Deriving Faà di Bruno’s formula for the derivative of a composite function via compositions of integers

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Abstract

We give yet another proof for Faà di Bruno’s formula for higher derivatives of composite functions. Our proof technique relies on reinterpreting the composition of two power series as the generating function for weighted integer compositions, for which a Faà di Bruno-like formula is quite naturally established.

1 Introduction

According to Faà di Bruno’s formula, the $n$th derivative of a composite function $G \circ F$ is given by

$$
\frac{d^n}{dx^n} G(F(x)) = \sum \frac{n!}{b_1! \cdots b_n!} G^{(r)}(F(x)) \prod_{i=1}^n \left( \frac{F^{(i)}(x)}{i!} \right)^{b_i},
$$

where the sum ranges over all different solutions in nonnegative integers $b_1, \ldots, b_n$ of $b_1 + 2b_2 + \cdots + nb_n = n$ and where $r$ is defined as $r = b_1 + \cdots + b_n$. For example, for $n = 3$, the three solutions for $(b_1, b_2, b_3)$ are $(0, 0, 1)$, $(1, 1, 0)$ and $(3, 0, 0)$, which correctly yields

$$G'(F(x)) \cdot F'''(x) + 3G''(F(x)) \cdot F'(x)F''(x) + G'''(F(x)) \cdot (F'(x))^3$$

as third derivative of $G \circ F$.

Many proofs of formula (1) have been given, both based on combinatorial arguments — such as via Bell polynomials [3] or set partitions — as well as on analytical; the latter, for example, using Taylor’s theorem [7]. Roman [8] gives a proof based on the umbral calculus. Johnson [7] summarizes the historical discoveries and re-discoveries of the formula as well as a variety of different proof techniques.

Herein, we give (yet) another proof of the formula, one that is based on the combinatorics of integer compositions and a particular interpretation of the composition of power series. The essence of our derivation is as follows: First, we consider the number $C_{f,g}(n)$ of (doubly weighted) integer compositions of the positive integer $n$, for which we derive a closed-form formula; this requires some notation and introduction of terminology, but the derivation and combinatorial interpretation of the formula is quite intuitive. Then, for two arbitrary power series $G(x) = \sum_{n \geq 0} g_n x^n$ and $F(x) = \sum_{n \geq 0} f_n x^n$, we argue that $G \circ F$ has a natural interpretation of denoting the generating function

$$C(x) = \sum_{n \geq 0} C_{f,g}(n) x^n$$

for $C_{f,g}(n)$. Hence, $\frac{d^n}{dx^n} C(0) = C_{f,g}(n)$. This yields formula (1) for $x = 0$, but we argue that it is clear that the formula must indeed hold for any $x$.

Two remarks are in order: first, as indicated, our derivation does not apply to arbitrary functions $F$ and $G$, but only to power series. While this may be considered a restriction, many interesting functions can indeed be represented as power series (those functions even have a name, real analytical functions). We also remark that, throughout, we ignore matters of convergence and treat all series as formal and assume that functions have sufficiently many derivatives. Finally, while we think that many derivations of Faà di Bruno’s
2 Integer compositions and partitions

An integer composition of a positive integer \( n \) is a tuple of positive integers \( (\pi_1, \ldots, \pi_k) \), typically called parts, whose sum is \( n \). For example, the eight integer compositions of \( n = 4 \) are

\[
(4), (1, 3), (3, 1), (2, 2), (1, 1, 2), (1, 2, 1), (2, 1, 1), (1, 1, 1, 1).
\]

An integer partition of \( n \) is a tuple of positive integers \( (\pi_1, \ldots, \pi_k) \) whose sum is \( n \) and such that \( \pi_1 \geq \pi_2 \geq \cdots \geq \pi_k \). For instance, there are (only) five integer partitions of \( n = 4 \), namely

\[
(4), (3, 1), (2, 2), (2, 1, 1), (1, 1, 1, 1).
\]

Both integer compositions and partitions are well-studied objects in combinatorics \([2, 6]\). Instead of considering ordinary partitions and compositions as defined, we may consider weighted compositions \([1, 4]\) and partitions, where each part value \( \pi_i \in \mathbb{N} = \{1, 2, 3, \ldots\} \) may have attributed with it a weight \( f(\pi_i) \in \mathbb{R} \), where \( \mathbb{R} \) denotes the set of real numbers. If weights are nonnegative integers, they may be interpreted as colors. For instance, when \( f(3) = 2 \) and \( f(1) = f(2) = f(4) = f(5) = \cdots = 1 \), then there are ten \( f \)-weighted compositions and six \( f \)-weighted partitions of \( n = 4 \). These are

\[
(4), (1, 3), (1, 3^*), (3, 1), (3^*, 1), (2, 2), (1, 1, 2), (1, 2, 1), (2, 1, 1), (1, 1, 1, 1)
\]

and

\[
(4), (3, 1), (3^*, 1), (2, 2), (2, 1, 1), (1, 1, 1, 1),
\]

respectively, where we use a star \( (\ast) \) to differentiate between the two colors of part value 3. When weights are nonintegral real numbers, they may simply be interpreted as ordinary ‘weights’ — possibly as probabilities if the range of \( f \) is the unit interval \([0, 1]\).

