A generalization of the Leibniz rule for derivatives

R. DYBOWSKI
School of Computing, University of East London,
Docklands Campus, London E16 2RD
e-mail: dybowski@uel.ac.uk

"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

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

(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:

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

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 \( \alpha_i \) balls \( (\alpha_i \geq 0) \) in the \( i \)-th box. The number of ways of allocating \( \alpha_1 \) labeled balls in the 1st box, \( \alpha_2 \) labeled balls in the 2nd box, \ldots, \( \alpha_m \) 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, \( \binom{\alpha_1, \ldots, \alpha_m}{n} \) of the \( m^n \) possible allocations have the occupancy vector \( (\alpha_1, \ldots, \alpha_m) \).
Let \([b_1|b_2| \cdots |b_m]\) represent an allocation of \(|b_1| + |b_2| + \cdots + |b_m| \leq n\) labeled balls in \(m\) boxes, where \(b_i\) is the set of labeled balls in the \(i\)-th box. The occupation vector corresponding to this allocation is \((|b_1|, |b_2|, \ldots, |b_m|)\). For example, \([\emptyset, \emptyset, \{c\}]\) is an allocation based on three boxes (the second box being empty), and its corresponding occupancy vector is \((2, 0, 1)\).

Let \(L_{\gamma}^*[b_1| \cdots |b_m]\) represent the set of allocations resulting from the \(m\) possible ways of allocating one labeled ball, say \(x\), to the boxes of \([b_1| \cdots |b_m]\):

\[
L_{\gamma}^*[b_1| \cdots |b_m] = [b_1 \cup \{x\}| \cdots |b_m], \ldots, [b_1| \cdots |b_m \cup \{x\}].
\]  

(2)

For example,

\[
L_{\gamma}^*[\{a, b\}|\varnothing|\{c\}] = \{[\{a, b, x\}|\varnothing|\{c\}], [\{a, b\}|\{x\}|\{c\}], [\{a, b\}|\varnothing|\{c, x\}\}\).
\]

We will extend the application of \(L_{\gamma}^*[\cdot]\) to a set of \(\gamma\) allocations \(\{u_1, \ldots, u_\gamma\}\):

\[
L_{\gamma}^*[u_1, \ldots, v_\gamma] = L_{\gamma}^*[u_1] \cup \cdots \cup L_{\gamma}^*[u_\gamma].
\]

For example,

\[
L_{\gamma}^*[\{a\}|\varnothing|\{a\}] = L_{\gamma}^*[\{a\}|\varnothing] \cup L_{\gamma}^*[\varnothing|\{a\}]
\]

\[
= \{[\{a, b\}|\varnothing], [\{a\}|\{b\}]\} \cup \{[\{b\}|\{a\}], [\varnothing|\{a, b\}]\}.
\]

We can use the \(L_{\gamma}^*\) operator to create 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 \(L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m\). Adding a second labeled ball to the elements of \(L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m\) in every possible way corresponds to \(L_{\gamma}^*[L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m]\), but this is equal to the set of all possible ways of allocating two labeled balls to \([\varnothing| \cdots |\varnothing]_m\) (See Figure 1):

\[
L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m = L_{\gamma}^*(L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m).
\]

Continuing in this manner, we obtain

\[
L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m = \underbrace{L_{\gamma}^*[L_{\gamma}^*[\cdots L_{\gamma}^*[\varnothing| \cdots |\varnothing]_m \cdots]}}_n.
\]  

(3)

Figure 1: Formation of possible elements of \(L_{\gamma}^*[\varnothing|\varnothing]_m\) from allocation \([\varnothing|\varnothing]_2\) via possible elements of \(L_{\gamma}^*[\varnothing|\varnothing]_m\).
2.1 Multisets of occupancy vectors

Let \( L_1(\alpha_1, \ldots, \alpha_m) \) denote the set (possibly multiset) of occupancy vectors resulting from firstly performing \( L_1^\ast \) 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 \( b_i \) is such that \( |b_i| = \alpha_i \) then

\[
L_1(\alpha_1, \ldots, \alpha_m) = L_1(|b_1|, \ldots, |b_m|) = \Gamma(L_1^\ast[|b_1| \cdots |b_m|]).
\]  \( (4) \)

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

\[
L_1(0, 0, 0, 0) = \{(1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)\}.
\]

Analogous to the case with \( L_1^\ast \), we will extend the application of \( L_1 \) to a multiset of \( \gamma \) occupancy vectors \( \{v_1, \ldots, v_\gamma\} \):

\[
L_1\{v_1, \ldots, v_\gamma\} = \bigcup_{i=1}^{\gamma} L_1 v_i.
\]  \( (5) \)

This can be rewritten as

\[
L_1 \bigcup_{i=1}^{\gamma} v_i = \bigcup_{i=1}^{\gamma} L_1 v_i,
\]

where \( \bigcup \) denotes the additive union operator of multisets [2].

