A generalization of the Leibniz rule for derivatives

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"I will shamelessly tell you what my bottom line is. It is placing balls into boxes . . . ." Gian-Carlo Rota (*Indiscrete Thoughts*)

1 Introduction

It is common knowledge that the first derivative of the product $f(x)g(x)$ is given by $f'(x)g(x) + f(x)g'(x)$, and that the second derivative is $f''(x)g(x) + 2f'(x)g'(x) + f(x)g''(x)$. We look at the more general case; namely, the n-th derivative of a product of m functions $f_1(x) \cdots f_m(x)$.

According to the Leibniz rule [e.g., 1, p. 534], the n-th derivative of a product of two functions is given by

$$\frac{d^n}{dx} f(x)g(x) = \sum_{r=0}^{n} \binom{n}{r} f^{(r)}(x) g^{(n-r)}(x) \ , \tag{1}$$

where $f^{(n)}(x)$ denotes the n-th derivative of function $f(x)$, with $f^{(0)}(x) = f(x)$, but what is the general form when we have m functions:

$$\frac{d^n}{dx} f_1(x) \cdots f_m(x) \ \ ?$$

We will answer this question by using the combinatorial tool of balls in boxes.

2 Balls and boxes

There are m^n ways of allocating n labeled balls to m empty boxes. Each possibility will be referred to as an *allocation*. The *occupancy vector* $(\alpha_1, \ldots, \alpha_m)$ denotes an allocation having α_i balls ($\alpha_i \geq 0$) in the i-th box. The number of ways of allocating α_1 labeled balls in the 1st box, α_2 labeled balls in the 2nd box, . . . , α_m labeled balls in the m-th box is given by the multinomial coefficient

$$\binom{n}{\alpha_1, \ldots, \alpha_m} = \frac{n!}{\alpha_1! \cdots \alpha_m!} \ ,$$

where $\alpha_1 + \cdots + \alpha_m = n$; thus, $\binom{n}{\alpha_1,\ldots,\alpha_m}$ of the m^n possible allocations have the occupancy vector $(\alpha_1, \ldots, \alpha_m)$.

Let $[\![\boldsymbol{b}_1|\boldsymbol{b}_2|\cdots|\boldsymbol{b}_m]\!]$ represent an allocation of $|\boldsymbol{b}_1|+|\boldsymbol{b}_2|+\cdots+|\boldsymbol{b}_m|\le n$ labeled balls in m boxes, where $\boldsymbol{b}_i$ is the set of labeled balls in the i-th box. The occupation vector corresponding to this allocation is $(|\boldsymbol{b}_1|,|\boldsymbol{b}_2|,\ldots,|\boldsymbol{b}_m|)$. For example, $[\![\{a,b\}|\varnothing|\{c\}]\!]$ is an allocation based on three boxes (the second box being empty), and its corresponding occupancy vector is $(2,0,1)$.

Let $\mathcal{L}_1^*[\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m]\!]$ represent the set of allocations resulting from the m possible ways of allocating one labeled ball, say x, to the boxes of $[\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m]\!]$:

$$\mathcal{L}_1^*[\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m]\!] = [\![\boldsymbol{b}_1\cup\{x\}|\cdots|\boldsymbol{b}_m]\!],\ldots,[\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m\cup\{x\}]\!] \quad . \tag{2}$$

For example,

$$\mathcal{L}_1^*[\![\{a,b\}|\varnothing|\{c\}]\!] = \{[\![\{a,b,x\}|\varnothing|\{c\}]\!],[\![\{a,b\}|\{x\}|\{c\}]\!],[\![\{a,b\}|\varnothing|\{c,x\}]\!]\}\,.$$

We will extend the application of $\mathcal{L}_1^*$ to a set of γ allocations $\{\boldsymbol{u}_1,\ldots,\boldsymbol{u}_\gamma\}$:

$$\mathcal{L}_1^*\{\boldsymbol{u}_1,\ldots,\boldsymbol{v}_\gamma\} = \mathcal{L}_1^*\boldsymbol{u}_1\cup\cdots\cup\mathcal{L}_1^*\boldsymbol{u}_\gamma\,.$$

