

1. Faa di Bruno Formulas

Around 1850 interest in new special functions was strong, and formulas for higher derivatives of $[f(x)]^n$, $[f(x)]^{-1}$, and $\log[f(x)]$ were produced, both for special and general choices of $f(x)$. Faa di Bruno trumped these formulas by publishing a general higher-order chain rule [3] for p th derivatives of $G(z) = F(u(z))$: $G^{(p)}(z) = \left(\frac{d}{dz}\right)^p F(u(z))$, in terms of $F^{(m)}(u(z))$, and, $u^{(n)}(z)$, where $1 \leq m \leq p$ and $1 \leq n \leq p$. Most applications were, and still are, for $2 \leq p \leq 4$. Exceptionally, $p = 5$ or 6 , in statistical or plasma physics. Bruno's condensed formula for general $p \geq 1$ involves a $(p+1)$ dimensional summation over indices m, k_1, k_2, \dots, k_p with $0 \leq m \leq p$ and $1 \leq k_1, k_2, \dots, k_p \leq p$, subject to two coupling conditions:

$$\sigma_p(\vec{k}) = k_1 + k_2 + \dots + k_p = m \quad (1)$$

$$\tau_p(\vec{k}) = k_1 + 2k_2 + \dots + pk_p = p \quad (2)$$

Characteristic here are the Bruno products,

$$B_{\vec{k},p}(u(z)) = \prod_{\nu=1}^p \left(\frac{d^\nu u(z)}{dz^\nu} \frac{1}{\nu!} \right)^{k_\nu}, \quad \vec{k} = (k_1, k_2, \dots, k_p) \quad (3)$$

These products appear in the Bruno formula for one intermediate variable and also in our multivariable analogs. The formula itself is, on recalling (1 – 3), takes the compressed form

$$\begin{aligned} G^{(p)}(z) &= \left(\frac{d}{dz} \right)^p F(u(z)) \\ &= \sum_{m=1}^p \sum_{k_1=1}^p \dots \sum_{k_p=1}^p F^{(m)}(u(z)) B_{\vec{k},p}(u(z)), \quad \sigma_p(\vec{k}) = m, \quad \tau_p(\vec{k}) = p \end{aligned} \quad (4)$$

For $p = 3(4)$ the number of additive terms in (4) under the σ and τ conditions are 3(5), respectively, each term with 3(4) symbolic multiplications involving the derivatives of $F(u)$ and Bruno products, plus numerical coefficients. Thus for functions of one variable, printing out the full expressions of $p(z)$ for $p = 3(4)$ is quite efficient, compared to the use of (4).

In the multivariable analogs, even for $p = 3(4)$, the number of additive terms becomes awkward and the derivation of the terms somewhat tiresome. This is evident already in the 2×2 case $\vec{u}(\vec{z}) = u_1(z_1, z_2), u_2(z_1, z_2)$. A “compressed” Bruno formula becomes more attractive as the multivariable dimensions m for \vec{u} or n for \vec{z} , and the order p is increased. Also, it can be used for symbolic computation instead of recursive application of the standard first-order chain rule. Certain features of the multivariable general chain rule, such as the type of cross-coupling between different intermediate variables in the τ conditions, are possibly more illuminating in a Bruno-type formula than in the full expression. Obviously, “pure” derivatives, such as $\frac{\partial^4 G(z_1, z_2)}{\partial z_1^4}$, are easier to deal with than mixed derivatives like $\frac{\partial^4 G}{\partial z_1^2 \partial z_2^2}$, which cannot always be avoided, as in calculation of $(\nabla^2)^2$ terms for elasticity and fluidics.

2. Proofs of the Single-Variable Bruno Formula

Bruno [3] has only a hazy proof of (4), neither rigorous nor algorithmically convincing. Königsberger [7] derived a more difficult formula for the general problem of calculating higher-order differentials, $d^p f(z_1, \dots, z_N)$, using a symbolic calculus and induction. Since differentials are invariant under differentiable transformations, this in principle should yield multivariable chain rules. However, higher differentials package together a variety of different orders of derivatives, which yield a Bruno formula conveniently only in the case $M = N = 1$. But for that case, Königsberger's proof also is an inductive proof of (4), as Bieberbach [2] pointed out. Somewhat later, de la Vallee Poussin [4] produced a concise proof of (4), based on a weak form of the Taylor expansion with remainder and a weak uniqueness theorem for “almost” power series of the form $a_0 + a_1 h + \dots + a_{q-1} h^{q-1} + M_q(h) h^q$, where $M_q(h) \rightarrow a_q$ as $h \rightarrow 0$ and $M_q(h)$ is bounded in h for small h .

