# A new algorithm for computing the multivariate Faà di Bruno's formula

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December 30, 2010

#### Abstract

A new algorithm for computing the multivariate Faà di Bruno's formula is provided. We use a symbolic approach based on the classical umbral calculus that turns the computation of the multivariate Faà di Bruno's formula into a suitable multinomial expansion. We propose a MAPLE procedure whose computational times are faster compared with the ones existing in the literature. Some illustrative applications are also provided.

**keywords**: multivariate composite function, Faà di Bruno's formula, multivariate cumulant, multivariate Hermite polynomial, classical umbral calculus

AMS subject classification: 68W30, 65C60, 05A40

# 1 Introduction

The multivariate Faà di Bruno's formula has been recently addressed by the following two approaches. Combinatorial methods are used by Costantine and Savits [1], and (only in the bivariate case) by Noschese and Ricci [12]. A treatment based on Taylor series is proposed by Leipnik and Pearce [10]. We refer to this last paper for a detailed list of references on this subject and for a detailed account of its applications. We just mention the paper of Savits [14] for statistical applications. A comprehensive survey of the use of univariate and multivariate series approximation methods in statistics is given in [9].

Computing the multivariate Faà di Bruno's formula by means of a symbolic software can be done by recursively applying a chain rule. Despite its conceptual plainess, applications of the chain rule become impractical also for small values, because the number of additive terms becomes awkward and the derivation of the terms somewhat tiresome. Moreover

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the output is often untidy, so further manipulations are required to simplify the result (see the example in Appendix 2). So a "compressed" version of the multivariate Faà di Bruno's formula becomes more attractive, as the multivariable dimensions or the derivation order increase. Here, a "compressed" version of the multivariate Faà di Bruno's formula is given by using the umbral methods, introduced and developed in [6, 7, 13]. These methods have been particularly suited in dealing with topics where the composition of the formal power series plays a crucial role, see for instance [2, 3] and [5]. Therefore it is quite natural to approach the multivariate Faà di Bruno's formula by means of these symbolic tools. The result is a new algorithm based on a suitable generalization of the well-known multinomial theorem:

$$(x_1 + x_2 + \dots + x_n)^i = \sum_{k_1 + k_2 + \dots + k_n = i} \binom{i}{k_1, k_2, \dots, k_n} x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n}$$

where the indeterminates are replaced by symbolic objects. Suitable choices of these objects give rise to an efficient computation of the following compositions: univariate with multivariate, multivariate with univariate, multivariate with the same multivariate, multivariate with different multivariates in an arbitrary number of components.

Finally, the connection between the multivariate Faà di Bruno's formula and the multinomial theorem allows us to give a closed form for the so-called *generalized Bell polynomial* introduced in [1]. Umbral versions of the multivariate Hermite polynomials are given as a special case of these generalized Bell polynomials.

A MAPLE implementation of all these formulae ends the paper. Comparisons with existing algorithms, based on the chain rule, show the improvement of the computational time due to the proposed approach.

#### 2 The umbral syntax

Umbral methods consist essentially of a symbolic technique to deal with sequences of numbers, indexed by nonnegative integers, where the subscripts are treated as powers.

More formally an umbral calculus consists of a set  $A = \{\alpha, \beta, \ldots\}$ , called *alphabet*, whose elements are named *umbrae*, and a linear functional E, called *evaluation*, defined on a polynomial ring R[A] and taking values in R, where R is a suitable ring. For the purpose of this paper, R denotes the real or complex field. The linear functional E is such that E[1] = 1 and

$$E[\alpha^{i}\beta^{j}\cdots\gamma^{k}] = E[\alpha^{i}] E[\beta^{j}]\cdots E[\gamma^{k}], \quad \text{(uncorrelation property)}$$
(1)

for any set of distinct umbrae in A and for i, j, k nonnegative integers. A sequence  $a_0 = 1, a_1, a_2, \ldots$  in R is umbrally represented by an umbra  $\alpha$  when

$$E[\alpha^n] = a_n$$

for all nonnegative integers n. The elements  $\{a_n\}_{n\geq 1}$  are called *moments* of the umbra  $\alpha$ . Special umbrae are

- i) the augmentation umbra  $\epsilon \in A$ , such that  $E[\epsilon^n] = \delta_{0,n}$ , for all nonnegative integers n;
- ii) the unity umbra  $u \in A$ , such that  $E[u^n] = 1$ , for all nonnegative integers n;
- *iii)* the singleton umbra  $\chi \in A$  such that  $E[\chi^n] = \delta_{1,n}$ , for all integers  $n \ge 1$ .

Note that a sequence of moments can be umbrally represented by two or more uncorrelated umbrae. Indeed, the umbrae  $\alpha$  and  $\gamma$  are said to be *similar* when

$$E[\alpha^n] = E[\gamma^n],$$
 (in symbols  $\alpha \equiv \gamma$ )

for all nonnegative integers n. An umbral polynomial p is such that  $p \in R[A]$ . The support of an umbral polynomial is the set of all umbrae which occur. Two umbral polynomials pand q are said to be *umbrally equivalent* if and only if

$$E[p] = E[q],$$
 (in symbols  $p \simeq q$ ). (2)

The classical umbral calculus has reached a more advanced level compared with the notions that we resume in the next paragraph. We only recall terminology, notation and basic definitions strictly necessary to deal with the topic of this paper. We skip the proofs, the reader interested in is referred to [6, 7, 13].

Univariate umbral calculus. The symbol  $\gamma^{\cdot n}$  denotes the product of n uncorrelated umbrae similar to  $\gamma$ , that is  $E[(\gamma^{\cdot n})^k] = g_k^n$  for all nonnegative integers k and n, where  $g_k = E[\gamma^k]$ . The auxiliary umbra  $\gamma^{\cdot n}$  is called the *n*-th dot power of  $\gamma$ . The summation of n uncorrelated umbrae similar to  $\gamma$  is denoted by the auxiliary umbra  $n \cdot \gamma$  and called the dot product of the integer n and the umbra  $\gamma$ . By using the umbral equivalence (2), we are able to expand powers of  $n \cdot \gamma$ . Indeed, let  $\lambda = (1^{r_1}, 2^{r_2}, \ldots)$  be an integer partition of length  $\nu_{\lambda}$  with multiplicities  $\mathfrak{m}(\lambda) = (r_1, r_2, \ldots)$ . Set  $\mathfrak{m}(\lambda)! = r_1!r_2! \cdots$  and  $\lambda! = (1!)^{r_1}(2!)^{r_2} \cdots$ . Then powers of  $n \cdot \gamma$  verify the following umbral equivalence:

$$(n \cdot \gamma)^i \simeq \sum_{\lambda \vdash i} \frac{i!}{\mathfrak{m}(\lambda)! \,\lambda!} (n)_{\nu_\lambda} \gamma_\lambda, \qquad i = 1, 2, \dots$$
(3)

where the summation is over all partitions  $\lambda$  of the integer *i*, the symbol  $(n)_{\nu_{\lambda}}$  denotes the lower factorial and  $\gamma_{\lambda} = (\gamma_1)^{\cdot r_1} (\gamma_2^2)^{\cdot r_2} \cdots$ , with  $\gamma_1, \gamma_2, \ldots$  uncorrelated umbrae similar to  $\gamma$ . Since  $E[(n,\chi)^i] = (n)_i$ , equivalence (3) can be rewritten as

$$(n \cdot \gamma)^{i} \simeq \sum_{\lambda \vdash i} \frac{i!}{\mathfrak{m}(\lambda)! \,\lambda!} (n \cdot \chi)^{\nu_{\lambda}} \gamma_{\lambda}.$$

$$\tag{4}$$

The main tool of the umbral syntax is summarized in the following construction. By equivalence (3),  $E[(n \cdot \gamma)^i]$  results to be a polynomial  $q_i(n) = \sum_{\lambda \vdash i} (n)_{\nu_\lambda} d_\lambda E[\gamma_\lambda]$  of degree *i* in *n*, where  $d_\lambda = i!/\mathfrak{m}(\lambda)!\lambda!$ . If the integer *n* is replaced by an umbra  $\alpha$ , the umbral polynomial  $q_i(\alpha)$  is such that  $q_i(\alpha) \simeq \sum_{\lambda \vdash i} (\alpha)_{\nu_\lambda} d_\lambda \gamma_\lambda$ . We denote by  $\alpha \cdot \gamma$  the auxiliary