For example,

$$\begin{aligned}\mathcal{L}_1^*\{[\![\{a\}|\varnothing]\!],[\![\varnothing|\{a\}]\!]\} &= \mathcal{L}_1^*[\![\{a\}|\varnothing]\!]\cup\mathcal{L}_1^*[\![\varnothing|\{a\}]\!]\\ &= \{[\![\{a,b\}|\varnothing]\!],[\![\{a\}|\{b\}]\!]\}\cup\{[\![\{b\}|\{a\}]\!],[\![\varnothing|\{a,b\}]\!]\}\,.\end{aligned}$$

We can use the $\mathcal{L}_1^*$ operator to create the the set of all possible allocations of n labeled balls in m boxes in a systematic, step-wise manner. Initially, the m boxes are empty: $[\![\varnothing|\cdots|\varnothing]\!]_m$. The m possible ways of allocating a labeled ball to $[\![\varnothing|\cdots|\varnothing]\!]_m$ is the set $\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m$. Adding a second labeled ball to the elements of $\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m$ in every possible way corresponds to $\mathcal{L}_1^*(\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m)$, but this is equal to the set of all possible ways of allocating two labeled balls to $[\![\varnothing|\cdots|\varnothing]\!]_m$ (See Figure 1):

$$\mathcal{L}_2^*[\![\varnothing|\cdots|\varnothing]\!]_m = \mathcal{L}_1^*(\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m)\,.$$

Continuing in this manner, we obtain

$$\mathcal{L}_n^*[\![\varnothing|\cdots|\varnothing]\!]_m = \underbrace{\mathcal{L}_1^*(\mathcal{L}_1^*(\cdots\mathcal{L}_1^*}_{n}[\![\varnothing|\cdots|\varnothing]\!]_m\cdots))\,. \tag{3}$$

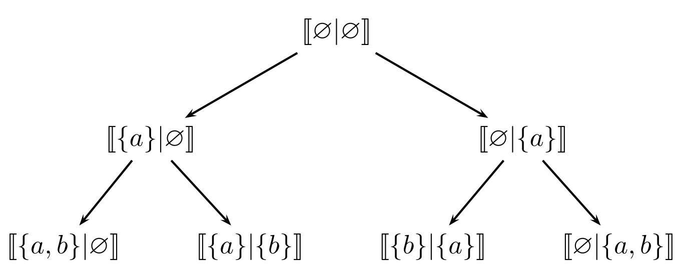

Figure 1: Formation of possible elements of $\mathcal{L}_2^*[\![\varnothing|\varnothing]\!]$ from allocation $[\![\varnothing|\varnothing]\!]$ via possible elements of $\mathcal{L}_1^*[\![\varnothing|\varnothing]\!]$.

2.1 Multisets of occupancy vectors

Let $\mathcal{L}_1(\alpha_1, \ldots, \alpha_m)$ denote the set (possibly multiset) of occupancy vectors resulting from firstly performing $\mathcal{L}_1^*$ on an allocation with occupancy vector $(\alpha_1, \ldots, \alpha_m)$ and then replacing each resulting allocation with its corresponding occupancy vector. Put another way, if a set of labeled balls $\boldsymbol{b}_i$ is such that $|\boldsymbol{b}_i| = \alpha_i$ then

$$\begin{aligned}\mathcal{L}_1(\alpha_1, \ldots, \alpha_m) &= \mathcal{L}_1(|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m|) \\ &= \Gamma(\mathcal{L}_1^* [\![\boldsymbol{b}_1| \cdots |\boldsymbol{b}_m]\!]) \quad .\end{aligned} \tag{4}$$

