Some extensions of Faà di Bruno’s formula with divided differences

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ABSTRACT

The well-known formula of Faà di Bruno’s for higher derivatives of a composite function has played an important role in combinatorics. In this paper we generalize the divided difference form of Faà di Bruno’s formula and give an explicit formula for the \(n\)-th divided difference of a multicomposite function. More generally, we establish the relationships of the Bell polynomials with respect to multicomposite functions. Applying these to multicomposite functions, we obtain some extensions of Faà di Bruno’s formula.

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1. Introduction

The problem of finding an explicit expression for the \(n\)-th derivative of a composite function is an old one. Let \(h = f \circ g\) be a composite function. There are several ways to represent the \(n\)-th derivative of the composite function \(h\). One of the best-known ways is given by Faà di Bruno’s formula [1–3]

\[
h^{(n)}(t) = \sum_{\pi(0)} \frac{n!}{k_1!k_2!\cdots k_n!} f^{(k_1)}(g(t)) \left( \frac{g'(t)}{1!} \right)^{k_1} \left( \frac{g''(t)}{2!} \right)^{k_2} \cdots \left( \frac{g^{(n)}(t)}{n!} \right)^{k_n},
\]

where the sum runs over all partitions \(\pi(0)\) of the integer \(n\), \(k_i\) denotes the number of parts of size \(i\), and \(k = k_1 + k_2 + \cdots + k_n\) denotes the number of parts of the partition considered.

Faà di Bruno’s formula is an identity in mathematics generalizing the chain rule to higher derivatives, named in honor of Francesco Faà di Bruno (1825–1888). As usual, Faà di Bruno’s formula is also described in terms of the Bell polynomials:

\[
h^{(n)}(t) = \sum_{k=1}^{n} f^{(k)}(g(t)) B_{n,k}(g'(t), g''(t), \ldots, g^{(n)}(t)),
\]

where the exponential partial Bell polynomial \(B_{n,k}(x_1, x_2, \ldots, x_n)\) is given by an explicit expression

\[
B_{n,k}(x_1, x_2, \ldots, x_n) = \sum_{c_1 + 2c_2 + \cdots + nc_n = n} \frac{n!}{c_1!(1!)^{c_1}c_2!(2!)^{c_2} \cdots c_n!(n!)^{c_n}} x_1^{c_1}x_2^{c_2} \cdots x_n^{c_n}.
\]

As such, this dates back to [4]. Faà di Bruno’s formula has played an important role in combinatorial analysis. By the formula, Hsu [5] found some strange identities. It has also been applied in many branches of mathematics such as in numerical
analysis [6, 7] and statistics [8, 9]. Recently, Faà di Bruno’s formula has even been applied to the computation of Lamé function derivatives of arbitrary order [10] and the singular behavior of k-th angular derivatives of analytic functions in the unit disk in the complex plane \( \mathbb{C} \) and positive harmonic functions in the unit ball in \( \mathbb{R}^n \) [11]. Consequently, Faà di Bruno’s formula has been widely studied and generalized. For instance, some extensions of the formula in the case of multicomposite functions were considered in [12]. Further results on the formula in several variables were also obtained by [13–19]. It is worth noting that a divided difference version of Faà di Bruno’s formula has been established by using the chain rule of divided differences in the recent papers [20, 21]. Further generalization is given by Wang and Xu [22].

In this paper, we will generalize the divided difference form of Faà di Bruno’s formula. Applying this to multicomposite functions, we obtain some extensions of Faà di Bruno’s formula which generalize the results in [12].