<sup>&</sup>lt;sup>1</sup>Here  $\delta_{i,j}$  denotes the Kronecker's delta.

umbra such that  $(\alpha \cdot \gamma)^i \simeq q_i(\alpha)$ , for all nonnegative integers *i*. The umbra  $\alpha \cdot \gamma$  is called the *dot product* of  $\alpha$  and  $\gamma$ . Since  $(\alpha \cdot \chi)^i \simeq (\alpha)_i$ , from equivalence (4) we have

$$q_i(\alpha) \simeq \sum_{\lambda \vdash i} \frac{i!}{\mathfrak{m}(\lambda)! \, \lambda!} \, (\alpha \cdot \chi)^{\nu_\lambda} \, \gamma_\lambda. \tag{5}$$

We repeat this construction, replacing the umbra  $\alpha$  in  $q_i(\alpha)$  with the dot product of  $\alpha$ and  $\delta$ , so we construct  $(\alpha \cdot \delta) \cdot \gamma$ . Since  $(\alpha \cdot \delta) \cdot \gamma \equiv \alpha \cdot (\delta \cdot \gamma)$ , parenthesis can be avoided.

A noteworthy dot product is the auxiliary umbra  $\alpha \cdot \beta \cdot \gamma$ , where  $\beta$  is the so-called Bell umbra. The moments of the umbra  $\beta$  are the Bell numbers. Indeed, since  $\beta \cdot \chi \equiv \chi \cdot \beta \equiv u$ then  $\alpha \cdot \beta \cdot \chi \equiv \alpha \cdot u \equiv \alpha$  and from equivalence (5) we have

$$q_i(\alpha,\beta) \simeq (\alpha,\beta,\gamma)^i \simeq \sum_{\lambda \vdash i} \frac{i!}{\mathfrak{m}(\lambda)!\,\lambda!} \,\alpha^{\nu_\lambda} \,\gamma_\lambda. \tag{6}$$

**Remark 2.1.** Equivalence (6) is the umbral version of the univariate Faà di Bruno's formula. In particular, let  $\{a_n\}, \{g_n\}, \{h_n\}$  denote respectively the moments of  $\alpha, \gamma$  and  $\alpha \cdot \beta \cdot \gamma$ . If we consider the formal power series

$$f(\alpha, t) = 1 + \sum_{n=1}^{\infty} a_n \frac{t^n}{n!}, \ f(\gamma, t) = 1 + \sum_{n=1}^{\infty} g_n \frac{t^n}{n!}, \ f(\alpha \cdot \beta \cdot \gamma, t) = 1 + \sum_{n=1}^{\infty} h_n \frac{t^n}{n!},$$

then we have

$$f(\alpha \cdot \beta \cdot \gamma, t) = f[\alpha, f(\gamma, t) - 1].$$
(7)

So  $E[(\alpha,\beta,\gamma)^n]$  is the *n*-th coefficient of  $f[\alpha, f(\gamma,t)-1]$ . This is why the dot product  $\alpha,\beta,\gamma$  is called the *composition umbra* of  $\alpha$  and  $\gamma$ .

Multivariate umbral calculus. In the univariate classical umbral calculus, the main device is to replace  $a_n$  with  $\alpha^n$  via the linear evaluation E. Similarly, in the multivariate case, the main device is to replace sequences like  $\{g_{i_1,i_2,\ldots,i_n}\}$ , where  $(i_1,i_2,\ldots,i_n) \in \mathbb{N}_0^n$  is a *multi-index*, with a product of powers  $\mu_1^{i_1}\mu_2^{i_2}\cdots\mu_n^{i_n}$ , where  $\{\mu_1,\mu_2,\ldots,\mu_n\}$  are umbral monomials in R[A]. Note that the supports of the umbral monomials in  $\{\mu_1,\mu_2,\ldots,\mu_n\}$  are not necessarily disjoint. In order to manage a product like  $\mu_1^{i_1}\mu_2^{i_2}\cdots\mu_n^{i_n}$ , as a power of an umbra, we will use a multi-index notation. Let  $\mathbf{i} \in \mathbb{N}_0^n$ . We set  $\mathbf{i}! = i_1!i_2!\cdots i_n!$  and  $(\mu_1,\mu_2,\ldots,\mu_n)^{\mathbf{i}} = \mu_1^{i_1}\mu_2^{i_2}\cdots\mu_n^{i_n}$ , where  $\mathbf{\mu} = (\mu_1,\mu_2,\ldots,\mu_n)$  denotes a *n*-tuple of umbral monomials. We define the  $\mathbf{i}$ -th power of  $\mathbf{\mu}$  as follows  $\mathbf{\mu}^{\mathbf{i}} = \mu_1^{i_1}\mu_2^{i_2}\cdots\mu_n^{i_n}$ .

A sequence  $\{g_i\}_{i\in\mathbb{N}_0^n} \in R$ , with  $g_i = g_{i_1,i_2,...,i_n}$  and  $g_0 = 1$ , is umbrally represented by the *n*-tuple  $\mu$  when

$$E[\boldsymbol{\mu}^{\boldsymbol{\imath}}] = g_{\boldsymbol{i}},$$

for all  $i \in \mathbb{N}_0^n$ . The elements  $\{g_i\}_{i \in \mathbb{N}_0^n}$  are called *multivariate moments* of  $\mu$ . Two *n*-tuples  $\nu$  and  $\mu$  of umbral monomials are said to be similar, if they represent the same sequence of multivariate moments, in symbols  $\nu \equiv \mu$ . If for all  $i, j \in \mathbb{N}_0^n$ , we have  $E[\nu^i \mu^j] = E[\nu^i]E[\mu^j]$ , then  $\nu$  and  $\mu$  are said to be uncorrelated.

In the univariate case we have defined the auxiliary umbra  $n \cdot \gamma$  and the composition umbra  $\alpha \cdot \beta \cdot \gamma$ . We follow the same steps in the multivariate case.

Let  $\{\mu', \mu'', \ldots, \mu'''\}$  be a set of *m* uncorrelated *n*-tuples similar to  $\mu$ . Define the *dot* product of *m* and  $\mu$  as the auxiliary umbra  $m \cdot \mu = \mu' + \mu'' + \cdots + \mu'''$  and the *m*-th *dot* power of  $\mu$  as the auxiliary umbra  $\mu \cdot m = \mu' \mu'' \cdots \mu'''$ .