For example from (2) and (4), we have

$$\mathcal{L}_1(0,0,0,0) = \{(1,0,0,0), (0,1,0,0), (0,0,1,0), (0,0,0,1)\} \,.$$

Analogous to the case with $\mathcal{L}_1^*$, we will extend the application of $\mathcal{L}_1$ to a multiset of γ occupancy vectors $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\gamma\}$:

$$\mathcal{L}_1\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\gamma\} = \mathcal{L}_1 \boldsymbol{v}_1 \uplus \cdots \uplus \mathcal{L}_1 \boldsymbol{v}_\gamma \,.$$

This can be rewritten as

$$\mathcal{L}_1 \biguplus_{i=1}^{\gamma} \{\boldsymbol{v}_i\} = \biguplus_{i=1}^{\gamma} \mathcal{L}_1 \boldsymbol{v}_i \quad , \tag{5}$$

where $\uplus$ denotes the additive union operator of multisets [2].

The operator $\mathcal{L}_1$ can be generalized to $\mathcal{L}_n$; namely, $\mathcal{L}_n(\alpha_1, \ldots, \alpha_m)$ is the multiset of occupancy vectors resulting from performing $\mathcal{L}_n^*$ on an allocation with occupancy vector $(\alpha_1, \ldots, \alpha_m)$ and then replacing each resulting allocation with its corresponding occupancy vector:

$$\begin{aligned}\mathcal{L}_n(\alpha_1, \ldots, \alpha_m) &= \mathcal{L}_n(|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m|) \\ &= \Gamma(\mathcal{L}_n^* [\![\boldsymbol{b}_1| \cdots |\boldsymbol{b}_m]\!]) \quad .\end{aligned} \tag{6}$$

Theorem 1

$$\mathcal{L}_1(\alpha_1, \ldots, \alpha_m) = \biguplus_{j=1}^{m} (\alpha_1 + \delta_{1j}, \ldots, \alpha_m + \delta_{mj}) \,,$$

where δ_{ij} is the Kronecker delta:

$$\delta_{ij} = \begin{cases} 1 & \textit{if } i = j, \\ 0 & \textit{otherwise.} \end{cases}$$

Proof. Let $\boldsymbol{b}_i$ be any set of labeled balls such that $|\boldsymbol{b}_i| = \alpha_i$, then

$$\begin{aligned}\mathcal{L}_1(\alpha_1, \ldots, \alpha_m) &= \Gamma(\mathcal{L}_1^* [\![\boldsymbol{b}_1| \cdots |\boldsymbol{b}_m]\!]) \text{ from (4)} \\ &= \Gamma\{[\![\boldsymbol{b}_1 \cup \{x\}| \cdots |\boldsymbol{b}_m]\!], \ldots, [\![\boldsymbol{b}_1| \cdots |\boldsymbol{b}_m \cup \{x\}]\!]\} \text{ from (2)} \\ &= \{\Gamma[\![\boldsymbol{b}_1 \cup \{x\}| \cdots |\boldsymbol{b}_m]\!], \ldots, \Gamma[\![\boldsymbol{b}_1| \cdots |\boldsymbol{b}_m \cup \{x\}]\!]\} \text{ from (5)} \\ &= \{(|\boldsymbol{b}_1| + 1, \ldots, |\boldsymbol{b}_m|), \ldots, (|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m| + 1)\} \\ &= \{(\alpha_1 + 1, \ldots, \alpha_m), \ldots, (\alpha_1, \ldots, \alpha_m + 1)\} \\ &= \biguplus_{j=1}^{m} (\alpha_1 + \delta_{1j}, \ldots, \alpha_m + \delta_{mj}) \,.\end{aligned}$$

□

An important relationship exists between $\mathcal{L}_1^*$ and $\mathcal{L}_1$, as shown by the following lemma.

LEMMA 1.
If $\boldsymbol{u}$ is an allocation then $\Gamma\mathcal{L}_1^*\boldsymbol{u} = \mathcal{L}_1\Gamma\boldsymbol{u}$.