That proof is less elementary than a longer one based on the integral form of the Taylor remainder, which latter can be made quite explicit, at the cost of assuming slightly more regularity than the minimum needed. The integral remainder version can be generalized quite well in the multivariable context.

An American book with a good collection of higher-derivative formulas, including many infinite series, is Schwatt [8]. Oddly, he does not list the Bruno formula, only various substitutes oriented to special cases of interest, and has little on the important topic of asymptotic series for higher-order derivatives, of interest in statistical mechanics (Fowler [6]).

Symbolic manipulation on computer via Macsyma, Maple, Mathematica, etc. can produce any required order of Bruno or Schwatt formulas. As shown later, a multivariable symbolic program produces multivariable versions of such formulas. In another direction, similar formulas appear in the Whitney [9], Dieudonné [5] theories of extensions of differentiable functions. See Abraham and Robbin [1] for a detailed account.

3. Integral Remainder Proof of the Bruno Formula

If $u(z)$ and $F(u)$ are $q+1$ times differentiable in suitable domains, the q th order Taylor expansions with integral remainder are given by

$$F(u+j) = \sum_{m=0}^q \frac{j^m}{m!} F^{(m)}(u) + R_q \left(F^{(q+1)}(u), u, j \right) \quad (5)$$

$$u(z+h) = \sum_{n=0}^q \frac{h^n}{n!} u^{(n)}(z) + R_q \left(u^{(q+1)}(z), z, h \right) \quad (6)$$

where

$$R_p(Y, v, k) = \frac{1}{p!} \int_v^{v+k} (v+k-y)^p Y(y) dy, \quad p = 0, 1, 2, \dots \quad (7)$$

is the integral remainder.

Based on (5–7), it will be shown that $G^{(p)}(z)$ is given by (4) for $p \leq q$. This will follow from

$$G(z+h) = \sum_{p=0}^q \frac{h^p}{p!} g_p(z) + S_q(G, z, h) \quad (8)$$

where $g_p(z)$ is given by the Bruno formula (4), and the fact that

$$\lim_{h \rightarrow 0} \left(\frac{d}{dh} \right)^p S_q(G, z, h) = 0, \quad 0 \leq p \leq q \quad (9)$$

First, (8) and (6) imply that

$$G^{(p)}(z) = \lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p G(z+h) = \lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p F(u(z+h)) \quad (10)$$

Second, setting $j = j(z, h) = u(z+h) - u(z)$, formulas (5) and (6) yield

$$F(u(z+h)) = \sum_{m=0}^q \frac{F^{(m)}(u(z))}{m!} \left[\sum_{n=1}^q \frac{h^n}{n!} u^{(n)}(z) + {}_u R_q \right]^m + {}_F R_q \quad (11)$$

where the remainders, ${}_u R_q$, ${}_F R_q$ are given (in the notation of (7)) more precisely by

$${}_u R_q = R_q \left(u^{(q+1)}(z), z, h \right) \quad (12)$$

$${}_F R_q = R_q \left(F^{(q+1)}(u), u, j \right) \Big|_{u=u(z)} \quad (13)$$

Multinomial expansion of the terms inside the brackets in (11) permits rewriting (11) as

$$F(u(z+h)) = \sum_{m=0}^q \frac{F^{(m)}(u)}{m!} \sum_{r=0}^m \sum_{\substack{k_1 \cdots k_q \\ k_1 + \cdots + k_q = m-r}} \frac{m!}{k_1! \cdots k_q! r!} \bullet \prod_{\nu=1}^q \left(\frac{h^\nu}{\nu!} \frac{d^\nu u(z)}{dz^\nu} \right)^{k_\nu} ({}_u R_q)^r + {}_F R_q \quad (14)$$

Each Bruno product term in (14) comes with the exponential $h^{\tau_q(\vec{k})}$, $\tau_q(\vec{k}) = k_1 + 2k_2 + \cdots + qk_q$, and the power $({}_u R_q)^r$ as factors. Thus application of $\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p$ to (14) reduces it to linear combinations of $\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p \left[h^{\tau_q(\vec{k})} ({}_u R_q)^r \right] = p! \delta(r, 0) \delta(p, \tau_q(\vec{k}))$ and $\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p ({}_F R_q) = 0$, for $p \leq q$.