2. Divided differences and the chain rule

Divided differences are often considered as the coefficients of the Newton interpolating polynomial. Assume that \( x_0, x_1, \ldots, x_n \) are distinct; then the divided differences of \( f \) are recursively given by the following formula:

\[
f[x_0] = f(x_0),
\]

\[
f[x_1, x_2, \ldots, x_j] = \frac{f[x_1, x_2, \ldots, x_j] - f[x_1, x_2, \ldots, x_{j-1}]}{x_j - x_i}.
\]

From the recursive formulas, it is clear that if \( x \neq x_0 \)

\[
f[x, x_0] = \frac{f(x) - f(x_0)}{x - x_0}.
\]

If repetitions are permitted in the arguments and the function \( f \) is smooth enough, then

\[
\lim_{x \to x_0} f[x, x_0] = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} = f'(x_0).
\]

This gives the definition of first-order divided differences with repeated points

\[
f[x_0, x_0] = f'(x_0).
\]

In general, let \( x_0 \leq x_1 \leq \cdots \leq x_n \); then the divided differences with repeated points obey this recursive formula:

\[
f[x_0, x_1, \ldots, x_n] = \begin{cases} f[x_1, x_2, \ldots, x_n] - f[x_0, x_1, \ldots, x_{n-1}] & \text{if } x_n \neq x_0, \\ f^{(n)}(x_0) \frac{x_n - x_0}{n!} & \text{if } x_n = x_0. \end{cases}
\]

Now let’s consider the composite function \( h = f \circ g \) with \( x = g(t) \) and \( y = f(x) \). Assume that \( g(t) \) and \( f(x) \) are sufficiently differentiable with respect to the relevant independent variables. Then

\[
h_{[t_0, t_1]} = f[g(t_0), g(t_1)]g_{[t_0, t_1]},
\]

\[
h_{[t_0, t_1, t_2]} = f[g(t_0), g(t_1), g(t_2)]g_{[t_0, t_1, t_2]} + f[g(t_0), g(t_1), g(t_2)]g_{[t_0, t_1]}g_{[t_1, t_2]},
\]

\[
h_{[t_0, t_1, t_2, t_3]} = f[g(t_0), g(t_1), g(t_2), g(t_3)]g_{[t_0, t_1, t_2, t_3]} + f[g(t_0), g(t_1), g(t_2), g(t_3)]g_{[t_0, t_1]}g_{[t_1, t_2]}g_{[t_2, t_3]},
\]

In a particular case, when \( t_0 = t_1 = t_2 = t_3 = t \), by the recurrence relations of divided differences one readily has the following formulas:

\[
h'(t) = f'(g(t))g'(t),
\]

\[
h''(t) = f''(g(t))g''(t) + f''(g(t))g'(t)^2,
\]

\[
h'''(t) = f'''(g(t))g'''(t) + 3f''(g(t))g'(t)g''(t) + f'''(g(t))g'(t)^3.
\]

The above example is for the case of solving the lower order derivatives of the composite function \( h \). More generally, for arbitrary \( n \), an interesting formula is explicitly given by:

**Proposition 1** ([20, 21]). If \( f \) and \( g \) are functions with a sufficient number of derivatives, then

\[
h_{[t_0, t_1, \ldots, t_n]} = \sum_{k=1}^{n} f[g(t_0), g(t_1), \ldots, g(t_k)]A_{n,k}(g; \{t_i\}_{i=0}^{n}),
\]

where

\[
A_{n,k}(g; \{t_i\}_{i=0}^{n}) = \sum_{k=0 \leq l_1 \leq \cdots \leq l_k \leq n} \prod_{i=1}^{k} g[t_{l_i-1}, t_{l_i-1}, t_{l_i-1+1}, \ldots, t_{l_i}].
\]

Observing this formula in the case \( t_0 = t_1 = \cdots = t_n = t \), we find \( A_{n,k}(g; \{t_i\}_{i=0}^{n}) \) reduces to \( \frac{k!}{n!} B_{n,k}(g'(t), g''(t), \ldots, g^{(n)}(t)) \).

Then the well-known Faà di Bruno’s formula is easily deduced.
3. Extensions of Faà di Bruno’s formula

Suppose that $\phi$ is a sufficiently smooth function. In this section, let’s first consider the term

$$A_{n,r}(\phi; \{t_i\}_{i=0}^n) = \sum_{r=\nu_0 \leq \nu_1 \leq \cdots \leq \nu_n = n} \prod_{i=1}^f \phi[t_{\nu_{i-1}}, t_{\nu_i}, t_{\nu_i+1}, \ldots, t_{\nu_f}]$$

for $r \geq 1$.