In the following we give an expansion of the *i*-th power of  $m.\mu$  in terms of partitions of a multi-index, see Definition 2.2. To this aim, we introduce the notion of generating function of the *n*-tuple  $\mu$ . The exponential multivariate formal power series

$$e^{\mu t^{T}} = e^{\mu_{1}t_{1} + \mu_{2}t_{2} + \dots + \mu_{n}t_{n}} = u + \sum_{k=1}^{\infty} \sum_{\substack{i \in \mathbb{N}_{0} \\ |i| = k}} \mu^{i} \frac{t^{i}}{i!}$$
(8)

is said to be the generating function of the *n*-tuple  $\mu$ , where  $\mathbf{t} = (t_1, t_2, \ldots, t_n)$  and  $\mathbf{t}^T$  denotes its transpose. Now, assume  $\{g_i\}_{i \in \mathbb{N}_0^n}$  umbrally represented by the *n*-tuple  $\mu$ . If the sequence  $\{g_i\}_{i \in \mathbb{N}_0^n}$  has exponential multivariate generating function

$$f(\boldsymbol{\mu}, \boldsymbol{t}) = 1 + \sum_{k=1}^{\infty} \sum_{\substack{\boldsymbol{i} \in \mathbb{N}_0^n \\ |\boldsymbol{i}| = k}} g_{\boldsymbol{i}} \frac{\boldsymbol{t}^{\boldsymbol{i}}}{\boldsymbol{i}!},$$

by suitably extending the action of E coefficientwise to generating functions (8), we have  $E[e^{\mu t^{T}}] = f(\mu, t)$ . Henceforth, when no confusion occurs, we refer to  $f(\mu, t)$  as the generating function of the *n*-tuple  $\mu$ .

**Proposition 2.1.** If  $\{\mu_1, \ldots, \mu_n\}$  are uncorrelated umbral monomials, then  $\boldsymbol{\mu} \equiv \tilde{\boldsymbol{\mu}}_1 + \cdots + \tilde{\boldsymbol{\mu}}_n$ , where the vectors  $\{\tilde{\boldsymbol{\mu}}_1, \ldots, \tilde{\boldsymbol{\mu}}_n\}$  are uncorrelated and such that  $\tilde{\boldsymbol{\mu}}_i = (\varepsilon, \ldots, \mu_i, \ldots, \varepsilon)$  is obtained from  $\boldsymbol{\mu}$  by replacing each umbral monomial with  $\varepsilon$ , except the *i*-th one.

*Proof.* From (8), we have  $f(\boldsymbol{\mu}, \boldsymbol{t}) = E[e^{\boldsymbol{\mu} \boldsymbol{t}^T}] = E[e^{\mu_1 t_1 + \mu_2 t_2 + \dots + \mu_n t_n}] = \prod_{i=1}^n E[e^{\mu_i t_i}] = \prod_{i=1}^n f(\mu_i, t_i)$ . The result follows by observing that  $f(\mu_i, t_i) = f(\tilde{\boldsymbol{\mu}}_i, \boldsymbol{t})$  for  $i = 1, 2, \dots, n$ .

In order to compute the coefficients of  $f(m.\mu, t)$ , we first introduce the notion of *composition of a multi-index* and then the notion of *partition of a multi-index*.

**Definition 2.1** (Composition of a multi-index). A composition  $\lambda$  of a multi-index i, in symbols  $\lambda \models i$ , is a matrix  $\lambda = (\lambda_{ij})$  of nonnegative integers and with no zero columns such that  $\lambda_{r1} + \lambda_{r2} + \cdots + \lambda_{rk} = i_r$  for r = 1, 2, ..., n.

The number of columns of  $\lambda$  is called the length of  $\lambda$  and denoted by  $l(\lambda)$ .

**Definition 2.2** (Partition of a multi-index). A partition of a multi-index i is a composition  $\lambda$ , whose columns are in lexicographic order, in symbols  $\lambda \vdash i$ .

Just as it is for integer partitions, the notation  $\lambda = (\lambda_1^{r_1}, \lambda_2^{r_2}, ...)$  means that in the matrix  $\lambda$  there are  $r_1$  columns equal to  $\lambda_1$ ,  $r_2$  columns equal to  $\lambda_2$  and so on, with  $\lambda_1 < \lambda_2 < \cdots$ . The integer  $r_i$  is the multiplicity of  $\lambda_i$ . We set  $\mathfrak{m}(\lambda) = (r_1, r_2, ...)$ .

**Proposition 2.2.** Let  $\mu$  be a n-tuple of umbral monomials. For  $i \in \mathbb{N}_0^n$  we have

$$(m \cdot \boldsymbol{\mu})^{\boldsymbol{i}} \simeq \sum_{\boldsymbol{\lambda} \vdash \boldsymbol{i}} \frac{\boldsymbol{i}!}{\mathfrak{m}(\boldsymbol{\lambda})! \, \boldsymbol{\lambda}!} (m \cdot \chi)^{l(\boldsymbol{\lambda})} \boldsymbol{\mu}_{\boldsymbol{\lambda}}, \tag{9}$$

where the sum is over all partitions  $\lambda$  of the multi-index i, and  $\mu_{\lambda} = (\mu'^{\lambda_1}) \cdot r_1(\mu''^{\lambda_2}) \cdot r_2 \cdots$ , with  $\mu', \mu'', \ldots$  uncorrelated n-tuples similar to  $\mu$ .

*Proof.* Due to the uncorrelation property, we have  $f(m.\mu, t) = [f(\mu, t)]^m$  and  $\{[f(\mu, t) - 1] + 1\}^m = 1 + \sum_{k=1}^m {m \choose k} [f(\mu, t) - 1]^k$ . Moreover, we have

$$[f(\boldsymbol{\mu}, \boldsymbol{t}) - 1]^k = \sum_{(\boldsymbol{\pi}_1, \dots, \boldsymbol{\pi}_k)} \frac{g_{\boldsymbol{\pi}_1}}{\boldsymbol{\pi}_1 !} \cdots \frac{g_{\boldsymbol{\pi}_k}}{\boldsymbol{\pi}_k !} \boldsymbol{t}^{\boldsymbol{\pi}_1} \cdots \boldsymbol{t}^{\boldsymbol{\pi}_k}$$

where the sum is over all vectors  $\{\pi_1, \ldots, \pi_k\} \in \mathbb{N}_0^n \setminus \{\mathbf{0}\}$ . If we denote by  $\pi$  the multi-index composition  $(\pi_1, \ldots, \pi_k) \models i$ , and we set  $g_{\pi} = g_{\pi_1} \cdots g_{\pi_k}$  and  $\binom{i}{\pi} = \frac{i!}{\pi!}$ , then we have

$$[f(\boldsymbol{\mu}, \boldsymbol{t}) - 1]^k = \sum_{\boldsymbol{i} > 0} \left[ \sum_{\substack{\boldsymbol{\pi} \models \boldsymbol{i} \\ l(\boldsymbol{\pi}) = k}} \binom{\boldsymbol{i}}{\boldsymbol{\pi}} g_{\boldsymbol{\pi}} \right] \frac{\boldsymbol{t}^{\boldsymbol{i}}}{\boldsymbol{i}!}.$$
 (10)