PROOF. Let $\boldsymbol{u} = [\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m]\!]$ then
$\mathcal{L}_1^*\boldsymbol{u} = \{[\![\boldsymbol{b}_1 \cup \{x\}|\cdots|\boldsymbol{b}_m]\!], \ldots, [\![\boldsymbol{b}_1|\cdots|\boldsymbol{b}_m \cup \{x\}]\!]\}$;
therefore, $\Gamma\mathcal{L}_1^*\boldsymbol{u} = \{(|\boldsymbol{b}_1|+1, \ldots, |\boldsymbol{b}_m|), \ldots, (|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m|+1)\}$.
However, $\Gamma\boldsymbol{u} = (|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m|)$;
therefore, $\mathcal{L}_1\Gamma\boldsymbol{u} = \{(|\boldsymbol{b}_1|+1, \ldots, |\boldsymbol{b}_m|), \ldots, (|\boldsymbol{b}_1|, \ldots, |\boldsymbol{b}_m|+1)\}$. □

The next lemma extends Lemma 1 so that sets of allocations can be included.

LEMMA 2.
If S is a set of allocations then $\Gamma\mathcal{L}_1^*S = \mathcal{L}_1\Gamma S$.

PROOF. Let $S = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_\gamma\}$ then $\mathcal{L}_1^*S = \mathcal{L}_1^*\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_\gamma\} = \biguplus_{i=1}^{\gamma} \mathcal{L}_1^*\boldsymbol{u}_i$ from (5); therefore, $\Gamma\mathcal{L}_1^*S = \Gamma\biguplus_{i=1}^{\gamma} \mathcal{L}_1^*\boldsymbol{u}_i = \biguplus_{i=1}^{\gamma} \Gamma\mathcal{L}_1^*\boldsymbol{u}_i$.
Now, $\Gamma S = \{\Gamma\boldsymbol{u}_1, \ldots, \Gamma\boldsymbol{u}_\gamma\}$; therefore, $\mathcal{L}_1\Gamma S = \mathcal{L}_1\{\Gamma\boldsymbol{u}_1, \ldots, \Gamma\boldsymbol{u}_\gamma\} = \biguplus_{i=1}^{\gamma} \mathcal{L}_1\Gamma\boldsymbol{u}_i = \biguplus_{i=1}^{\gamma} \Gamma\mathcal{L}_1^*\boldsymbol{u}_i$ from Lemma 1. □

Lemma 2 allows a version of (3) for $\mathcal{L}_n$ to be established.

Theorem 2
$\mathcal{L}_n(0, \ldots, 0)_m = \underbrace{\mathcal{L}_1\mathcal{L}_1\cdots\mathcal{L}_1}_{n}(0, \ldots, 0)_m$.

PROOF.

$$\begin{aligned}
\mathcal{L}_n(0, \ldots, 0)_m &= \Gamma\mathcal{L}_n^*[\![\varnothing|\cdots|\varnothing]\!]_m \text{ from (4)} \\
&= \Gamma\mathcal{L}_1^*\cdots\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m \text{ from (3)} \\
&= \mathcal{L}_1\Gamma\mathcal{L}_1^*\cdots\mathcal{L}_1^*[\![\varnothing|\cdots|\varnothing]\!]_m \text{ from Lemma 2} \\
&= \cdots\cdots \\
&= \mathcal{L}_1\cdots\mathcal{L}_1\Gamma[\![\varnothing|\cdots|\varnothing]\!]_m \text{ from Lemma 2} \\
&= \mathcal{L}_1\cdots\mathcal{L}_1(0, \ldots, 0)_m
\end{aligned}$$