Notice that

$$A_{n,1}(\phi; \{t_i\}_{i=0}^n) = \phi[t_0, t_1, \ldots, t_n].$$

Then Eq. (2.1) can be rewritten as

$$A_{n,1}(h; \{t_i\}_{i=0}^n) = \sum_{k=1}^n A_{k,r}(f; \{g(t_i)\}_{i=0}^k)A_{n,k}(g; \{t_i\}_{i=0}^n).$$

This result is very interesting and important. We think $A_{n,r}(\phi; \{t_i\}_{i=0}^n)$ maybe possess good properties. This motivation makes us therefore try to look for a more general result. It is fortunate that we find that the following theorem holds:

**Theorem 1.** If $f$ and $g$ are functions with a sufficient number of derivatives, then

$$A_{n,r}(h; \{t_i\}_{i=0}^n) = \sum_{k=1}^n A_{k,r}(f; \{g(t_i)\}_{i=0}^k)A_{n,k}(g; \{t_i\}_{i=0}^n).$$

If we let $t_0 = t_1 = \cdots = t_n = t$, then the following corollary is immediately obtained.

**Corollary 1.** If $f$ and $g$ are functions with a sufficient number of derivatives, then

$$B_{n,r}(h(t), h''(t), \ldots, h^{(r)}(t)) = \sum_{k=1}^n B_{k,r}(f'(g(t)), f''(g(t)), \ldots, f^{(k)}(g(t)))B_{n,k}(g'(t), g''(t), \ldots, g^{(k)}(t)).$$

By the expressions for the Bell polynomials, one obtains $B_{n,1}(x_1, \ldots, x_n) = x_n$. Thus, letting $r = 1$ in Eq. (3.1) we will obtain Faà di Bruno’s formula again. In other words, Eq. (3.1) can be viewed as an extension of Faà di Bruno’s formula.

Before we give the proof of Theorem 1, two necessary lemmas are presented now.

**Lemma 1.** Let $\chi(t) = \varphi(t)\psi(t)$. If $\varphi$ and $\psi$ are sufficiently smooth functions, then for arbitrary nodes $t_0, t_1, \ldots, t_n$, we have

$$\chi[t_0, t_1, \ldots, t_n] = \sum_{i=0}^n \varphi[t_0, t_1, \ldots, t_i]\psi[t_i, t_{i+1}, \ldots, t_n].$$

This is called the Steffensen formula [23] which is a generalization of the Leibniz formula. When $t_0 = t_1 = \cdots = t_n = t$, the classical Leibniz formula holds, namely,

$$\chi^{(n)}(t) = \sum_{i=0}^n \binom{n}{i} \varphi^{(i)}(t)\psi^{(n-i)}(t).$$

Furthermore, considering the multiplication of the $m$ functions $\varphi_1, \varphi_2, \ldots, \varphi_m$, the generalized Steffensen formula is easily obtained by induction.

**Lemma 2.** Let $\chi(t) = \prod_{i=1}^m \varphi_i(t)$. If $\varphi_i$ ($i = 1, 2, \ldots, m$) are sufficiently smooth functions, then for arbitrary nodes $t_0, t_1, \ldots, t_n$, we have

$$\chi[t_0, t_1, \ldots, t_n] = \sum_{0=\nu_0 \leq \nu_1 \leq \cdots \leq \nu_{m-1} \leq \nu_m = n} \prod_{k=0}^{m-1} \varphi_k[t_{\nu_k}, t_{\nu_k+1}, \ldots, t_{\nu_{k+1}}].$$

**Proof of Theorem 1.** Assume initially that the $t_i$ are distinct. Letting $Q_r(t) = \prod_{i=0}^{r-1} (h(t) - h(t_i))$, $r \geq 1$, it is clear that $Q_r[t_0, t_1, \ldots, t_j] = 0$, $j \leq r - 1$. 
Then the Newton interpolating polynomial of $Q_r$ at the nodes $t_0, t_1, \ldots, t_n$ is described as

$$N_n(Q_r; t; \{t_i\}_{i=0}^n) = Q_r(t_0) + \sum_{j=1}^{n} Q_r[t_0, t_1, \ldots, t_j]\omega_j(t),$$

where

$$\omega_0(t) = 1, \omega_j(t) = (t - t_0)(t - t_1) \cdots (t - t_{j-1}), \quad j \geq 1.$$

