Elemente der Mathematik

A new Faà di Bruno type formula

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1 Introduction

Faà di Bruno's formula for the derivatives of composite functions has an interesting history and a rich literature (see, e.g., the survey by Johnson [8], the revealing paper on the predecessors of Faà di Bruno by Craik [4] and the long list of references therein); some recent papers are [13] and [11]. If f and g are functions with a sufficient number of derivatives, then we have, for $n \in \mathbb{N}$,

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \sum_{k=0}^{n} f^{(k)}(g(x)) P_{n,k}(g; x)$$

with

$$P_{n,k}(g; x) = n! \sum \prod_{\nu=1}^{n} \frac{1}{a_\nu!} \left(\frac{g^{(\nu)}(x)}{\nu!}\right)^{a_\nu},$$

Die Formel von Leibniz für die höheren Ableitungen eines Produkts von zwei oder mehr Funktionen ist wohlbekannt und handlich, da nur Binomial- respektive Multinomialkoeffizienten auftreten. Ihr Gegenstück ist die Verallgemeinerung der Kettenregel, nämlich der Formel für die höheren Ableitungen zusammengesetzter Funktionen. Auch diese Formel, die nach Faà di Bruno benannt ist, gehört zum Standardrepertoire der Analysis. Aufgrund ihrer kombinatorischen Komplexität hat sie trotz ihrer langen Geschichte nichts von ihrem Reiz verloren und zieht immer wieder Mathematikerinnen und Mathematiker an. Neben der üblichen expliziten Form gibt es zahlreiche geschlossene Darstellungen, die in speziellen Fällen unterschiedliche Vor- und Nachteile aufweisen. Der nachstehende Aufsatz enthält eine in der bekannten Literatur bisher nicht vertretene Darstellung und illustriert sie durch eine konkrete Anwendung.

where the sum is over all different solutions in non-negative integers $a_1, \ldots, a_n$ of $a_1 + \cdots + a_n = k$ and $a_1 + 2a_2 + \cdots + na_n = n$. A different notation uses the Bell polynomials (see, e.g., [5, p. 137] or [8, Equation (2.2)]). Spindler [13] published a short elementary proof of Faà di Bruno's formula. Mortini [11] found a representation of $P_{n,k}(g; x)$ which uses a simpler summation order so that the cumbersome condition $a_1 + 2a_2 + \cdots + na_n = n$ does not appear.

There are several closed representations of $P_{n,k}$. One of them is Meyer's formula

$$P_{n,k}(g; x) = \frac{1}{k!} \left[\left(\frac{d}{dy} \right)^n (g(y) - g(x))^k \right]_{|y=x} \tag{1}$$

([10]; see also [8, Sect. 3, p. 224]) which is called Schlömilch's formula in Jordan's book [9, pp. 31–32]. It can easily be derived by expansion of f in a power series $f(y) = \sum_{k=0}^{\infty} f_k \cdot (y - g(x))^k$ with $f_k = f^{(k)}(g(x))/k!$ and differentiating n times $F = f \circ g$. The slightly different form

$$P_{n,k}(g; x) = \binom{n}{k} \left[\left(\frac{d}{dy} \right)^{n-k} \left(\frac{g(y) - g(x)}{y - x} \right)^k \right]_{|y=x} \tag{2}$$

of Formula (1) follows by applying the Leibniz rule to

$$\left(\frac{d}{dy} \right)^n \left[(y - x)^k \left(\frac{g(y) - g(x)}{y - x} \right)^k \right]$$

and evaluating at $y = x$. Representation (2) was given as early as 1800 by Arbogast [3, p. 34] when notational changes are taken into account (cf. [4, p. 121]). It was rediscovered by J.F.C. Tiburce Abadie ([1], [2]; see also [8, Sect. 3, p. 223]). Equation (2) can be rewritten in the usual form

$$P_{n,k}(g; x) = \binom{n}{k} \left[\left(\frac{d}{dh} \right)^{n-k} (\Delta_h g(x))^k \right]_{|h=0}, \tag{3}$$

where Δ_h denotes the divided difference $\Delta_h g(x) := (g(x + h) - g(x))/h$ with step size h. An equivalent result, which also predates [1], was given by J. West (see [4, p. 121]).

A further representation

$$P_{n,k}(g; x) = \frac{1}{k!} \sum_{j=0}^{k} \binom{k}{j} (-g(x))^{k-j} \left(\frac{d}{dx} \right)^n (g(x))^j \tag{4}$$

known as Hoppe's formula, is commonly attributed to Hoppe ([7]; see also [8, Sect. 3, p. 224]), but appears already in the work of West [14, vol. 1, Theorem 8, p. 138] (cf. [4, p. 127]).