The latter result follows from Leibnitz's differentiation rule: for $q > 0$

$$\begin{aligned} \frac{\partial}{\partial h} [{}_F R_q(u, j)] &= \frac{\partial}{\partial h} \left[\frac{1}{q!} \int_u^{u+j(z, h)} [u + j(z, h) - y] F^{(q+1)}(y) dy \right] \\ &= \frac{1}{q!} \frac{\partial j(z, h)}{\partial h} \left\{ [u + j(z, h) - (u + j(z, h))]^q F^{(q+1)}(u(z+h)) \right. \\ &\quad \left. + q \int_u^{u+j(z, h)} [u + j(z, h) - y]^{q-1} F^{(q+1)}(y) dy \right\} \\ &= [{}_F R_{q-1}(u, j)] \quad u'(z+h) \end{aligned} \quad (15)$$

However, $\frac{\partial}{\partial h} [{}_F R_0] = F^{(q+1)}(u(z+h))$. (This recursion resembles that for derivatives of $T_q(h) = C \frac{j^q(z, h)}{q!}$, a simple special case of the Faa di Bruno formula). Since $\lim_{h \rightarrow 0} {}_F R_0(u, j) = \lim_{h \rightarrow 0} \int_u^{u+j(z, h)} F^{(q+1)}(y) dy = \lim_{h \rightarrow 0} [F^{(q)}(u(z+h)) - F^{(q)}(u(z))] = 0$, induction of (15) easily yields

$$\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p ({}_F R_q) = 0, \quad \text{for } q > 0, \quad p \leq q \quad (16)$$

A special case of the above argument, with F replaced by u , u replaced by z , and j replaced by h , leads to

$$\left(\frac{\partial}{\partial h} \right) [{}_u R_q(z, h)] = {}_u R_{q-1}(z, h) \quad (17)$$

and

$$\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p ({}_u R_q) = 0, \quad \text{for } q > 0, \quad p \leq q \quad (18)$$

Leibnitz's product rule then produces

$$\begin{aligned} L_{p, \tau(\vec{k}), \nu} &= \left(\frac{\partial}{\partial h} \right)^p [h^{\tau(\vec{k})} ({}_u R_q)^r] \\ &= \sum_{s=0}^p \binom{p}{s} \left(\frac{\partial}{\partial h} \right)^{p-s} h^{\tau(\vec{k})} \left(\frac{\partial}{\partial h} \right)^s ({}_u R_q)^r \\ &= \sum_{s=0}^p \binom{p}{s} \frac{[\tau(\vec{k})]!}{[\tau(\vec{k}) - p + s]!} h^{\tau(\vec{k}) - p + s} \left(\frac{\partial}{\partial h} \right)^s ({}_u R_q)^r \end{aligned} \quad (19)$$

and thus

$$\lim_{h \rightarrow 0} L_{p, \tau(\vec{k}), \nu} = \frac{p!}{[p - \tau(\vec{k})]!} \lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^{p - \tau(\vec{k})} ({}_u R_q)^r \quad (20)$$

If $r > 0$, every term in the finite Leibnitz expansion of the above derivative (if $p > \tau(\vec{k})$) will contain ${}_u R_q$ itself (and its derivative) which tend to zero with h . If $r = 0$, the limit is zero unless $p = \tau(\vec{k})$, in which case it is $p!$, as stated previously.

Insertion of these limits in (14) gives

$$\lim_{h \rightarrow 0} \left(\frac{\partial}{\partial h} \right)^p [F(u(z+h)) - F(u(z))] = \frac{d^p G(z)}{dz^p} = p! \sum_{m=0}^q \frac{d^m F(u)}{du^m} \sum_{\substack{k_1 \dots k_q \\ \sigma_q(\vec{k})=m \\ \tau_q(\vec{k})=p}} \frac{1}{k_1! \dots k_q!} B_{\vec{k},q} (u(z)) \quad (21)$$

which is close to (4). However, if $p < q$, then $\tau_q(\vec{k}) = k_1 + 2k_2 + \dots + pk_p + (p+1)k_{p+1} + \dots + qk_q = p$ implies that in the summation, all indices k_{p+1}, \dots, k_q must be zero. For if any of them is non-zero, $\tau_q(\vec{k})$ will exceed p . This adjustment in the summation limits and indices from q to p converts (21) into (4). The proof can now be modified for the multivariable situation.