Replacing (10) in  $f(m \cdot \mu, t) = 1 + \sum_{k=1}^{m} \frac{(m)_k}{k!} [f(\mu, t) - 1]^k$ , we have

$$f(m.\boldsymbol{\mu},\boldsymbol{t}) = 1 + \sum_{\boldsymbol{i}>0} \left[ \sum_{\boldsymbol{\pi}\models\boldsymbol{i}} {\binom{\boldsymbol{i}}{\boldsymbol{\pi}}} \frac{(m)_{l(\boldsymbol{\pi})}}{l(\boldsymbol{\pi})!} g_{\boldsymbol{\pi}} \right] \frac{\boldsymbol{t}^{\boldsymbol{i}}}{\boldsymbol{i}!}.$$
 (11)

Observe that for each  $\pi \models i$ , any other composition  $\tau \models i$ , obtained by permuting the columns of  $\pi$ , is such that  $g_{\pi} = g_{\tau}$ . If  $\pi = (c_1^{r_1}, c_2^{r_2}, ...)$  then the number of distinct permutations of  $\pi$  are  $l(\pi)!/\mathfrak{m}(\pi)!$ . So indexing the last summation in (11) by partitions  $\lambda$  of i, instead of compositions  $\pi$ , we have

$$f(m.\boldsymbol{\mu}, \boldsymbol{t}) = 1 + \sum_{\boldsymbol{i}>0} \left[ \sum_{\boldsymbol{\lambda}\vdash\boldsymbol{i}} \frac{(m)_{l(\boldsymbol{\lambda})}}{\mathfrak{m}(\boldsymbol{\lambda})! \, \boldsymbol{\lambda}!} g_{\boldsymbol{\lambda}} \right] \frac{\boldsymbol{t}^{\boldsymbol{i}}}{\boldsymbol{i}!}.$$
 (12)

Recalling that  $E[(m,\chi)^{l(\lambda)}] = (m)_{l(\lambda)}$  and  $E[\mu_{\lambda}] = g_{\lambda}$ , equivalence (9) follows.

### 3 Multivariate Faà di Bruno's formula

We start by introducing the auxiliary umbra  $\alpha \boldsymbol{.} \beta \boldsymbol{.} \boldsymbol{\mu}$ . We define

$$(\alpha \boldsymbol{.} \beta \boldsymbol{.} \boldsymbol{\mu})^{\boldsymbol{i}} \simeq \sum_{\boldsymbol{\lambda} \vdash \boldsymbol{i}} \frac{\boldsymbol{i}!}{\mathfrak{m}(\boldsymbol{\lambda})! \, \boldsymbol{\lambda}!} \, \alpha^{l(\boldsymbol{\lambda})} \boldsymbol{\mu}_{\boldsymbol{\lambda}}, \tag{13}$$

where  $\beta$  is the Bell umbra and  $\alpha \in A$ .

**Theorem 3.1** (Univariate composite Multivariate). Let  $\boldsymbol{\mu}$  be a n-tuple of umbral monomials with generating function  $f(\boldsymbol{\mu}, \boldsymbol{t})$ . The auxiliary umbra  $\alpha \boldsymbol{.} \beta \boldsymbol{.} \boldsymbol{\mu}$  has generating function  $f(\alpha \boldsymbol{.} \beta \boldsymbol{.} \boldsymbol{\mu}, \boldsymbol{t}) = f[\alpha, f(\boldsymbol{\mu}, \boldsymbol{t}) - 1].$ 

*Proof.* The proof follows the same path outlined in the proof of Proposition 2.2, by taking backward. Indeed if we set  $E[\alpha^{l(\lambda)}] = a_{l(\lambda)}$  and  $E[\mu_{\lambda}] = g_{\lambda}$ , from (12) and equivalence (13), the result follows taking into account (10) and (11) and also by observing that

$$\begin{aligned} f(\alpha,\beta,\boldsymbol{\mu},\boldsymbol{t}) &= 1 + \sum_{i>0} \left[ \sum_{\boldsymbol{\lambda}\vdash i} \frac{a_{l(\boldsymbol{\lambda})}}{\boldsymbol{\lambda}!\mathfrak{m}(\boldsymbol{\lambda})!} g_{\boldsymbol{\lambda}} \right] \frac{\boldsymbol{t}^{i}}{\boldsymbol{i}!} = 1 + \sum_{k\geq 1} \frac{a_{k}}{k!} \sum_{i>0} \left[ \sum_{\substack{\boldsymbol{\pi}\vdash i\\l(\boldsymbol{\pi})=k}} \binom{i}{\boldsymbol{\pi}} g_{\boldsymbol{\pi}} \right] \frac{\boldsymbol{t}^{i}}{\boldsymbol{i}!} \\ &= 1 + \sum_{k\geq 1} \frac{a_{k}}{k!} [f(\boldsymbol{\mu},\boldsymbol{t}) - 1]^{k} = f[\alpha,f(\boldsymbol{\mu},\boldsymbol{t}) - 1]. \end{aligned}$$

Theorem 3.1 and equivalence (13) generalize equation (7) and equivalence (6) respectively. Indeed the generating function  $f(\alpha \cdot \beta \cdot \mu, t)$  is the composition of a univariate formal power series with a multivariate formal power series and equivalence (13) gives its *i*-th coefficient.

The following theorem characterizes the auxiliary umbra, whose generating function is the composition of a multivariate formal power series and a univariate formal power series.

**Theorem 3.2** (Multivariate composite Univariate). Let  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)$  be a n-tuple of umbral monomials with generating function  $f(\boldsymbol{\mu}, \boldsymbol{t})$ . The auxiliary umbra  $(\mu_1 + \dots + \mu_n) \cdot \beta \cdot \gamma$  has generating function

$$f[(\mu_1 + \dots + \mu_n) \cdot \beta \cdot \gamma, t] = f[\boldsymbol{\mu}, (f(\gamma, t) - 1, \dots, f(\gamma, t) - 1)].$$

$$(14)$$

Proof. From Remark 2.1, we have  $f[(\mu_1 + \dots + \mu_n) \cdot \beta \cdot \gamma, t] = E\{\exp[(\mu_1 + \dots + \mu_n)(f(\gamma, t) - 1)]\} = E\{\exp(\mu_1[f(\gamma, t) - 1] + \dots + \mu_n[f(\gamma, t) - 1])\}$ . Hence, the result follows from (8).  $\Box$ 

The *i*-th coefficient of  $f[(\mu_1 + \dots + \mu_n) \cdot \beta \cdot \gamma, t]$  can be computed by evaluating equivalence (6) after having replaced  $\alpha$  with  $(\mu_1 + \dots + \mu_n)$ .

In (14), if we replace the umbra  $\gamma$  with the *n*-tuple  $\boldsymbol{\nu} = (\nu_1, \dots, \nu_n)$ , we obtain a characterization of an auxiliary umbra whose generating function is the composition of a multivariate formal power series and a different multivariate formal power series. This characterization is given in the following theorem, where the first multivariate formal power series is umbrally represented by the *n*-tuple  $\boldsymbol{\mu}$  and the second multivariate formal power series is umbrally represented by the *n*-tuple  $\boldsymbol{\nu}$ .

