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Applications of a Generalized Leibniz Rule

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The central point of this short paper is a generalization of the Leibniz Rule for the derivative of a product of differentiable functions. As applications we present several combinatorial identities. Among the consequences are the celebrated Abel identity and the Rothe identity.

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1. Introduction and Main Formula

Let $n \in \mathbb{N}_0$, $r \in \mathbb{N}$, and let h, f_i $(i = 1, \ldots, r)$ be functions which are n-times differentiable in $x_0 \in \mathbb{R}$ with $h(x_0) \neq 0$. The main formula considered in this short note is

$$\sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \prod_{i=1}^{r} \left(h^{k_i} f_i\right)^{(k_i)}(x_0) = \left(\left(\frac{d}{dx}\right)^n \frac{h^{n+r-1}(x) \prod_{i=1}^{r} f_i(x)}{\left(h(x) - h'(x)(x - x_0)\right)^{r-1}} \right)\Bigg|_{x=x_0}. \tag{1}$$

Obviously, if h is a constant function, Eq. (1) reduces to the well-known Leibniz Rule

$$\left(\prod_{i=1}^{r} f_i\right)^{(n)} = \sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \prod_{i=1}^{r} f_i^{(k_i)} \qquad (n = 0, 1, 2, \ldots), \tag{2}$$

for several n-times differentiable functions f_i $(i = 1, \ldots, r)$.

Throughout the paper $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{N}_0^r$ denotes a multi-index, $|\mathbf{k}| = k_1 + \cdots + k_r$, and the multinomial coefficient is defined by

$$\binom{n}{\mathbf{k}} = \binom{n}{k_1, \ldots, k_r} := \frac{n!}{k_1! \cdots k_r! (n - |\mathbf{k}|)!}.$$

A proof of the intriguing formula (1) can be found in [2]. It is essentially based on methods of complex analysis. Therefore, in the derivation h,

f_i $(i = 1, \ldots, r)$ are assumed to be functions analytic in a neighborhood of $x_0 \in \mathbb{C}$ with $h(x_0) \neq 0$. However, the identity (1) is of an algebraic nature among the derivatives (Taylor coefficients) and hence automatically extends to non-analytic functions of sufficient smoothness by a general principle. Therefore, Eq. (1) is valid also for real functions h and f_i possessing a continuous derivative of order n in $x_0 \in \mathbb{R}$. It would be desirable to find a proof using only combinatorial methods.

Remark 1. If h is a linear function we have

$$h(x) - h'(x)(x - x_0) = h(x_0),$$

and Eq. (1) simplifies to

$$h^{r-1} \sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \prod_{i=1}^{r} \big(h^{k_i} f_i\big)^{(k_i)} = \Big(h^{n+r-1} \prod_{i=1}^{r} f_i\Big)^{(n)}.$$

The special case $r = 2$, $h(x) = x$, i.e., the amazing identity

$$x \sum_{k=0}^{n} \binom{n}{k} \big(x^k f(x)\big)^{(k)} \big(x^{n-k} g(x)\big)^{(n-k)} = \big(x^{n+1} f(x) g(x)\big)^{(n)}$$

was discovered by the author while studying asymptotic expansions for sequences of certain approximation operators.

2. Applications

2.1. Abel Identity

As applications, we obtain remarkable identities. The most prominent example is the Abel identity

$$\sum_{k=0}^{n} \binom{n}{k} a(a - kc)^{k-1} (b + kc)^{n-k} = (a + b)^n, \tag{3}$$

published in 1826 [1]. It is valid in commutative rings. A multivariate variant of this deep generalization of the binomial formula follows as a direct consequence of Eq. (1). If

$$\begin{aligned} h(x) &= e^{-cx}, \\ f_i(x) &= e^{a_i x} h^{-1}(x)\big(h(x) - h'(x)(x - x_0)\big) \\ &= e^{a_i x}(1 + c(x - x_0)), \qquad \text{for } 1 \leq i \leq r - 1, \\ f_r(x) &= e^{(a_r + nc)x}, \end{aligned}$$

we obtain the following

Conclusion 1. *For* $n = 0, 1, 2, \ldots$, $r \geq 2$, *and all* $\mathbf{a} = (a_1, \ldots, a_r) \in \mathbb{C}^r$, $c \in \mathbb{C}$, *it follows that*

$$\sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \left[\prod_{i=1}^{r-1} \left(a_i (a_i - k_i c)^{k_i - 1}\right) \right] \left(a_r + (n - k_r)c\right)^{k_r} = |\mathbf{a}|^n.$$