□

From Theorem 1, Theorem 2 and (5), we now have the following system (System 1) that generates the elements of the multiset $\mathcal{L}_n(0, \ldots, 0)_m$:

$$\text{System 1} \begin{cases} \mathcal{L}_n(0, \ldots, 0)_m = \underbrace{\mathcal{L}_1\mathcal{L}_1\cdots\mathcal{L}_1}_{n}(0, \ldots, 0)_m \\ \text{where } \mathcal{L}_1(\alpha_1, \ldots, \alpha_m) = \biguplus_{j=1}^{m}(\alpha_1 + \delta_{1j}, \ldots, \alpha_m + \delta_{mj}) \\ \text{and } \mathcal{L}_1 \biguplus_{i=1}^{\gamma}\{\boldsymbol{v}_i\} = \biguplus_{i=1}^{\gamma} \mathcal{L}_1\boldsymbol{v}_i \ , \\ \boldsymbol{v}_i \text{ denoting an occupancy vector.} \end{cases}$$

This generation of elements is illustrated in Figure 2.

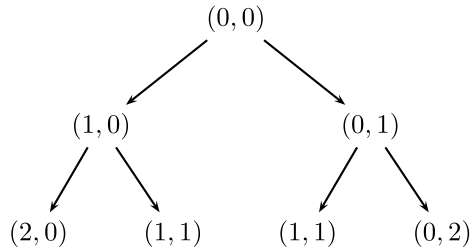

Figure 2: Formation of the elements of multiset $\mathcal{L}_2(0,0)$ from occupancy vector $(0,0)$ via the elements of $\mathcal{L}_1(0,0)$.

3 Beyond the Leibniz rule

In order to see more clearly the link between the n-th derivative of $f_1(x)\cdots f_m(x)$ and $\mathcal{L}_n(0,\ldots,0)_m$, we will use a special notation. The product $f_1^{(\alpha_1)}(x)\cdots f_m^{(\alpha_m)}(x)$ will be written as the *derivative-order tuple* $\langle\alpha_1,\ldots,\alpha_m\rangle$; for example, the derivation

$$\frac{d}{dx}f_1^{(a)}(x)f_2^{(b)}(x) = f_1^{(a+1)}(x)f_2^{(b)}(x) + f_1^{(a)}(x)f_2^{(b+1)}(x)$$

can be written more succinctly as

$$\frac{d}{dx}\langle a,b\rangle = \langle a+1,b\rangle + \langle a,b+1\rangle \ .$$

Furthermore, using this notation, the n-th derivative of $f_1(x)\cdots f_m(x)$ can be redefined as

$$\frac{d^n}{dx^n}\langle 0,\ldots,0\rangle_m = \underbrace{\frac{d}{dx}\frac{d}{dx}\cdots\frac{d}{dx}}_{n}\langle 0,\ldots,0\rangle_m \ . \tag{7}$$

The sum rule of differential calculus can be written as

$$\frac{d}{dx}\sum_{i=1}^{\gamma}\boldsymbol{w}_i = \sum_{i=1}^{\gamma}\frac{d}{dx}\boldsymbol{w}_i \ , \tag{8}$$

where $\boldsymbol{w}_j$ is a derivative-order tuple.

Lemma 3.

$$\frac{d}{dx}\langle\alpha_1,\ldots,\alpha_m\rangle = \sum_{j=1}^{m}\langle\alpha_1+\delta_{1j},\ldots,\alpha_m+\delta_{mj}\rangle \ ,$$

where δ_{ij} is the Kronecker delta.

Proof. $\frac{d}{dx}\langle\alpha_1,\ldots,\alpha_m\rangle = \langle\alpha_1+1,\alpha_2,\ldots,\alpha_m\rangle + \langle\alpha_1,\alpha_2+1,\ldots,\alpha_m\rangle + \cdots + \langle\alpha_1,\alpha_2,\ldots,\alpha_m+1\rangle$. $\square$