**Theorem 3.3** (Multivariate composite Multivariate). Let  $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$  be a n-tuple of umbral monomials with generating function  $f(\boldsymbol{\mu}, \boldsymbol{t})$  and  $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_n)$  be a n-tuple of umbral monomials with generating function  $f(\boldsymbol{\nu}, \boldsymbol{t})$ . The auxiliary umbra  $(\mu_1 + \cdots + \mu_n) \cdot \beta \cdot \boldsymbol{\nu}$  has generating function

$$f[(\boldsymbol{\mu}_1 + \cdots + \boldsymbol{\mu}_n) \boldsymbol{\cdot} \boldsymbol{\beta} \boldsymbol{\cdot} \boldsymbol{\nu}, \boldsymbol{t}] = f[\boldsymbol{\mu}, (f(\boldsymbol{\nu}, \boldsymbol{t}) - 1, \dots, f(\boldsymbol{\nu}, \boldsymbol{t}) - 1)].$$

The *i*-th coefficient of  $f[(\mu_1 + \cdots + \mu_n) \cdot \beta \cdot \nu, t]$  can be computed by evaluating equivalence (13) after having replaced  $\mu$  with  $\nu$  and the umbra  $\alpha$  with  $(\mu_1 + \cdots + \mu_n)$ .

In Theorem 3.3, we can also choose a *m*-tuple  $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_m)$ , with  $m \neq n$ . To this aim, from now on we denote by  $\boldsymbol{t}_{(n)}$  the vector  $(t_1, t_2, \ldots, t_n)$  of length *n*.

**Theorem 3.4** (Multivariate composite Multivariate). Let  $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$  be a n-tuple of umbral monomials with generating function  $f(\boldsymbol{\mu}, \boldsymbol{t}_{(n)})$  and  $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_m)$  be a m-tuple of umbral monomials with generating function  $f(\boldsymbol{\nu}, \boldsymbol{t}_{(m)})$ . The auxiliary umbra  $(\mu_1 + \cdots + \mu_n) \cdot \beta \cdot \boldsymbol{\nu}$  has generating function

$$f[(\mu_1 + \dots + \mu_n) \cdot \beta \cdot \nu, t_{(m)}] = f[\mu, (f(\nu, t_{(m)}) - 1, \dots, f(\nu, t_{(m)}) - 1)].$$
(15)

The auxiliary umbra  $(\mu_1 + \cdots + \mu_n) \cdot \beta \cdot \nu$  is a first umbral expression of the generalized Bell polynomials, introduced in [1]. A more general expression can be obtained from equation (15), by replacing each occurrence of the umbral monomial  $\nu$  with a *m*-tuple of umbral monomials. In other words, we deal with the composition of a multivariate formal power series in *n* variables and *n* distinct multivariate formal power series in *m* variables.

**Theorem 3.5** (Multivariate composite different multivariates). Let  $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$  be a *n*-tuple of umbral monomials with generating function  $f(\boldsymbol{\mu}, \boldsymbol{t}_{(n)})$  and  $\{\boldsymbol{\nu}_1, \boldsymbol{\nu}_2, \ldots, \boldsymbol{\nu}_n\}$  be a set of *m*-tuples of umbral monomials with generating function  $f(\boldsymbol{\nu}_i, \boldsymbol{t}_{(m)})$ , for  $i = 1, 2, \cdots, n$ . The auxiliary umbra  $\mu_1 \cdot \beta \cdot \boldsymbol{\nu}_1 + \cdots + \mu_n \cdot \beta \cdot \boldsymbol{\nu}_n$  has generating function

$$f[\mu_1 \cdot \beta \cdot \nu_1 + \dots + \mu_n \cdot \beta \cdot \nu_n, t_{(m)}] = f[\mu, (f(\nu_1, t_{(m)}) - 1, \dots, f(\nu_n, t_{(m)}) - 1)].$$

*Proof.* If we replace the real or complex field R with the polynomial ring  $R[x_1, \ldots, x_n]$ , then the uncorrelation property (1) has to be rewritten as [6]

$$E[x_i^k x_j^m \cdots \alpha^s \beta^t \cdots] = x_i^k x_j^m \cdots E[\alpha^s] E[\beta^t] \cdots,$$

for any set of distinct umbrae in A, and for nonnegative integers k, m, s, t. In  $R[x_1, \ldots, x_n][A]$ , the following property holds

$$(x_1 + \dots + x_n) \cdot \beta \cdot \alpha \equiv (x_1 \cdot \beta \cdot \alpha + \dots + x_n \cdot \beta \cdot \alpha).$$

In particular we have

$$f(x_1 \cdot \beta \cdot \nu_1 + \dots + x_n \cdot \beta \cdot \nu_n, t) = \exp\{x_1[f(\nu_1, t) - 1] + \dots + x_n[f(\nu_n, t) - 1]\},\$$

where  $\{\nu_1, \ldots, \nu_n\}$  are umbral monomials with supports not necessarily disjoint. If we replace  $\nu_i$  with the *m*-tuple  $\boldsymbol{\nu}_i$ , then we still have

$$f(x_1 \cdot \beta \cdot \boldsymbol{\nu}_1 + \dots + x_n \cdot \beta \cdot \boldsymbol{\nu}_n, \boldsymbol{t}_{(m)}) = \exp\left\{\sum_{i=1}^n x_i [f(\boldsymbol{\nu}_i, \boldsymbol{t}_{(m)}) - 1]\right\}.$$
 (16)

Equation (16) still holds if we replace the variables  $\{x_1, \ldots, x_n\}$  with the symbols  $\{\mu_1, \ldots, \mu_n\}$ and define the evaluation E on the polynomial ring  $R[\mu_1, \ldots, \mu_n][A]$  taking values in  $R[\mu_1, \ldots, \mu_n]$ , that is

$$f(\mu_1 \cdot \beta \cdot \boldsymbol{\nu}_1 + \dots + \mu_n \cdot \beta \cdot \boldsymbol{\nu}_n, \boldsymbol{t}_{(m)}) = \exp\left\{\sum_{i=1}^n \mu_i [f(\boldsymbol{\nu}_i, \boldsymbol{t}_{(m)}) - 1]\right\}.$$
 (17)

Now, if we apply the linear functional E, defined on the polynomial ring  $R[\mu_1, \ldots, \mu_n]$  and taking values in R, to equation (17) we have

$$E[f(\mu_1 \cdot \beta \cdot \nu_1 + \dots + \mu_n \cdot \beta \cdot \nu_n, t_{(m)})] = f[\mu, (f(\nu_1, t_{(m)}) - 1, \dots, f(\nu_n, t_{(m)}) - 1)]$$

by which the result follows.

In [1], the *i*-th coefficient  $B_i(x_1, \ldots, x_n)$  of exp  $\left\{\sum_{i=1}^n x_i[f(\boldsymbol{\nu}_i, \boldsymbol{t}_{(m)}) - 1]\right\}$  is called *generalized Bell polynomial*. From equation (16), the following corollary is immediately stated.

**Corollary 3.1** (Umbral representation of generalized Bell polynomials). If  $B_i(x_1, \ldots, x_n)$  denotes the generalized Bell polynomial, then we have

$$B_i(x_1,\ldots,x_n) \simeq (x_1 \cdot \beta \cdot \nu_1 + \cdots + x_n \cdot \beta \cdot \nu_n)^i$$

From Theorem 3.5, the general expression of the multivariate Faà di Bruno's formula can be computed by evaluating the generalized Bell polynomial  $B_i(\mu_1, \ldots, \mu_n)$ , as the following corollary states.