The bivariate specialization with $\mathbf{a} = (a, b) \in \mathbb{C}^2$ *is Eq. (3).*

2.2. Rothe-Hagen Identity

In 1793 Rothe [10] published the convolution formula

$$\sum_{k=0}^{n} \frac{a}{a - kc} \binom{a - kc}{k} \binom{b + kc}{n - k} = \binom{a + b}{n}, \tag{4}$$

which is also called Rothe-Hagen identity because it appears in Hagen's three-volume 1891 publication [9, Formula 17, pp. 64–68, vol. I]. There are many proofs of this famous identity in the literature as well as various extensions. It was rediscovered by Gould [6] in 1956. Recently, Chu [3] gave an elementary proof. We put

$$\begin{aligned} h(x) &= x^{-c}, \\ f_i(x) &= x^{a_i} h^{-1}(x) \big(h(x) - h'(x)(x - x_0)\big) \\ &= x^{a_i} (1 + c - c x_0 / x), \qquad \text{for } 1 \leq i \leq r - 1, \\ f_r(x) &= x^{a_r + nc} \end{aligned}$$

and formula (1) implies the following generalization of the Rothe identity.

Conclusion 2. *For* $n = 0, 1, 2, \ldots$, $r \geq 2$, *and all* $\mathbf{a} = (a_1, \ldots, a_r) \in \mathbb{C}^r$, $c \in \mathbb{C}$, *it follows that*

$$\sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \left[\prod_{i=1}^{r-1} \left(\frac{a_i}{a_i - k_i c} \binom{a_i - k_i c}{k_i} \right) \right] \binom{a_r + (n - k_r)c}{k_r} = \binom{|\mathbf{a}|}{n}.$$

The special case $r = 2$ with $\mathbf{a} = (a, b) \in \mathbb{C}^2$ is the Rothe identity (4).

2.3. A Binomial Identity

If $h(x) = x$ and $f_i(x) = x^{a_i}$ $(i = 1, \ldots, r)$ we obtain the following

Conclusion 3. *For* $n = 0, 1, \ldots$ *and all* $\mathbf{a} = (a_1, \ldots, a_r) \in \mathbb{C}^r$, *it follows that*

$$\sum_{|\mathbf{k}|=n} \prod_{i=1}^{r} \binom{k_i + a_i}{k_i} = \binom{n + |\mathbf{a}| + r - 1}{n}.$$

The bivariate specialization is given by

$$\sum_{k=0}^{n} \binom{k+a}{k} \binom{n-k+b}{n-k} = \binom{n+a+b+1}{n}.$$

2.4. A First Problem by Graham, Knuth and Patashnik

In their textbook [8, Ex. 5.47, p. 246] Graham, Knuth and Patashnik pose the following problem: Show that the sum

$$P_n(a,b) := \sum_{k=0}^{n} \binom{ak+b}{k} \binom{a(n-k)-b}{n-k},$$

which is a polynomial in the both variables a and b, is independent of b. The sum is similar to the left-hand side of the Rothe identity (4). A direct consequence is the formula

$$\sum_{k=0}^{n} \binom{ak+b}{k} \binom{a(n-k)-b}{n-k} = \sum_{k=0}^{n} \binom{ak}{k} \binom{a(n-k)}{n-k}.$$

We put $h(x) = x^a$, $f_1(x) = x^b$, $f_2(x) = x^{-b}$ and apply identity (1) with $r = 2$. We have

$$\begin{aligned} n! x^{(a-1)n} P_n(a,b) &= \sum_{k=0}^{n} \binom{n}{k} (x^{ak+b})^{(k)} (x^{a(n-k)-b})^{(n-k)} \\ &= \sum_{k=0}^{n} \binom{n}{k} \big(h^k(x) f_1(x)\big)^{(k)} \big(h^{n-k}(x) f_2(x)\big)^{(n-k)}. \end{aligned}$$

Because of $f_1(x) f_2(x) = 1$ the right-hand side of Eq. (1) is equal to

$$\left(\left(\frac{d}{dt}\right)^n \frac{h^{n+1}(t)}{h(t) - h'(t)(t-x)} \right)\Bigg|_{t=x},$$

which is independent of b.