Its direct consequence,

$$P_{n,k}(g; x) = \frac{1}{k!} \left[\left(\frac{d}{dx} \right)^n (g(x))^k \right]_{|g(x)=0}, \tag{5}$$

a streamlined version of Equation (4), is called Scott's formula ([12]; see also [8, Sect. 3, p. 226]).

2   Main result and proof

The purpose of this short note is the derivation of a rather different closed representation of $P_{n,k}$. The proof uses complex methods. Therefore, the main result is stated for analytic functions defined on subsets of the complex plane.

Theorem 1. *Let x be a complex number. Furthermore, let f and g be analytic functions on (complex) neighborhoods of $g(x)$ and x, respectively, with $g'(x) \neq 0$. Then the composite function $f \circ g$ has the derivatives*

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \sum_{k=0}^{n} f^{(k)}(g(x)) P_{n,k}(g; x),$$

where $P_{n,k}$ possesses the representation

$$P_{n,k}(g; x) = \binom{n}{k}\left(\frac{d}{dy}\right)^{n-k}\left[\left(\frac{y - g(x)}{g^{-1}(y) - x}\right)^{n+1} \left(g^{-1}\right)'(y)\right]_{|y=g(x)}. \tag{6}$$

Remark 2. Note that the representation (6) is valid also for real functions f and g possessing a continuous derivative of order n in a (real) neighborhood of $x \in \mathbb{R}$. This is a consequence of the fact that each function $f \in C^n(I)$, where I is any real interval, can be simultaneously approximated with arbitrary precision by an analytic function $\hat{f}$ on each compact set $K \subset I$, i.e., for each $\varepsilon > 0$, there exists $\hat{f}$ analytic in a region containing K, such that

$$\left|f^{(k)}(x) - \hat{f}^{(k)}(x)\right| < \varepsilon \qquad (x \in K, \; k = 0, \ldots, n)$$

Remark 3. Note that the condition $g'(x) \neq 0$ assures that g is one-to-one on a certain neighborhood of the point x.

Obviously, for fixed x, the function $\tilde{g}_x(y) := (y - g(x))/\left(g^{-1}(y) - x\right)$ is analytic in a deleted neighborhood of $g(x)$. Because of $\left(g^{-1}\right)'(g(x)) = 1/g'(x)$ the isolated singularity at $y = g(x)$ can be removed by defining $\tilde{g}_x(g(x)) := g'(x)$. Setting $G_{n,x}(y) := (\tilde{g}_x(y))^{n+1}\left(g^{-1}\right)'(y)$, Formula (6) can be rewritten in the concise form

$$P_{n,k}(g; x) = \binom{n}{k} G_{n,x}^{(n-k)}(g(x)). \tag{7}$$

Proof of Theorem 1. Let $r > 0$ such that $f \circ g$ is analytic with $g'(z) \neq 0$ in a region containing the closed disk $\bar{D}_r(x) = \{z \in \mathbb{C} \mid |z - x| \leq r\}$. Applying the Cauchy integral formula we obtain

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \frac{n!}{2\pi i}\int_{\partial D_r(x)}\frac{f(g(z))}{(z-x)^{n+1}}dz.$$

Because $g'(z) \neq 0$ on $\partial D_r(x)$ we can change the variable $z = g^{-1}(y)$, and the latter contour integral is equal to

$$\int_W \frac{f(y)}{\left(g^{-1}(y) - x\right)^{n+1}} \left(g^{-1}\right)'(y)\, dy$$

$$= \int_W \frac{f(y)}{(y - g(x))^{n+1}} \left(\frac{y - g(x)}{g^{-1}(y) - x}\right)^{n+1} \left(g^{-1}\right)'(y)\, dy,$$

where $W = g(\partial D_r(x))$ is a closed integration path encircling $g(x)$. As in Remark 3 we note that $y \neq g(x)$, for all $y \in W$. Furthermore, $h(y) := \left(\frac{y - g(x)}{g^{-1}(y) - x}\right)^{n+1}$ is analytic in a region containing $g\left(\bar{D}_r(x)\right) \smallsetminus \{g(x)\}$. The point $y = g(x)$ is a removable singularity. If we define $h(g(x)) = (g(x))^{n+1}$ the function h becomes analytic at $y = g(x)$. Therefore, the Cauchy integral formula implies that

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \left(\frac{d}{dy}\right)^n \left[f(y) \left(\frac{y - g(x)}{g^{-1}(y) - x}\right)^{n+1} \left(g^{-1}\right)'(y) \right]_{|y = g(x)}.$$

An application of the Leibniz rule for differentiation leads to

$$\left(\frac{d}{dx}\right)^n f(g(x))$$

$$= \sum_{k=0}^{n} \binom{n}{k} f^{(k)}(g(x)) \left(\frac{d}{dy}\right)^{n-k} \left[\left(\frac{y - g(x)}{g^{-1}(y) - x}\right)^{n+1} \left(g^{-1}\right)'(y) \right]_{|y = g(x)}$$

which proves Formula (6). $\square$

3 An application

As an example showing the advantage of Formula (6) against other representations we take $g(x) = \sqrt{x}$, for $x > 0$.