**Corollary 3.2** (Multivariate Faà di Bruno's formula). If  $B_i(x_1, \ldots, x_n)$  denotes the generalized Bell polynomial, then we have

$$B_{\boldsymbol{i}}(\mu_1,\ldots,\mu_n) \simeq (\mu_1 \boldsymbol{\cdot} \boldsymbol{\beta} \boldsymbol{\cdot} \boldsymbol{\nu}_1 + \cdots + \mu_n \boldsymbol{\cdot} \boldsymbol{\beta} \boldsymbol{\cdot} \boldsymbol{\nu}_n)^{\boldsymbol{i}}.$$
(18)

Note that the umbral polynomial  $B_{i}(\mu_{1}, \ldots, \mu_{n})$  is umbrally equivalent to the *i*-th coefficient of the formal power series exp  $\{\sum_{i=1}^{n} \mu_{i}[f(\boldsymbol{\nu}_{i}, \boldsymbol{t}_{(m)}) - 1]\}$  in (17). How to compute by means of a symbolic software the "compressed" multivariate Faà di Bruno's formula (18) is the object of the last section.

#### 4 Examples and applications.

**Randomized compound Poisson random variable.** As observed in [6], the moments of a randomized Poisson random variable are umbrally represented by the composition umbra  $\alpha \cdot \beta \cdot \gamma$ . A randomized Poisson random variable is a random sum  $S_N = X_1 + \cdots + X_N$ of independent and identical distributed random variables  $\{X_i\}$ , where N is a Poisson random variable with random parameter Y. In  $\alpha \cdot \beta \cdot \gamma$  the moments of Y, if they exist, are umbrally represented by the umbra  $\alpha$  as well as the moments of  $X_i$ , if they exist, are umbrally represented by the umbra  $\gamma$ . Similarly, the umbra  $\alpha \cdot \beta \cdot \mu$  is the umbral counterpart of a multivariate randomized compound Poisson random variable, that is a random sum  $S_N = X_1 + \cdots + X_N$  of independent and identical distributed random vectors  $\{X_i\}$ . The evaluation E, applied to both sides of equivalence (13), gives the moments of a randomized compound Poisson random variable in terms of moments of  $\{X_i\}$  and N. This result is the same stated in Theorem 4.1 of [1], by using a different proof and different methods. Let us underline that all auxiliary umbrae, constructed in the previous section, admit probabilistic counterpart. Multivariate Laplace transform. In multivariate probability theory, the verification of sign alternation in derivatives of Laplace transform of densities is one of the applications for which multivariate Faà di Bruno's formula of all orders is desirable. As it is well-known, the Laplace transform  $L_{\mathbf{X}}(t)$  of multivariate densities is given by its moment generating function, with t replaced by -t, that is  $L_{\mathbf{X}}(t) = f(\mu, -t)$ , if the moments of the random vector  $\mathbf{X}$  are umbrally represented by the *n*-tuple  $\mu$ . Since  $f(\mu, -t) = f(-1.\mu, t) =$  $f(-1.\chi.\beta.\mu, t)$ , equivalence (13) can be again used in order to find the derivatives of Laplace transform, recalling that  $E[(-1.\chi)^n] = (-1)^n n!$ .

Multivariate cumulants. If  $\chi$  denotes the singleton umbra, multivariate moments of  $\chi \cdot \mu$  are the so-called *multivariate cumulants* of  $\mu$ . Indeed from Proposition 3.1 we have  $f(\chi \cdot \mu, t) = 1 + \log[f(\mu, t)]$ , by recalling that  $\chi \cdot \mu \equiv \chi \cdot \chi \cdot \beta \cdot \mu$  and  $f(\chi \cdot \chi, t) = 1 + \log(t + 1)$ . The equations giving multivariate cumulants in terms of multivariate moments and viceversa are considered in [11]. See [2] for a recent symbolic treatment of this topic. Here, we remark that also equivalence (13) allows us to express multivariate cumulants in terms of multivariate moments, and vice-versa. Indeed, since  $\chi \cdot \chi \cdot \beta \cdot \mu \equiv \chi \cdot \mu$ , multivariate cumulants in terms of multivariate moments are obtained by applying the evaluation E to both sides of equivalence (13), where the umbra  $\alpha$  has to be replaced by the umbra  $\chi \cdot \chi$ . Analogously, multivariate moments in terms of multivariate cumulants are obtained by applying the evaluation E to both sides of equivalence (13), where the umbra  $\alpha$  has to be replaced by the umbra u and the *n*-tuple  $\mu$  has to be replaced by  $\chi \cdot \mu$ , taking into account that  $u \cdot \beta \cdot (\chi \cdot \mu) \equiv \mu$ .

The multivariate analogous of the well-known semi-invariance property of cumulants is stated in Proposition 4.1. First we have to define the *disjoint sum*  $\mu + \nu$  of two *n*-tuples  $\mu$ and  $\nu$ . As in the univariate case, the auxiliary umbra  $\mu + \nu$  is such that  $(\mu + \nu)^i \simeq \mu^i + \nu^i$ . Note that the contribution of mixed products in the disjoint sum is zero.

**Proposition 4.1.** If  $\mu$  and  $\nu$  are uncorrelated n-tuples of umbral monomials, then  $\chi_{\cdot}(\mu + \nu) \equiv \chi_{\cdot}\mu + \chi_{\cdot}\nu$ .

*Proof.* The result follows by observing that  $f(\mu + \nu, t) = f(\mu, t) + f(\nu, t) - 1$ .

Thus multivariate cumulants linearize convolutions of uncorrelated n-tuples of umbral monomials. By using Propositions 2.1 and 4.1, we are able to state that mixed cumulants are zero in the case of uncorrelated components.

**Corollary 4.1.** If  $\{\mu_i\}_{i=1}^n$  are uncorrelated umbral monomials, then  $\chi \cdot \boldsymbol{\mu} \equiv \chi \cdot \tilde{\boldsymbol{\mu}}_1 + \cdots + \chi \cdot \tilde{\boldsymbol{\mu}}_n$ , where  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)$  and the uncorrelated vectors  $\{\tilde{\boldsymbol{\mu}}_i\}_{i=1}^n$  are obtained from  $\boldsymbol{\mu}$  by replacing each component with  $\varepsilon$ , except the *i*-th one, that is  $\tilde{\boldsymbol{\mu}}_i = (\varepsilon, \dots, \mu_i, \dots, \varepsilon)$ .

Multivariate Hermite polynomials. The *i*-th Hermite polynomial  $H_i(\boldsymbol{x}, \Sigma)$  is defined as  $H_i(\boldsymbol{x}, \Sigma) = (-1)^{|\boldsymbol{i}|} D_{\boldsymbol{x}}^{(\boldsymbol{i})} \phi(\boldsymbol{x}; \boldsymbol{0}, \Sigma) / \phi(\boldsymbol{x}; \boldsymbol{0}, \Sigma)$ , where  $\phi(\boldsymbol{x}; \boldsymbol{0}, \Sigma)$  denotes the multivariate gaussian density with **0** mean and covariance matrix  $\Sigma$  of full rank *n*. These polynomials are orthogonal with respect to  $\phi(\boldsymbol{x}; \boldsymbol{0}, \Sigma)$  if we consider the polynomials  $\tilde{H}_i(\boldsymbol{x}, \Sigma) = H_i(\boldsymbol{x}\Sigma^{-1}, \Sigma^{-1})$ , where  $\Sigma^{-1}$  denotes the inverse matrix of  $\Sigma$ . The following result is proved in [15]

$$H_{\boldsymbol{i}}(\boldsymbol{x},\boldsymbol{\Sigma}) = E[(\boldsymbol{x}\boldsymbol{\Sigma}^{-1} + i\boldsymbol{Y})^{\boldsymbol{i}}] \qquad \tilde{H}_{\boldsymbol{i}}(\boldsymbol{x},\boldsymbol{\Sigma}) = E[(\boldsymbol{x} + i\boldsymbol{Z})^{\boldsymbol{i}}]$$
(19)

where *i* is the imaginary unit and  $\mathbf{Z} \sim N(\mathbf{0}, \Sigma)^2$  and  $\mathbf{Y} \sim N(\mathbf{0}, \Sigma^{-1})$ . By keeping the length of the present paper within bounds, we use (19) in order to get the umbral expression of multivariate Hermite polynomials.