Moreover, one can proceed with calculating the latter expression. Denote

$$R(x) := \left(\left(\frac{d}{dt}\right)^n \frac{h^{n+1}(t)}{h(t) - h'(t)(t-x)} \right)\Bigg|_{t=x} = \left(\left(\frac{d}{dt}\right)^n \frac{t^{an+1}}{(1-a)t + ax} \right)\Bigg|_{t=x}.$$

We distinguish two cases.

Case $|(a-1)/a| < 1$: We have

$$\begin{aligned} R(x) &= \frac{1}{ax} \left(\left(\frac{d}{dt}\right)^n \left[t^{an+1} \sum_{k=0}^{\infty} \Big(\frac{a-1}{a} \frac{t}{x}\Big)^k \right] \right)\Bigg|_{t=x} \\ &= \frac{n!}{a} x^{(a-1)n} \sum_{k=0}^{\infty} \binom{an+k+1}{n} \Big(\frac{a-1}{a}\Big)^k \end{aligned}$$

and thus

$$P_n(a,b) = a^{-1} \sum_{k=0}^{\infty} \binom{an+k+1}{n} \Big(\frac{a-1}{a}\Big)^k, \qquad \text{if } \Big|\frac{a-1}{a}\Big| < 1.$$

Case $|(a-1)/a| > 1$: We have

$$\begin{aligned} R(x) &= \frac{-1}{a-1} \left(\Big(\frac{d}{dt}\Big)^n \left[t^{an} \sum_{k=0}^{\infty} \Big(\frac{a}{a-1}\frac{x}{t}\Big)^k \right] \right) \Bigg|_{t=x} \\ &= \frac{-n!}{a-1}\, x^{(a-1)n} \sum_{k=0}^{\infty} \binom{an-k}{n} \Big(\frac{a}{a-1}\Big)^k \end{aligned}$$

and thus

$$P_n(a,b) = \frac{-1}{a-1} \sum_{k=0}^{\infty} \binom{an+k+1}{n} \Big(\frac{a-1}{a}\Big)^k, \qquad \text{if } \Big|\frac{a-1}{a}\Big| > 1.$$

Alternatively, we can apply the Leibniz Rule to $R(x)$ in order to obtain

$$\begin{aligned} R(x) &= n! \sum_{k=0}^{n} (-1)^k \binom{an+1}{n-k} \frac{(1-a)^k}{((1-a)t+ax)^{k+1}}\, t^{an+1-(n-k)} \Bigg|_{t=x} \\ &= n!\, x^{(a-1)n} \sum_{k=0}^{n} \binom{an+1}{n-k} (a-1)^k. \end{aligned}$$

As conclusion we obtain

$$P_n(a,b) = \sum_{k=0}^{n} \binom{an+1}{k} (a-1)^{n-k}$$

which is valid for all values $a \in \mathbb{C}$.

When it happens that a is an integer greater than 1 an elementary calculation leads to the representation

$$P_n(a,b) = \frac{a^{(a-1)n}}{(a-1)^{(a-1)n+1}} \left[-1 + \sum_{k=0}^{(a-1)n} (-1)^k \binom{an+1}{k+n+1} \binom{k+n}{n} a^{-k} \right],$$

which is a finite sum.