Letting $\bar{Q}_r(t) = Q_r(t)/\omega_r(t)$, it is not difficult to obtain that

$$\bar{Q}_r(t) = \prod_{i=0}^{r-1} h[t_i].$$

By the Steffensen formula, we have

$$Q_r[t_0, t_1, \ldots, t_r] = \sum_{v=0}^{r} \bar{Q}_r[t_v, t_{v+1}, \ldots, t_r]\omega_r[t_0, t_1, \ldots, t_r].$$

Since

$$\omega_r[t_0, t_1, \ldots, t_r] = \begin{cases} 0 & v \neq r, \\ 1 & v = r, \end{cases}$$

we have

$$Q_r[t_0, t_1, \ldots, t_r] = \bar{Q}_r[t_r, t_{r+1}, \ldots, t_r].$$

By the generalized Steffensen formula, we arrive at

$$\bar{Q}_r[t_r, t_{r+1}, \ldots, t_r] = \sum_{f=r+2 \leq i_1 \leq \cdots \leq i_r} \prod_{k=1}^{r} h[t_{i_k-1}, t_{i_k-1+1}, \ldots, t_{i_k}].$$

Consequently, by (3.3) and (3.4), we have

$$Q_r[t_0, t_1, \ldots, t_r] = A_{r,r}(h; \{t_i\}_{i=0}^r).$$

On the other hand, letting $x = g(t), x_i = g(t_i), i = 0, 1, \ldots, n$, we have

$$Q_r(t) = \tilde{Q}_r(x) = \prod_{i=0}^{r-1} (f(x) - f(x_i)).$$

Thus, the Newton interpolating polynomial of $\tilde{Q}_r(x)$ at the nodes $x_0, x_1, \ldots, x_n$ is given by

$$N_n(\tilde{Q}_r; x; \{x_i\}_{i=0}^n) = \tilde{Q}_r(x_0) + \sum_{k=1}^{n} \tilde{Q}_r(x_0, x_1, \ldots, x_k)\omega_k(x),$$

where

$$\tilde{Q}_r[x_0, x_1, \ldots, x_k] = A_{k,r}(f; \{x_i\}_{i=0}^k).$$

Considering the Newton interpolating polynomial of $\omega_k(x) = \Omega_k(t) = \prod_{i=0}^{k-1} (g(t) - g(t_i))$ at the nodes $t_0, t_1, \ldots, t_n$, it follows that

$$N_n(\Omega_k; t; \{t_i\}_{i=0}^n) = \sum_{j=k}^{n} \Omega_k[t_0, t_1, \ldots, t_j]\omega_j(t).$$
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\[
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\]
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\[
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\]
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\[
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because
\[
\text{NataliniandRiccil12established}
\]
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\[\text{Theorem 2.}\quad\text{For}\quad1 \leq j \leq m\quad(\text{m} \geq 2),\quad\text{if}\quad f_{j}\quad\text{are functions with a sufficient number of derivatives, then}
\]
\[
A_{n,r}(F_{m};\{t_{i}\}_{i=0}^{n}) = \sum_{s_{0} \leq s_{1} \leq \ldots \leq s_{m-1} \leq s_{m} \leq s_{m+1}} \prod_{j=1}^{m} A_{j,s_{j-1}}(f_{j};\{(f_{j+1} \circ \cdots \circ f_{m})(t_{j})\}_{i=0}^{n}),
\]
where we assume that\(s_{0} = r,\quad s_{m} = n\) and \((f_{m+1} \circ \cdots \circ f_{m})(t) = t\).