**Proposition 4.2.** If  $\boldsymbol{\nu}$  is a n-tuple of umbral monomials such that  $f(\boldsymbol{\nu}, t) = 1 + \frac{1}{2}t\Sigma^{-1}t^T$ and  $\boldsymbol{\mu}$  is a n-tuple of umbral monomials such that  $f(\boldsymbol{\mu}, t) = 1 + \frac{1}{2}t\Sigma t^T$ , then we have

$$H_{i}(\boldsymbol{x},\boldsymbol{\Sigma}) \simeq (-1.\beta.\boldsymbol{\nu} + \boldsymbol{x}\boldsymbol{\Sigma}^{-1})^{i} \qquad \tilde{H}_{i}(\boldsymbol{x},\boldsymbol{\Sigma}) \simeq (-1.\beta.\boldsymbol{\mu} + \boldsymbol{x})^{i}.$$
(20)

*Proof.* Equivalences (20) follows by observing that from (19) we have

$$1 + \sum_{k=1}^{\infty} \sum_{\substack{i \in \mathbb{N}_{0}^{n} \\ |i| = k}} H_{i}(\boldsymbol{x}, \Sigma) \frac{\boldsymbol{t}^{i}}{\boldsymbol{i}!} = \exp\left(\boldsymbol{x}\Sigma^{-1}\boldsymbol{t}^{T} - \frac{1}{2}\boldsymbol{t}\Sigma^{-1}\boldsymbol{t}^{T}\right), \qquad (21)$$
$$1 + \sum_{k=1}^{\infty} \sum_{\substack{i \in \mathbb{N}_{0}^{n} \\ |i| = k}} \tilde{H}_{i}(\boldsymbol{x}, \Sigma) \frac{\boldsymbol{t}^{i}}{\boldsymbol{i}!} = \exp\left(\boldsymbol{x}\boldsymbol{t}^{T} - \frac{1}{2}\boldsymbol{t}\Sigma\boldsymbol{t}^{T}\right).$$

In [4], it is proved that Appell polynomials are umbrally represented by the polynomial umbra  $x + \alpha$ . It is well-known that univariate Hermite polynomials are Appell polynomials. Then equivalences (20) show that also multivariate Hermite polynomials are of Appell type. Let us underline that the umbra  $-1.\beta$  allows us a simple expression of multivariate Hermite polynomials, without the employment of the imaginary unit of equations (19). Moreover, since the moments of  $\mathbf{Z} \sim N(\mathbf{0}, \Sigma)$  are umbrally represented by the umbra  $\beta.\mu$ , then the *n*-th tuple  $\boldsymbol{\mu} \equiv \chi_{\bullet}(\beta.\boldsymbol{\mu})$  umbrally represents the multivariate cumulants of  $\mathbf{Z}$ .

The following proposition states that the multivariate Hermite polynomials are special generalized Bell polynomials.

**Proposition 4.3.** If  $\boldsymbol{\mu}$  is a n-tuple of umbral polynomials such that  $f(\boldsymbol{\mu}, \boldsymbol{t}) = 1 + \frac{1}{2} \boldsymbol{t} \Sigma^{-1} \boldsymbol{t}$ and  $\boldsymbol{\mu}_{\boldsymbol{x}}$  is a n-tuple of umbral polynomials such that  $f(\boldsymbol{\mu}_{\boldsymbol{x}}, \boldsymbol{t}) = 1 + f(\boldsymbol{\mu}, \boldsymbol{t} + \boldsymbol{x}) - f(\boldsymbol{\mu}, \boldsymbol{t})$ , then  $H_{\boldsymbol{i}}(\boldsymbol{x}, \Sigma) \simeq (-1)^{|\boldsymbol{i}|} (-1.\beta \cdot \boldsymbol{\mu}_{\boldsymbol{x}})^{\boldsymbol{i}}$ .

*Proof.* We have

$$1 + \sum_{k \ge 1} \sum_{i:|i|=k} (-1)^{|i|} (-1.\beta \cdot \mu_x)^i \frac{t^i}{i!} = 1 + \sum_{k \ge 1} \sum_{i:|i|=k} (-1.\beta \cdot \mu_x)^i \frac{-t^i}{i!}$$

where  $-t = (-t_1, -t_2, \dots, -t_n)$ . The result follows from (21) since we have

$$1 + \sum_{k \ge 1} \sum_{i:|i|=k} E[(-1.\beta \cdot \mu_x)^i] \frac{-t^i}{i!} = f(-1.\beta \cdot \mu_x, -t) = \exp\left(x\Sigma^{-1}t^T - \frac{1}{2}t\Sigma^{-1}t^T\right).$$

Finally we remark that computing efficiently the multivariate Hermite polynomials via equivalences (20) or Proposition 4.3 helps in constructing multivariate Edgeworth approximation of multivariate density functions, see [9].

<sup>&</sup>lt;sup>2</sup> Here  $\boldsymbol{Z} \sim N(\boldsymbol{0}, \Sigma)$  denotes a multivariate gaussian vector  $\boldsymbol{Z}$  with  $\boldsymbol{0}$  mean and covariance matrix  $\Sigma$ .

#### 5 The UMFB algorithm.

In this last section, we present a MAPLE algorithm for the computation of the multivariate Faà di Bruno's formula by using the umbral equivalence (18). The main steps can be summarized as followed:

i) to the right-hand-side of equivalence (18), we apply the multivariate version of the well-known multinomial theorem:

$$(\mu_{1}\boldsymbol{\cdot}\boldsymbol{\beta}\boldsymbol{\cdot}\boldsymbol{\nu}_{1}+\cdots+\mu_{n}\boldsymbol{\cdot}\boldsymbol{\beta}\boldsymbol{\cdot}\boldsymbol{\nu}_{n})^{i} = \sum_{(\boldsymbol{k}_{1},\ldots,\boldsymbol{k}_{n}):\sum_{i=1}^{n}\boldsymbol{k}_{i}=i} \binom{i}{\boldsymbol{k}_{1},\ldots,\boldsymbol{k}_{n}} (\mu_{1}\boldsymbol{\cdot}\boldsymbol{\beta}\boldsymbol{\cdot}\boldsymbol{\nu}_{1})^{\boldsymbol{k}_{1}}\cdots(\mu_{n}\boldsymbol{\cdot}\boldsymbol{\beta}\boldsymbol{\cdot}\boldsymbol{\nu}_{n})^{\boldsymbol{k}_{n}}.$$
 (22)

The procedure mkT finds all the vectors  $(k_1, \ldots, k_n)$  such that  $\sum_{i=1}^n k_i = i$ .

*ii)* Then, it is necessary to expand powers like  $(\mu_j \cdot \beta \cdot \nu_j)^{k_j}$ . The procedure MFB realizes this computation by using equivalence (13), with  $\alpha$  replaced by  $\mu_j$ . This procedure makes use of the procedure makeTab, available online at

```
http://www.maplesoft.com/applications/view.aspx?SID=33039
```

We will add more details on the output of procedure makeTab later on.