In the trivial cases $a \in \{0,1\}$ we obtain

$$\begin{aligned} P_n(1,b) &= \sum_{k=0}^{n} \binom{k+b}{k} \binom{n-k-b}{n-k} = n+1, \\ P_n(2,b) &= \sum_{k=0}^{n} \binom{2k+b}{k} \binom{2(n-k)-b}{n-k} = 4^n. \end{aligned}$$

A proof of the latter formula can be found in [5] (see also [4]). I am grateful to Dr. V. Kushnirevych for pointing out that the sequences $(P_n(a,b))_{n=0}^{\infty}$, for $a = 3, \ldots, 7$, are listed in *The On-Line Encyclopedia of Integer Sequences* [11] as Sequence A006256, A078995, A079678, A079679, A079563, respectively.

2.5. A Second Problem by Graham, Knuth and Patashnik

As an example for the Gosper-Zeilberger algorithm Graham, Knuth and Patashnik [8, Ex. 5.104, p. 255] present the equation

$$\sum_{k=0}^{n}(-1)^k\binom{r-s-k}{k}\binom{r-2k}{n-k}\frac{1}{r-n-k+1}=\binom{s}{n}\frac{1}{r-2n+1}, \tag{5}$$

which they call a "remarkable identity". With $r=b$ and $s=a+b$ and using upper negation

$$(-1)^k\binom{-a-k}{k}=\binom{a+2k-1}{k},$$

the identity can be rewritten in the form

$$\sum_{k=0}^{n}\binom{a-1+2k}{k}\binom{b-2k}{n-k}\frac{1}{b-n-k+1}=\binom{a+b}{n}\frac{1}{b-2n+1},$$

which reveals Eq. (5) to be a variant of the Rothe identity (4). Nevertheless, the original representation can be deduced as a direct consequence of Eq. (1) if we put

$$\begin{aligned}
r &= 2,\\
h(x) &= x^2,\\
f_1(x) &= x^{s-r-1},\\
f_2(x) &= x^{r-2n-1}\big(h(x)-h'(x)(x-x_0)\big)=x^{r-2n-1}(2xx_0-x^2).
\end{aligned}$$

Then we have

$$\begin{aligned}
\big(h^k(x)f_1(x)\big)^{(k)} &= (x^{2k+s-r-1})^{(k)}=k!\binom{2k+s-r-1}{k}x^{k+s-r-1}\\
&= (-1)^k k!\binom{r-s-k}{k}x^{k+s-r-1},
\end{aligned}$$

and

$$\begin{aligned}
&\big(h^{n-k}(x)f_2(x)\big)^{(n-k)}\\
&\quad= \big(x^{-2k+r-1}(2xx_0-x^2)\big)^{(n-k)}\\
&\quad= \big(2x_0x^{-2k+r}-x^{-2k+r+1}\big)^{(n-k)}\\
&\quad= (n-k)!\left[2\binom{-2k+r}{n-k}x_0x^{-n-k+r}-\binom{-2k+r+1}{n-k}x^{-n-k+r+1}\right].
\end{aligned}$$

Thus, one can calculate the left-hand side of Eq. (1)

$$
\begin{aligned}
\mathrm{LHS} &= \sum_{k=0}^{n} \binom{n}{k} (h^k f_1)^{(k)}(x_0)(h^{n-k} f_2)^{(n-k)}(x_0) \\
&= n!\, x_0^{s-n} \sum_{k=0}^{n} (-1)^k \binom{r-s-k}{k} \binom{-2k+r}{n-k} \frac{r-2n+1}{r-n-k+1},
\end{aligned}
$$

where we used that

$$
2\binom{-2k+r}{n-k} - \binom{-2k+r+1}{n-k} = \frac{r-2n+1}{r-n-k+1} \binom{-2k+r}{n-k}.
$$

The right-hand side of (1) is equal to RHS $= \left((d/dx)^n x^s\right)\big|_{x=x_0} = n!\binom{s}{n} x_0^{s-n}$. Equating both sides proves Eq. (5).