In what follows we sometimes use the notation

$$z^{\underline{n}} = z(z-1)\cdots(z-n+1), \quad z^{\overline{n}} = z(z+1)\cdots(z+n-1), \quad n \in \mathbb{N},$$

$$z^{\underline{0}} = z^{\overline{0}} = 1,$$

for the falling and rising factorial, respectively.

The common form of Faà di Bruno's formula yields

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \sum_{k=0}^{n} f^{(k)}(\sqrt{x}) \sum_{a_v} n! \prod (a_v!)^{-1} \left(\binom{1/2}{v} x^{1/2 - v}\right)^{a_v},$$

where the summation runs over all non-negative integers a_v satisfying $\sum a_v = k$ and $\sum v a_v = n$. After a simplification we arrive at

$$P_{n,k}(g; x) = (-1)^{n-k} n! 2^{-2n-k} x^{(k-2n)/2} \sum_{a_v} n! \prod (a_v!)^{-1} \left(\frac{(2v - 2)!}{v!\,(v-1)!}\right)^{a_v},$$

where $\sum a_v = k$ and $\sum v a_v = n$.

Meyer's formula (1) requires nth order derivatives of $\left(\sqrt{y} - \sqrt{x}\right)^k$ with respect to y.
Abadie's formula (2) requires derivatives of $\left(\frac{\sqrt{y}-\sqrt{x}}{y-x}\right)^k = \left(\sqrt{y} + \sqrt{x}\right)^{-k}$ with respect to y.

Hoppe's formula (4) leads to

$$P_{n,k}(g;x) = \frac{1}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} x^{(k-j)/2} \left(\frac{d}{dx}\right)^n x^{j/2}$$

$$= \frac{x^{k/2-n}}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} \left(\frac{j}{2}\right)^{\underline{n}},$$

while Scott's formula (5) seemingly doesn't provide any advantage.

Formula (6) with $\frac{y-\sqrt{x}}{y^2-x} = \left(y + \sqrt{x}\right)^{-1}$ and $g^{-1}(y) = y^2$ yields after an application of the Leibniz rule

$$\binom{n}{k}^{-1} P_{n,k}(g;x) = \left(\frac{d}{dy}\right)^{n-k} \left[\frac{2y}{(y+\sqrt{x})^{n+1}}\right]_{|y=\sqrt{x}}$$

$$= \left[2y \left(\frac{d}{dy}\right)^{n-k} \frac{1}{(y+\sqrt{x})^{n+1}} + \binom{n-k}{1} \cdot 2 \left(\frac{d}{dy}\right)^{n-k-1} \frac{1}{(y+\sqrt{x})^{n+1}}\right]_{|y=\sqrt{x}}$$

$$= 2\sqrt{x} (-n-1)^{\underline{n-k}} \left(2\sqrt{x}\right)^{-n-1-(n-k)}$$

$$+ (n-k) \cdot 2 (-n-1)^{\underline{n-k-1}} \left(2\sqrt{x}\right)^{-n-1-(n-k-1)}$$

$$= (-1)^{n-k} k (n+1)^{\overline{n-k-1}} \left(2\sqrt{x}\right)^{-2n+k}$$

and finally

$$P_{n,k}(g;x) = (-1)^{n-k} \frac{k}{n} \binom{n}{k} n^{\overline{n-k}} \left(2\sqrt{x}\right)^{-2n+k}, \tag{8}$$

which is valid for $0 \le k \le n$.

Remark 4. Comparison of the outcome of Hoppe's formula with the rewritten form of Equation (8)

$$P_{n,k}(g;x) = (-1)^{n-k} \frac{n!}{(k-1)!} \frac{1}{2n-k} \binom{2n-k}{n} \left(2\sqrt{x}\right)^{-2n+k}$$

leads to the remarkable equation

$$\sum_{j=0}^{k} (-1)^j \binom{k}{j} \binom{j/2}{n} = \frac{(-1)^n}{2^{2n-k}} \frac{k}{2n-k} \binom{2n-k}{n},$$

for $0 \le k \le n$ and $n \in \mathbb{N}$. This is the Rosenstock–Gray–Riordan identity [6, p. 43, Equation (3.164)].

Acknowledgement

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