Let us note that integer partitions of an integer \( n \) admit an alternative, equivalent representation. Instead of writing a partition of \( n \) as a tuple \( (\pi_1, \ldots, \pi_k) \) with \( \pi_1 \geq \pi_2 \geq \cdots \geq \pi_k \), we may represent it as a tuple \( (k_1, \ldots, k_n) \), with \( 0 \leq k_i \leq n \), for all \( i = 1, \ldots, n \), whereby \( k_i \) denotes the multiplicity of (type) \( i \in \{1, 2, \ldots, n\} \) in the composition of \( n \). For instance, the above five integer partitions of \( n = 4 \) may be represented as

\[
(0, 0, 0, 1), (1, 0, 1, 0), (0, 2, 0, 0), (2, 1, 0, 0), (4, 0, 0, 0).
\]

Obviously, each such tuple \( (k_1, \ldots, k_n) \) must satisfy \( 1 \cdot k_1 + 2 \cdot k_2 + \cdots + n \cdot k_n = n \). Assuming that the weighting function \( f \) takes on only integral values, for the moment, how many \( f \)-weighted integer partitions of \( n \) are there? Apparently, this number is given by

\[
\sum_{k_1+2k_2+\cdots+nk_n=n} f(1)^{k_1} \cdots f(n)^{k_n}, \tag{2}
\]

since the solutions, in positive numbers, of \( k_1 + 2k_2 + \cdots + nk_n = n \) are precisely the integer partitions of \( n \) and the product \( f(1)^{k_1} \cdots f(n)^{k_n} \) assigns the different colors to a given partition \( (k_1, \ldots, k_n) \). How many \( f \)-weighted integer compositions of \( n \) are there? Note that, in the representation \( (k_1, \ldots, k_n) \) of a partition, \( k_1 \) denotes the number of ‘type’ 1, \( k_2 \) denotes the number of ‘type’ 2, ..., and \( k_n \) denotes the number of

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1Technically, the approach most similar to our own appears to be the one due to Flanders \([3]\), which is, however, conceptually substantially different from our own.
‘type’ $n$ used in the partition of $n$. Since compositions are ordered partitions, for compositions, we need to distribute the $k_1$ types 1, ..., $k_n$ types $n$ in a sequence of length $(k_1 + \cdots + k_n)$. Therefore, the number of $f$-weighted integer compositions is simply:

$$
\sum_{k_1 + 2k_2 + \cdots + nk_n = n} \binom{k_1 + \cdots + k_n}{k_1, \ldots, k_n} f(1)^{k_1} \cdots f(n)^{k_n},
$$

where $\binom{r}{k_1, \ldots, k_n} = \frac{r!}{k_1! \cdots k_n!}$ (for $r = k_1 + \cdots + k_n$) denote the multinomial coefficients.

Finally, let us assume that integer partitions/compositions with a given, fixed number $k$ of parts are (additionally) weighted (e.g., colored) by $g(k)$, for a weighting function $g : \mathbb{N} \to \mathbb{R}$. For instance, we might double count the $f$-weighted partitions/compositions with exactly $k_1 + \cdots + k_n = 4$ parts (or assign them higher/lower probability). Then, the number of $f$-weighted integer compositions of $n$ where parts are $g$-weighted is simply given by

$$
C_{f,g}(n) = \sum_{k_1 + 2k_2 + \cdots + nk_n = n} \binom{k_1 + \cdots + k_n}{k_1, \ldots, k_n} g(k_1 + \cdots + k_n) \prod_{i=1}^{n} f(i)^{k_i}.
$$

If $f$ and/or $g$ take on nonintegral values, 2 and 3 denote the total weight of all $f$-weighted integer partitions/compositions, and 4 denotes the total weight of all $f$-weighted integer compositions of $n$ where parts are $g$-weighted. Henceforth, for brevity, we also call such compositions simply $(f, g)$-weighted.

3 Derivation of Faà di Bruno’s formula

We assume that $F(x)$ and $G(x)$ are the power series

$$
F(x) = f_0 + f_1 x^1 + f_2 x^2 + \cdots = \sum_{n \geq 0} f_n x^n,
$$

$$
G(x) = g_0 + g_1 x^1 + g_2 x^2 + \cdots = \sum_{n \geq 0} g_n x^n,
$$

for some real coefficients $f_0, f_1, f_2, \ldots$ and $g_0, g_1, g_2, \ldots$. In the remainder, for ease of interpretation, we speak of the $f_n$ and $g_n$ values as if they were nonnegative and integral, but keep in mind that they may be arbitrary real numbers.