Gathering together (7), (8) and Lemma 3, we obtain the following system (System 2) that generates the terms of $\frac{d^n}{dx^n}\langle 0,\ldots,0\rangle_m$ (See Figure 3):

$$\text{System 2}\begin{cases} \frac{d^n}{dx^n}\langle 0,\ldots,0\rangle_m = \underbrace{\frac{d}{dx}\frac{d}{dx}\cdots\frac{d}{dx}}_{n}\langle 0,\ldots,0\rangle_m \\ \text{where } \frac{d}{dx}\langle \alpha_1,\ldots,\alpha_m\rangle = \sum_{j=1}^{m}\langle \alpha_1+\delta_{1j},\ldots,\alpha_m+\delta_{mj}\rangle\ , \\ \text{and } \frac{d}{dx}\sum_{i=1}^{\gamma}\boldsymbol{w}_i = \sum_{i=1}^{\gamma}\frac{d}{dx}\boldsymbol{w}_i\ , \\ \boldsymbol{w}_i \text{ denoting a derivative-order tuple.} \end{cases}$$

Lemma 4.
There are $\binom{n}{\alpha_1,\ldots,\alpha_m}$ allocation vectors in $\mathcal{L}_n(0,\ldots,0)_m$ equal to $(\alpha_1,\ldots,\alpha_m)$.

Proof. $\mathcal{L}_n(0,\ldots,0)_m = \Gamma\mathcal{L}_n^*[\![\varnothing|\cdots|\varnothing]\!]_m$, and, as previously stated early in Section 2, $\binom{n}{\alpha_1,\ldots,\alpha_m}$ of the m^n possible allocations in $\mathcal{L}_n^*[\![\varnothing|\cdots|\varnothing]\!]_m$ have occupancy vector $(\alpha_1,\ldots,\alpha_m)$. □

We now have in place the material required to prove the main goal of this paper; namely, the n-th derivative of $f_1(x)\cdots f_m(x)$.

Theorem 3

$$\frac{d^n}{dx^n}\langle 0,\ldots,0\rangle_m = \sum_{\substack{\alpha_1+\cdots+\alpha_m=n\\ \alpha_i\geq 0}}\binom{n}{\alpha_1,\ldots,\alpha_m}\langle \alpha_1,\ldots,\alpha_m\rangle$$

Proof. By inspection, it is clear that System 1 and System 2 are isomorphous, with $\frac{d^n}{dx^n} \leftrightarrow \mathcal{L}_n$ and $\sum \leftrightarrow \uplus$; therefore, since $\binom{n}{\alpha_1,\ldots,\alpha_m}$ of the elements in multiset $\mathcal{L}_n(0,\ldots,0)_m$ are equal to $(\alpha_1,\ldots,\alpha_m)$ (Lemma 4), it follows that $\binom{n}{\alpha_1,\ldots,\alpha_m}$ of the terms in series $\frac{d^n}{dx^n}\langle 0,\ldots,0\rangle_m$ are equal to $\langle \alpha_1,\ldots,\alpha_m\rangle$. □

Theorem 3 can be rewritten as

$$\frac{d^n}{dx^n}f_1(x)\cdots f_m(x) = \sum_{\substack{\alpha_1+\cdots+\alpha_m=n\\ \alpha_i\geq 0}}\binom{n}{\alpha_1,\ldots,\alpha_m} f_1^{\alpha_1}(x)\cdots f_m^{\alpha_m}(x).$$

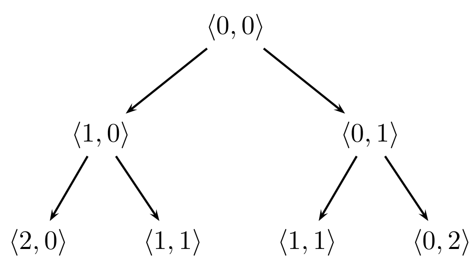

Figure 3: Formation of the terms of $\frac{d^2}{dx^2}\langle 0,0\rangle$ from derivative-order tuple $\langle 0,0\rangle$ via the terms of $\frac{d}{dx}\langle 0,0\rangle$. Compare with Figure 2.

References

[1] W. Kaplan. *Advanced Calculus*. Addison-Wesley, Reading, MA, 4th edition, 1993.

[2] W.D. Blizard. Multiset theory. *Notre Dame Journal of Formal Logic*, 30(1):36–66, 1988.