The operator \( L_1 \) can be generalized to \( L_n \): namely, \( L_n(\alpha_1, \ldots, \alpha_m) \) is the multiset of occupancy vectors resulting from performing \( L_n^\ast \) on an allocation with occupancy vector \( (\alpha_1, \ldots, \alpha_m) \) and then replacing each resulting allocation with its corresponding occupancy vector:

\[
L_n(\alpha_1, \ldots, \alpha_m) = L_n(|b_1|, \ldots, |b_m|) = \Gamma(L_n^\ast[|b_1| \cdots |b_m|]).
\]  \( (6) \)

**Theorem 1**

\[
L_1(\alpha_1, \ldots, \alpha_m) = \bigcup_{j=1}^{m} (\alpha_1 + \delta_{ij}, \ldots, \alpha_m + \delta_{mj}),
\]

where \( \delta_{ij} \) is the Kronecker delta:

\[
\delta_{ij} = \begin{cases} 
1 & \text{if } i = j, \\
0 & \text{otherwise.}
\end{cases}
\]

**PROOF.** Let \( b_i \) be any set of labeled balls such that \( |b_i| = \alpha_i \), then

\[
L_1(\alpha_1, \ldots, \alpha_m) = \Gamma(L_n^\ast[|b_1| \cdots |b_m|]) \text{ from (4)}
\]

\[
= \Gamma([b_1 \cup \{x\}] \cdots [b_m], \ldots, [b_1 \cdots b_m \cup \{x\}]) \text{ from (2)}
\]

\[
= \{\Gamma([b_1 \cup \{x\}] \cdots [b_m], \ldots, [b_1 \cdots b_m \cup \{x\}]) \text{ from (5)}
\]

\[
= \{(|b_1| + 1, \ldots, |b_m|), \ldots, (|b_1|, \ldots, |b_m| + 1)\}
\]

\[
= \{(|\alpha_1 + 1, \ldots, |\alpha_m|), \ldots, (|\alpha_1|, \ldots, |\alpha_m| + 1)\}
\]

\[
= \bigcup_{j=1}^{m} (\alpha_1 + \delta_{ij}, \ldots, \alpha_m + \delta_{mj}).
\]
An important relationship exists between $\mathcal{L}_1$ and $\mathcal{L}_1$, as shown by the following lemma.

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

**Proof.** Let $u = [b_1, \ldots, b_m]$ then

$\mathcal{L}_1^* u = \{ [b_1 \cup \{x\}], [b_1] \cdot [b_m] \}$; therefore, $\Gamma \mathcal{L}_1^* u = \{ ([b_1] + 1, \ldots, [b_m]), ([b_1], \ldots, [b_m] + 1) \}$.

However, $\Gamma u = ([b_1], \ldots, [b_m])$; therefore, $\mathcal{L}_1 \Gamma u = \{ ([b_1] + 1, \ldots, [b_m]), ([b_1], \ldots, [b_m] + 1) \}$.

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 $S = \{u_1, \ldots, u_r\}$ then $\mathcal{L}_1^* S = \mathcal{L}_1^* \{u_1, \ldots, u_r\} = \bigcup_{i=1}^r \mathcal{L}_1^* u_i$ from (5); therefore, $\Gamma \mathcal{L}_1^* S = \Gamma \bigcup_{i=1}^r \mathcal{L}_1^* u_i$. Now, $\Gamma S = \{ \Gamma u_1, \ldots, \Gamma u_r \}$; therefore, $\mathcal{L}_1 \Gamma S = \mathcal{L}_1 \{ \Gamma u_1, \ldots, \Gamma u_r \} = \bigcup_{i=1}^r \mathcal{L}_1 \Gamma u_i = \bigcup_{i=1}^r \mathcal{L}_1^* u_i$ from Lemma 1.