We interpret $F$ and $G$ as follows. The function $F$ is the generating function for the number of $f$-weighted integer compositions of $n$ with exactly one part, whereby $f(n) = f_n$. In fact, the coefficient $f_n$ of $x^n$ of $F(x)$ gives the number of $f$-weighted integer compositions of $n$ with exactly one part. We assume that $f_0 = 0$ (that is, integer compositions admit only positive integers).

In the context $G \circ F$, we interpret the function $G$ as follows: $G \circ F$ represents, for $G(x) = x^k$, the generating function for the number of $f$-weighted integer compositions with exactly $k$ parts; for $G(x) = a_k x^k$, it represents the generating function for the number of $f$-weighted integer compositions with exactly $k$ parts, where $f$-weighted compositions with $k$ parts are weighted by the factor $a_k$; and, finally, for $G(x) = x^j + x^k$, it represents the generating function for the number of $f$-weighted integer compositions with either $j$ or $k$ parts (union). This interpretation of $G$, in the context $G \circ F$, is a natural interpretation, since, for example, the coefficients of $x^n$ of $(F(x))^2$ have the form $\sum_{i=0}^{n} f_{n-i} f_i$, and all combinations of the number of $f$-weighted compositions of $n - i$ with one part and the number of $f$-weighted compositions of $i$ with one part yield the number of $f$-weighted compositions of $(n - i) + i = n$ with two parts. Then, the interpretation of $(F(x))^k$ follows inductively. Similarly, if $(F(x))^k$ denotes the generating function for the number of $f$-weighted

\[\text{This is in fact a critical point of our proof; if we interpreted } F(x) \text{ as the generating function for other combinatorial objects, such as integer partitions, then } G(x) = x^k, \text{ in the context } G \circ F, \text{ could not have the same interpretation as the one we have outlined.}\]
compositions of \( n \) with exactly \( k \) parts and \((F(x))^j\) denotes the analogous generating function for \( j \) parts, then their sum obviously denotes the generating function for \( k \) or \( j \) parts.

Hence, to summarize, we interpret \( G \circ F \) as the generating function for the number of \( f \)-weighted integer compositions with arbitrary number of parts (recall that the ‘+’ mean union over number of parts) and where compositions with \( k \) parts are weighted by \( g(k) = g_k \). Then, by virtue of the definition of generating functions, we know that \( \frac{1}{n!} \frac{d^n}{dx^n} (G \circ F)(0) \) gives the number of \((f,g)\)-weighted integer compositions of \( n \). This is the number \( C_{f,g}(n) \), whence by formula (4), we know that

\[
\frac{1}{n!} \frac{d^n}{dx^n} (G \circ F)(0) = C_{f,g}(n) = \sum_{k_1 + 2k_2 + \cdots + nk_n = n} \binom{k_1 + \cdots + k_n}{k_1, \ldots, k_n} g(k_1 + \cdots + k_n) \prod_{i=1}^n f(i)^{k_i},
\]

or, equivalently,

\[
\frac{d^n}{dx^n} (G \circ F)(0) = \sum_{k_1 + 2k_2 + \cdots + nk_n = n} \frac{n!}{k_1! \cdots k_n!} r^\prime g(r) \prod_{i=1}^n f(i)^{k_i}, \tag{5}
\]

where we write \( r = k_1 + \cdots + k_n \). We note that

\[
f(i) = \frac{1}{i!} F^{(i)}(0), \quad \forall \, i = 1, \ldots, n,
\]

\[
r^\prime g(r) = G^{(r)}(0) = G^{(r)}(F(0)),
\]

whence we can rewrite (5) as

\[
\frac{d^n}{dx^n} (G \circ F)(0) = \sum_{k_1 + 2k_2 + \cdots + nk_n = n} \frac{n!}{k_1! \cdots k_n!} G^{(r)}(F(0)) \prod_{i=1}^n \left( F^{(i)}(0) \right)^{k_i}, \tag{6}
\]

which is Faà di Bruno’s formula (1) evaluated at \( x = 0 \). Now, from \((G \circ F)'(x) = G'(F(x)) \cdot F'(x)\), and then \((G \circ F)''(x) = G''(F(x)) F'(x) + G'(F(x)) F''(x)\), etc., it is clear that \( \frac{d^n}{dx^n} (G \circ F)(x) \) is a sum of products of factors \( G^{(j)}(F(x)) \) and \( F^{(m)}(x) \). It is also clear that, whatever the precise form of \( \frac{d^n}{dx^n} (G \circ F)(x) \), evaluating it at \( x = 0 \) will simply yield the same sum of products of factors \( G^{(j)}(F(x)) \) and \( F^{(m)}(x) \), evaluated at \( x = 0 \). Hence, (6) must in fact hold for all \( x \), not only for \( x = 0 \).

4 Discussion

We argued that \( G \circ F \) has, for arbitrary power series \( G \) and \( F \) with coefficients \( g_n \) and \( f_n \), respectively, a natural interpretation as denoting the generating function for \((f,g)\)-weighted integer compositions, whereby \( f(n) = f_n \) and \( g(n) = g_n \), for whose coefficients Faà di Bruno-like formulas quite effortlessly arise.

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