4. Multivariable Bruno Formulas - Two Variable Proof

The basic first order multivariable chain rule formula for $G(\vec{z}) = F(\vec{u}(\vec{z}))$, with scalar F , where $\vec{u}(\vec{z}) = (u_1(\vec{z}), \dots, u_M(\vec{z}))$ and $\vec{z} = (z_1, \dots, z_N)$, is of course

$$\frac{\partial G}{\partial z_k} = \sum_{j=1}^M \frac{\partial F(\vec{u})}{\partial u_j} \frac{\partial u_j(\vec{z})}{\partial z_k} = (D_{\vec{u}}) (D_{\vec{z}} \vec{u})_{\bullet k} \quad (22)$$

or just

$$D_{\vec{z}} G = (D_{\vec{u}}) (D_{\vec{z}} \vec{u}) \quad (23)$$

where $(D_{\vec{z}} \vec{u})_{\bullet k}$ is the k th column of the $(M \times N)$ first derivative matrix, $D_{\vec{z}} \vec{u}$.

If \vec{F} is a L -component vector of functions, then $D_{\vec{u}} \vec{F}$ is an $L \times M$ matrix, and in matrix form the first order chain rule is again

$$D_{\vec{z}} \vec{G} = \left(D_{\vec{u}} \vec{F} \right) (D_{\vec{z}} \vec{u}) \Big|_{\vec{u}=\vec{u}(\vec{z})} \quad (24)$$

The formulas (23) and (24) can be iterated by symbolic computation to produce all partial derivatives of the form

$$\frac{\partial^{i_1}}{\partial z_1^{i_1}} \frac{\partial^{i_2}}{\partial z_2^{i_2}} \dots \frac{\partial^{i_N}}{\partial z_N^{i_N}} \vec{G}(\vec{z}) = D_{\vec{z}}^{\vec{i}} \vec{G}, \quad \text{where } \vec{i} = (i_1, i_2, \dots, i_N) \quad (25)$$

A few programming tricks can help considerably in producing convenient print-outs. This approach will be discussed in Section 4, following a derivation of a condensed form of the result, resembling (4), from the Taylor expansion with integral remainder method of Section 2, limited to the case $M = N = 2$ with a scalar F , so that $G(z_1, z_2) = F(u_1(z_1, z_2), u_2(z_1, z_2))$, the basic two-dimensional scalar version of the Bruno problem. This result, of some interest for its exact combinatorial form, is useful in checking that a symbolic program is producing the right numerical coefficients as well as the right algebraic expressions. The general M, N case is similar, and the results will be merely described.

The obvious application of the 2×2 case for derivative orders $p = 2, 3, 4$ is to physically meaningful two-dimensional Laplacians, and to curls and repeated curls. For orthogonal coordinates, such as polar, confocal, elliptic, the results are well-known and more easily found by variational integral methods. When coordinates are significantly non-orthogonal or non-conformal, or only isolated partial derivatives are needed, an approach by computer iteration or -as detailed here- by Taylor series plus coefficient matching, appears preferable to Königsberger or Dieudonné methods.

The first stage is to obtain a "double integral" remainder form for a double Taylor expansion. Let

$$f(z_1 + h_1, z_2 + h_2) = \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{h_1^{m_1} h_2^{m_2}}{m_1! m_2!} D_{\vec{z}}^{\vec{m}} f(\vec{z}) + R_{q_1, q_2} \quad (26)$$

where the form of R_{q_1, q_2} is to be determined. If f has the product form $f_0(z_1, z_2) = f_1(z_1)f_2(z_2)$, then

$$\begin{aligned}
& f_0(z_1 + h_1, z_2 + h_2) = f_1(z_1 + h_1)f_2(z_2 + h_2) \\
& = \left(\sum_{m_1=0}^{q_1} \frac{h_1^{m_1}}{m_1!} D_{z_1}^{m_1} f_1(z_1) + R_{q_1}(D_{z_1}^{q_1+1} f_1, z_1, h_1) \right) \left(\sum_{m_2=0}^{q_2} \frac{h_2^{m_2}}{m_2!} D_{z_2}^{m_2} f_2(z_2) + R_{q_2}(D_{z_2}^{q_2+1} f_2, z_2, h_2) \right) \\
& = \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{h_1^{m_1} h_2^{m_2}}{m_1! m_2!} D_{z_1, z_2}^{m_1, m_2} f_0(z_1, z_2) \\
& \quad + \sum_{m_1=0}^{q_1} \frac{h_1^{m_1}}{m_1!} D_{z_1}^{m_1} f_1(z_1) \bullet \frac{1}{q_2!} \int_{z_2}^{z_2+h_2} (z_2 + h_2 - y_2)^{q_2} D_{y_2}^{q_2+1} f_2(y_2) dy_2 \\
& \quad + \sum_{m_2=0}^{q_2} \frac{h_2^{m_2}}{m_2!} D_{z_2}^{m_2} f_2(z_2) \bullet \frac{1}{q_1!} \int_{z_1}^{z_1+h_1} (z_1 + h_1 - y_1)^{q_1} D_{y_1}^{q_1+1} f_1(y_1) dy_1 \\
& \quad + \frac{1}{q_1! q_2!} \int_{z_1}^{z_1+h_1} \int_{z_2}^{z_2+h_2} (z_1 + h_1 - y_1)^{q_1} (z_2 + h_2 - y_2)^{q_2} D_{y_1, y_2}^{q_1+1, q_2+1} f_0(y_1, y_2) dy_1 dy_2
\end{aligned} \tag{27}$$