**Proof.** We shall prove it by induction on \(m\). For \(m = 2\), it holds by Theorem 1. We assume the correctness of (4.1) for \(m = k\), and we now prove it for \(k + 1\). Let \(G_{k} = f_{2} \circ f_{3} \circ \cdots \circ f_{k+1}\), and by assumption we have
\[
A_{n,s}(G_{k};\{t_{i}\}_{i=0}^{n}) = \sum_{s_{1} \leq s_{2} \leq \ldots \leq s_{k} \leq s_{k+1}} \prod_{j=2}^{k+1} A_{j,s_{j-1}}(f_{j};\{(f_{j+1} \circ \cdots \circ f_{k+1})(t_{j})\}_{i=0}^{n})
\]
with \(s_{1} = s,\quad s_{k+1} = n\). Since \(F_{k+1} = f_{1} \circ G_{k}\), by using Theorem 1 again we therefore have
\[
A_{n,r}(F_{k+1};\{t_{i}\}_{i=0}^{n}) = \sum_{s_{0} \leq s_{1} \leq \ldots \leq s_{k} \leq s_{k+1}} \prod_{j=1}^{k+1} A_{j,s_{j-1}}(f_{j};\{(f_{j+1} \circ \cdots \circ f_{k+1})(t_{j})\}_{i=0}^{n})
\]
Substituting (4.2) into (4.3) yields
\[
A_{n,r}(F_{k+1};\{t_{i}\}_{i=0}^{n}) = \sum_{s_{0} \leq s_{1} \leq \ldots \leq s_{k} \leq s_{k+1}} \prod_{j=1}^{k+1} A_{j,s_{j-1}}(f_{j};\{(f_{j+1} \circ \cdots \circ f_{k+1})(t_{j})\}_{i=0}^{n})
\]
with \(s_{0} = r,\quad s_{k+1} = n\). Hence, Eq. (4.1) holds true for \(m = k + 1\), and this completes the proof. \(\Box\)
Since \( F_m(t_0, t_1, \ldots, t_n) = A_{n,1}(F_m; [t_i]_{i=0}^n) \), then an explicit expression for the \( n \)-th divided difference of the multicomposite function \( F_m \) is given by:

**Theorem 3.** For \( 1 \leq j \leq m \ (m \geq 2) \), if \( f_j \) are functions with a sufficient number of derivatives, then

\[
F_m(t_0, t_1, \ldots, t_n) = \sum_{s_0 \leq t_1 \leq \cdots \leq s_{m-1} \leq s_m} \prod_{j=1}^{m} A_{s_j, s_{j-1}} \left( f_j ; (f_{j+1} \circ \cdots \circ f_m)(t_1) \right) [t_i]_{i=0}^n,
\]

where \( s_0 = 0 \), \( s_m = n \) and \( (f_{m+1} \circ \cdots \circ f_m)(t) = t \).

In particular, when \( t_0 = t_1 = \cdots = t_n = t \), an extension of Faà di Bruno’s formula for multicomposite functions is as follows:

**Corollary 2.** For \( 1 \leq j \leq m \ (m \geq 2) \), if \( f_j \) are functions with a sufficient number of derivatives, then

\[
F_m^{(n)}(t) = \sum_{s_0 \leq t_1 \leq \cdots \leq s_{m-1} \leq s_m} \prod_{j=1}^{m} B_{s_j, s_{j-1}} \left( f_j ; (f_{j+1} \circ \cdots \circ f_m)(t) \right),
\]

where \( s_0 = 1 \), \( s_m = n \) and \( f_{m+1}(\cdots (f_m(t))) = t \).

In [12], Natalini et al. used Faà di Bruno’s formula to establish the relations between the \( n \)-th derivative of the multicomposite function and the derivatives of order less than \( n \). Here, we give the above explicit formula for the \( n \)-th derivative of the multicomposite function. More generally, we establish the relationships of the Bell polynomials with respect to multicomposite functions and include the above formula as a special case for \( r = 1 \).

**Corollary 3.** For \( 1 \leq j \leq m \ (m \geq 2) \), if \( f_j \) are functions with a sufficient number of derivatives, then

\[
B_{n,r}(F'_m(t), F''_m(t), \ldots, F^{(n)}_m(t)) = \sum B_{s_0, s_1} \left( f_j ; (f_{j+1} \circ \cdots \circ f_m)(t) \right) \prod_{j=1}^{m} f_j^{(s_j)}(f_{j+1} \circ \cdots \circ f_m(t)),
\]

where \( s_0 = r \), \( s_m = n \) and \( f_{m+1}(\cdots (f_m(t))) = t \).

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**References**


