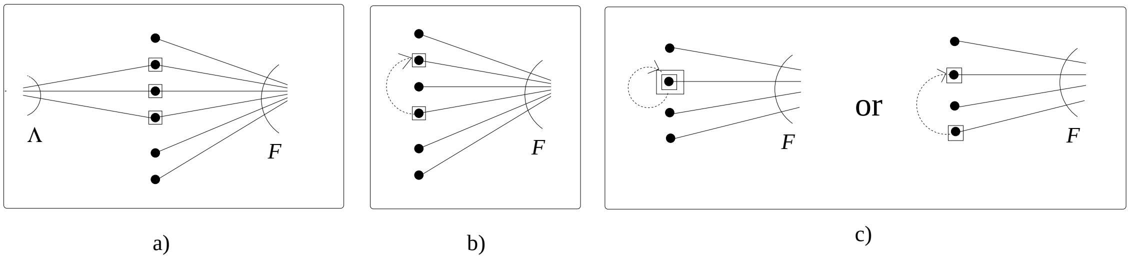


FIGURE 9. a) Λ-pointed F-structure, b) $(XD)^2F$-structure and c) $(XD \odot XD)F$-structure

cycles of an automorphism of the F-structure. They applied this unbiased pointing to the uniform random generation of classes of unlabelled structures.

3.3. Low degree operators. Let K be a subgroup of $\mathbb{S}_{n,k}$. By definition, the number k is called the *degree* of the molecular differential operator X^nD^k/K. More generally, the degree of the differential operator $\Omega(X, D)$, is the supremum (possibly infinite) of the degrees occurring in its molecular expansion $\Omega(X, D) = \sum_K \omega_K X^nD^k/K$. If all the degrees involved are k, the operator is said to be *homogeneous of degree k*. Degree 0 operator are simply the multiplication operators $H(X)$ which are adjoint, as we saw before, to the Hammond operators $H(D)$. Homogeneous operators of degree 1 are easily classified. They are of the form $H(X)D$, since every species $\Omega(X, T)$, homogeneous of degree 1 in T is of the form $H(X)T$. Homogeneous operator of degree 2 are a little more involved. We call them *handle operators* for obvious reasons (see Figure 10). The molecular handle operators X^nD^2/K fall into two classes:

a) the oriented ones, for which the second projection $\pi_2(K)$ is trivial in $\mathbb{S}_2$;
b) the unoriented ones, for which $\pi_2(K) \simeq \mathbb{S}_2$.

For example, $C_3(X)D^2$ is oriented and $E_2(XD)$ is unoriented. Explicit tables of molecular differential operators X^nD^k/K, for small n and k and their $\odot$-composition are under construction by the authors.

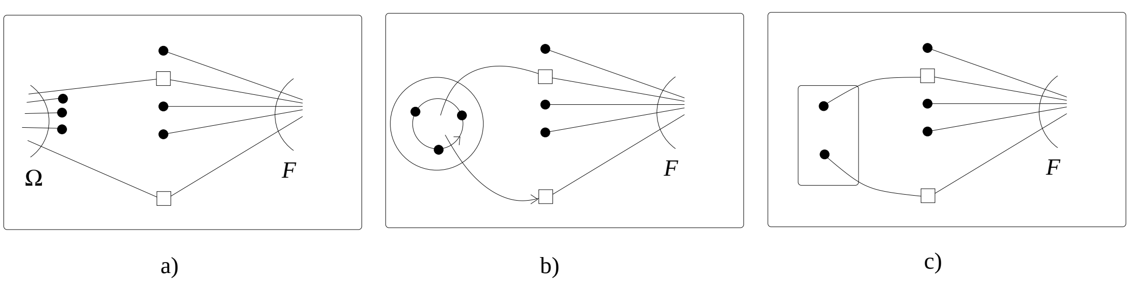


FIGURE 10. a) Handle, b) oriented handle and c) unoriented handle

3.4. Finite differences operators. We saw in Section 3.1, that $E(D)$ is the translation operator on species (of finite degree): $E(D)F(X) = F(X + 1)$. Hence, we can define the difference operator Δ by the equation

$$\Delta = E_+(D),$$

where $E_+ = E - 1$ is the species of non-empty finite sets. We obviously have

$$\Delta F(X) = F(X + 1) - F(X). \tag{3.5}$$

Note that the right-hand side of (3.5) is not a virtual species since $F(X)$ is always a subspecies of $F(X + 1)$. Conversely, we can write $D = E_+^{<-1>}(\Delta)$, where $E_+^{<-1>}$ is the inverse under substitution of the species E_+ (see [**2**] for a description of $E_+^{<-1>}$). This opens the way to a completely new theory of general combinatorial difference operators of the form $\Phi(X, \Delta) = \Phi(X, E_+(D))$ where $\Phi(X, T)$ is an arbitrary species.

3.5. Splittable and classical operators. Let us say that a molecular operator X^nD^k/K is *splittable* if it can be written in the form of a product

$$\frac{X^nD^k}{K} = \frac{X^n}{K_1}\cdot\frac{D^k}{K_2}$$

where $K_1 \leq \mathbb{S}_n$ and $K_2 \leq \mathbb{S}_k$. More generally, any linear combination of splittable operators is called splittable. For example, X^3D^2 and $C(X)E_2(D)+E(D)$ are splittable but $E(XD)$ and the operator X^3D^3/K where $K =< (123)(456) >\leq \mathbb{S}_{3,3}$ are not splittable. Of course, the adjoint of a splittable operator is always splittable. In particular, every Hammond operator $H(D)$ is splittable as well as every multiplication $H(X)$. However, splittable operators are not closed under composition $\odot$. To see this, consider the composition of the splittable operators $C_4(D)$ and $C_4(X)$. Some computations gives

$$C_4(D)\odot C_4(X) = C_4(X)C_4(D) + X^3D^3 + 4X^2D^2 + E_2(XD) + 6XD + 3,$$

which is not splittable since

$$E_2(XD) = \frac{X^2D^2}{< (12)(34) >}$$

is not.

An important subclass of splittable combinatorial operators are those for which $K_2 = \{\mathrm{id}\}$. These operators are closed under $\odot$ and form an algebra:

$$(A(X)D^k)\odot(B(X)D^\ell) = \sum_{i=0}^{k}\binom{k}{i}A(X)B^{(i)}(X)D^{k+\ell-i}.$$

Such operators have been used by Mishna to define a notion of holonomic species [**9**]. When both subgroups K_1 and K_2 are trivial, the corresponding operators are said to be *classical*. They also form an algebra (using complex coefficients in molecular expansions) under $+$ and $\odot$ which is isomorphic to the classical Weyl $\mathbb{C}$-algebra generated by X and D.

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