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

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

**Proof.**

\[
\mathcal{L}_n(0, \ldots, 0)_m = \Gamma \mathcal{L}_n^* [\emptyset] \cdots [\emptyset]_m \text{ from (4)}
= \Gamma \mathcal{L}_1^* \cdots \mathcal{L}_1^* [\emptyset] \cdots [\emptyset]_m \text{ from (3)}
= \mathcal{L}_1 \Gamma \mathcal{L}_1^* \cdots \mathcal{L}_1^* [\emptyset] \cdots [\emptyset]_m \text{ from Lemma 2}
= \ldots \ldots
= \mathcal{L}_1 \cdots \mathcal{L}_1 \Gamma [\emptyset] \cdots [\emptyset]_m \text{ from Lemma 2}
= \mathcal{L}_1 \cdots \mathcal{L}_1(0, \ldots, 0)_m
\]

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

\[
\mathcal{L}_n(0, \ldots, 0)_m = \mathcal{L}_1 \mathcal{L}_1 \cdots \mathcal{L}_1(0, \ldots, 0)_m
\]

System 1

where $\mathcal{L}_1(\alpha_1, \ldots, \alpha_m) = \bigcup_{j=1}^m (\alpha_1 + \delta_{ij}, \ldots, \alpha_m + \delta_{mj})$
and $\mathcal{L}_1(\mathcal{L}_1(\mathcal{L}_1(\mathcal{L}_1(\cdots \mathcal{L}_1(\mathcal{L}_1(v_1)), \ldots), \ldots), \ldots), v_i$ denoting an occupancy vector.

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

$$\frac{d^n}{dx^n}(0, \ldots, 0)_m = \frac{d}{dx} \frac{d}{dx} \cdots \frac{d}{dx} \langle 0, \ldots, 0 \rangle_m. \tag{7}$$

The sum rule of differential calculus can be written as

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

where $w_j$ 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 $\delta_{ij}$ is the Kronecker delta.

**Proof.**

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

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

\[
\text{System 2} \left\{ \begin{array}{l}
\frac{d^n}{dx^n}(0, \ldots, 0)_m = \frac{d}{dx} \frac{d}{dx} \cdots \frac{d}{dx} (0, \ldots, 0)_m \\
\text{where } \frac{d}{dx} (\alpha_1, \ldots, \alpha_m) = \sum_{j=1}^{m} (\alpha_1 + \delta_{1j}, \ldots, \alpha_m + \delta_{mj}), \\
\text{and } \frac{d}{dx} \sum_{i=1}^{\gamma} w_i = \sum_{i=1}^{\gamma} \frac{d}{dx} w_i,
\end{array} \right.
\]

where \( \{0, \ldots, 0\}_m \) denote a derivative-order tuple.

**Lemma 4.**
There are \( (\alpha_1, \ldots, \alpha_m)^n \) allocation vectors in \( L_n(0, \ldots, 0)_m \) equal to \( (\alpha_1, \ldots, \alpha_m) \).

**Proof.** \( L_n(0, \ldots, 0)_m = \Gamma L^*_n[\varnothing] \cdots [\varnothing]_m \), and, as previously stated early in Section 2, \( (\alpha_1, \ldots, \alpha_m)^n \) of the \( m^n \) possible allocations in \( L^*_n[\varnothing] \cdots [\varnothing]_m \) 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**

\[
\frac{d^n}{dx^n}(0, \ldots, 0)_m = \sum_{\alpha_1 + \cdots + \alpha_m = n, \alpha_i \geq 0} \binom{n}{\alpha_1, \ldots, \alpha_m} (\alpha_1, \ldots, \alpha_m)
\]

**Proof.** By inspection, it is clear that System 1 and System 2 are isomorphic, with \( \frac{d^n}{dx^n} L_n \leftrightarrow \sum \leftrightarrow \emptyset \); therefore, since \( (\alpha_1, \ldots, \alpha_m)^n \) of the elements in multiset \( L_n(0, \ldots, 0)_m \) are equal to \( (\alpha_1, \ldots, \alpha_m) \) (Lemma 4), it follows that \( (\alpha_1, \ldots, \alpha_m)^n \) of the terms in series \( \frac{d^n}{dx^n}(0, \ldots, 0)_m \) are equal to \( (\alpha_1, \ldots, \alpha_m) \). □

Theorem 3 can be rewritten as

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

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