- *iii)* The procedure joint provides a way to multiply the factors  $(\mu_1 \cdot \beta \cdot \nu_1)^{k_1} \cdots (\mu_n \cdot \beta \cdot \nu_n)^{k_n}$  in (22), previously expanded in *ii*).
- *iv)* Finally, occurrences of products like  $\mu_1^{j_1}\mu_2^{j_2}\cdots\mu_n^{j_n}$  are replaced by  $g_{j_1,j_2,\ldots,j_n}$  while occurrences of products like  $(\boldsymbol{\nu}_i)_{\boldsymbol{\lambda}}$ , where  $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_1^{r_1}, \boldsymbol{\lambda}_2^{r_2}, \ldots)$ , are replaced by  $(h_{\boldsymbol{\lambda}_1}^{(i)})^{r_1} (h_{\boldsymbol{\lambda}_2}^{(i)})^{r_2} \cdots$ , where  $h_{\boldsymbol{i}}^{(i)}$  denotes the  $\boldsymbol{j}$ -th coefficient of  $f(\boldsymbol{\nu}_i, \boldsymbol{t}_{(m)})$ .

All these steps are combined in the procedure UMFB. Some computational results are given in Table 1. All tasks have been performed on a PC Pentium(R)4 Intel(R), CPU 2.3 Ghz, 2.0 GB Ram with MAPLE version 12.0. The procedure diff of Table 1 is a MAPLE routine by which the multivariate Faà di Bruno's formula is computable making use of the chain rule.

Now let us give more details on the quoted procedure makeTab. This procedure gives multiset subdivisions. A multiset M is a pair  $(\overline{M}, f)$ , where  $\overline{M}$  is a set, called *support* of the multiset, and f is a function  $f : \overline{M} \to \mathbb{N}_0$ . For each  $\mu \in \overline{M}$ , the integer  $f(\mu)$  is called the *multiplicity* of  $\mu$ . The notion of multiset subdivision is quite natural and it is equivalent to split the multiset into disjoint blocks (submultisets) whose union gives the whole multiset. For a formal definition, the reader is referred to [2]. As example, for the multiset  $M = \{\mu_1, \mu_1, \mu_2\}$ , the subdivisions are

$$\{\{\mu_1, \mu_1, \mu_2\}\}; \{\{\mu_1, \mu_1\}, \{\mu_2\}\}; \{\{\mu_1, \mu_2, \}\{\mu_1\}\}; \{\{\mu_1\}, \{\mu_1\}, \{\mu_2\}\}.$$
(23)

If the input parameter is the vector i, the output of the procedure makeTab gives all the subdivisions of a multiset having the vector i as vector of multiplicities, that is  $f(\mu_j) = i_j$  for

i	m	# terms in output	Time (UMFB)	Time (diff)
(6,5)	2	14089	0.7	1.6
(7, 6)	2	60190	3.2	29.8
(7, 7)	2	123134	8.1	75.4
(5, 4)	3	20208	0.7	2.3
(6,5)	3	122034	6.3	62.5
(5, 4)	4	86768	4.5	26.9
(5, 4)	5	288370	25.9	130.9
(4, 4, 3)	2	95138	6.3	12.3
(4, 4, 4)	2	257854	22.8	41.1
(4, 3, 3)	3	313866	22.5	54.5
(4, 2, 2)	4	106912	6.5	17.3

Table 1:	Comparison	of com	putational	$\operatorname{times}$	in seconds.
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j = 1, 2, ..., n. At a first glance, a multiset subdivision does not seem to have any relation with multi-index partitions. But any subdivision of a multiset M, having i as vector of multiplicities, corresponds to a suitable partition of the multi-index i. As example, the multiset  $M = \{\mu_1, \mu_1, \mu_2\}$  corresponds to the multi-index (2, 1), and the subdivisions in (23) correspond to the multi-index partitions

$$\binom{2}{1}, \binom{2,0}{0,1}, \binom{1,1}{1,0}, \binom{1,1,0}{0,0,1}.$$

Therefore the procedure makeTab allows us to compute all the partitions of a multi-index *i*. On the other hand, the connection between the combinatorics of multisets and the Faà di Bruno's formula was already remarked in [8].

## 6 Appendix 1.

The UMFB algorithm.

```
joint := proc()
local p1,p2,M,V;
V := 'if'(nargs=1, [[args]], [args]);
p1 := mul(add(y,y=x)!, x=ListTools[Transpose](V));
p2 := mul(x!, x=ListTools['Flatten'](V));
M := max(seq( add(y,y=x), x=V ));
expand(p1/p2*mul( eval(MFB(op(V[i])) ,[g=g||i,
    seq(f[j]=f||i^j,j=1..M)]), i=1..nargs ));
end:
>
mkT := proc(V,n)
local vE,L,nV;
nV:=nops(V);
vE:=[seq(alpha[i],i=1..nV)];
L:=seq( 'if'(nops(x[1])<=n,x[1],NULL), x=makeTab( op(V) ));</pre>
L:=seq([seq([seq(degree(y,z),z=vE)],y=x),[0$nV]$(n-nops(x))],x=[L]);
L:=seq( op(combinat[permute](x)),x=[L]);
end:
>
UMFB := proc(V, n)
  local S,vE;
  if n=1 then
     return(expand(eval(MFB(op(V)),[g=g1]))); fi;
  vE:=[seq(f||i=1,i=1..n)];
  S:=add(joint( op(x) ), x=[mkT(V,n)]);
  add( f[ seq(degree(x,f||i),i=1..n) ]*
          eval(x,vE), x=S );
```

end:

# 7 Appendix 2.

The output of the routine diff of MAPLE, for  $\frac{\partial^2}{\partial x_1 \partial x_2} f(g_1(x_1, x_2), g_2(x_1, x_2))$  is

$$\begin{array}{l} \left(\frac{\partial}{\partial x_{1}}g1\left(x1,x2\right)\right)\left(D_{1,1}\right)\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial}{\partial x^{2}}g1\left(x1,x2\right) \\ + & \left(\frac{\partial}{\partial x_{1}}g1\left(x1,x2\right)\right)\left(D_{1,2}\right)\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial}{\partial x^{2}}g2\left(x1,x2\right) \\ + & D_{1}\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial^{2}}{\partial x1\partial x^{2}}g1\left(x1,x2\right) \\ + & \left(\frac{\partial}{\partial x1}g2\left(x1,x2\right)\right)\left(D_{1,2}\right)\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial}{\partial x^{2}}g1\left(x1,x2\right) \\ + & \left(\frac{\partial}{\partial x1}g2\left(x1,x2\right)\right)\left(D_{2,2}\right)\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial}{\partial x^{2}}g2\left(x1,x2\right) \\ + & D_{2}\left(f\right)\left(g1\left(x1,x2\right),g2\left(x1,x2\right)\right)\frac{\partial^{2}}{\partial x1\partial x^{2}}g2\left(x1,x2\right). \end{array}$$

The output of the routine UMFB for  $\frac{\partial^2}{\partial x 1 \partial x 2} f(g1(x1,x2),g2(x1,x2))$  is:

$$f_{1,0}g1_{1,1} + f_{2,0}g1_{1,0}g1_{0,1} + f_{0,1}g2_{1,1} + f_{0,2}g2_{1,0}g2_{0,1} + f_{1,1}g1_{1,0}g2_{0,1} + f_{1,1}g1_{0,1}g2_{1,0}g2_$$

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