3. Deduction of the Main Identity from a Simplified Special Case

In this section we show that the main identity (1) can be deduced from a simplified variant depending only on the function h. It is sufficient to prove Eq. (1) in the special case that all functions f_i $(i = 1, \ldots, r)$ are powers of the function h with non-negative integer exponents. The statement is as follows: For all $\alpha = (\alpha_1, \ldots, \alpha_r) \in \mathbb{N}_0^r$ satisfying $|\alpha| \leq n$, and for all $m \leq n - |\alpha|$,

$$
\sum_{|\mathbf{k}|=m} \binom{m}{\mathbf{k}} \prod_{i=1}^{r} (h^{k_i+\alpha_i})^{(k_i)}(x_0) = \left(\left(\frac{d}{dx}\right)^m \frac{h^{m+|\alpha|+r-1}(x)}{\big(h(x) - h'(x)(x-x_0)\big)^{r-1}} \right)\Bigg|_{x=x_0}.
$$

Proof. We start with the left-hand side of Eq. (1), where we neglect, for the moment, the variable x_0. Application of the Leibniz Rule yields

$$
\begin{aligned}
\mathrm{LHS} &= \sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \prod_{i=1}^{r} \left[\sum_{\alpha_i=0}^{k_i} \binom{k_i}{\alpha_i} f_i^{(\alpha_i)} (h^{k_i})^{(k_i-\alpha_i)} \right] \\
&= \sum_{|\alpha|\leq n} \left(\prod_{i=1}^{r} f_i^{(\alpha_i)} \right) \sum_{\substack{|\mathbf{k}|=n,\\ \mathbf{k}\geq\alpha}} n! \prod_{i=1}^{r} \left[\frac{1}{\alpha_i!(k_i-\alpha_i)!} (h^{k_i})^{(k_i-\alpha_i)} \right] \\
&= \sum_{\ell=0}^{n} \sum_{|\alpha|=\ell} \left(\prod_{i=1}^{r} \frac{f_i^{(\alpha_i)}}{\alpha_i!} \right) \sum_{|\mathbf{k}|=n-|\alpha|} n! \prod_{i=1}^{r} \left[\frac{1}{k_i!} (h^{k_i+\alpha_i})^{(k_i)} \right] \\
&= \sum_{\ell=0}^{n} \frac{n!}{(n-\ell)!} \sum_{|\alpha|=\ell} \left(\prod_{i=1}^{r} \frac{f_i^{(\alpha_i)}}{\alpha_i!} \right) \sum_{|\mathbf{k}|=n-\ell} \binom{n-\ell}{\mathbf{k}} \prod_{i=1}^{r} (h^{k_i+\alpha_i})^{(k_i)},
\end{aligned}
$$

where $\mathbf{k} \geq \alpha$ means $k_i \geq \alpha_i$ $(i = 1, \ldots, r)$. On the other hand, application of the Leibniz Rule to the right-hand side of Eq. (1)

$$\mathrm{RHS} = \left(\frac{d}{dx}\right)^n \left[Q(x) \prod_{i=1}^{r} f_i(x)\right],$$

where, for fixed n, r, x_0,

$$Q(x) := \frac{h^{n+r-1}(x)}{\big(h(x) - h'(x)(x - x_0)\big)^{r-1}},$$

yields

$$\begin{aligned}
\mathrm{RHS} &= \sum_{\ell=0}^{n} \binom{n}{\ell} \left(\prod_{i=1}^{r} f_i\right)^{(\ell)} Q^{(n-\ell)} \\
&= \sum_{\ell=0}^{n} \binom{n}{\ell} \sum_{|\alpha|=\ell} \binom{\ell}{\alpha} \left(\prod_{i=1}^{r} f_i^{(\alpha_i)}\right) Q^{(n-\ell)} \\
&= \sum_{\ell=0}^{n} \frac{n!}{(n-\ell)!} \sum_{|\alpha|=\ell} \left(\prod_{i=1}^{r} \frac{f_i^{(\alpha_i)}}{\alpha_i!}\right) Q^{(n-\ell)}.
\end{aligned}$$

Comparison of both sides leads to

$$\sum_{|\mathbf{k}|=n-|\alpha|} \binom{n-|\alpha|}{\mathbf{k}} \prod_{i=1}^{r} (h^{k_i+\alpha_i})^{(k_i)}(x_0) = Q^{(n-|\alpha|)}(x_0).$$

Putting $m = n - |\alpha|$ we obtain the desired result. $\square$

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