from the integral remainder formula for functions of one variable. Since

$$D_{z_1}^{m_1} f_1(z_1) D_{y_2}^{q_2+1} f_2(y_2) = D_{z_1, y_2}^{m_1, q_2+1} f_0(z_1, y_2) \tag{28}$$

and

$$D_{z_2}^{m_2} f_2(z_2) D_{y_1}^{q_1+1} f_1(y_1) = D_{y_1, z_2}^{q_1+1, m_2} f_0(y_1, z_2) \tag{29}$$

the remainder can be written as

$$\begin{aligned}
R_{q_1, q_2}(f) &= \frac{1}{q_2!} \sum_{m_1=0}^{q_1} \int_{z_2}^{z_2+h_2} \frac{h_1^{m_1}}{m_1!} (z_2 + h_2 - y_2)^{q_2} D_{z_1, y_2}^{m_1, q_2+1} f(z_1, y_2) dy_2 \\
& \quad + \frac{1}{q_1!} \sum_{m_2=0}^{q_2} \int_{z_1}^{z_1+h_1} \frac{h_2^{m_2}}{m_2!} (z_1 + h_1 - y_1)^{q_1} D_{y_1, z_2}^{q_1+1, m_2} f(y_1, z_2) dy_1 \\
& \quad + \frac{1}{q_1! q_2!} \int_{z_1}^{z_1+h_1} \int_{z_2}^{z_2+h_2} (z_1 + h_1 - y_1)^{q_1} (z_2 + h_2 - y_2)^{q_2} D_{y_1, y_2}^{q_1+1, q_2+1} f(y_1, y_2) dy_1 dy_2
\end{aligned} \tag{30}$$

for $f = f_0$. Clearly, (30) contains two simple sums of single integrals of mixed derivatives and one double integral of mixed derivatives, which holds when f is multiplicatively separable and $\frac{\partial^{q_1+1+q_2+1} f}{\partial z_1^{q_1+1} \partial z_2^{q_2+1}}$ is continuous jointly in z_1 and z_2 . Note that for $q_1 = q_2 = 0$, formula (30) reduces to

$$R_{00} = \int_{z_1}^{z_1+h_1} \frac{\partial f(y_1, z_2)}{\partial y_1} dy_1 + \int_{z_2}^{z_2+h_2} \frac{\partial f(z_1, y_2)}{\partial y_2} dy_2 + \int_{z_1}^{z_1+h_1} \int_{z_2}^{z_2+h_2} \frac{\partial^2 f(y_1, y_2)}{\partial y_1 \partial y_2} dy_1 dy_2 \tag{31}$$

where hopefully

$$f(z_1 + h_1, z_2 + h_2) = f(z_1, z_2) + R_{00} \tag{32}$$

for non-multiplicative functions f . For $h_1 = h_2 = 0$, (31) holds for all f such that $\frac{\partial^2 f(y_1, y_2)}{\partial y_1 \partial y_2}$ is continuous. Fixing h_2 ,

$$\begin{aligned}
\frac{\partial R_{00}}{\partial h_1} &= \left. \frac{\partial f}{\partial y_1}(y_1, y_2) \right|_{y_1=z_1+h_1} + \int_{z_2}^{z_2+h_2} \frac{\partial^2 f(y_1, y_2)}{\partial y_1 \partial y_2} dy_2 \Big|_{y_1=z_1+h_1} \\
&= \left. \frac{\partial f}{\partial y_1}(y_1, y_2) \right|_{y_1=z_1+h_1} + \left[\frac{\partial f}{\partial y_1}(y_1, z_2 + h_2) - \frac{\partial f}{\partial y_1}(y_1, z_2) \right] \Big|_{y_1=z_1+h_1}
\end{aligned}$$

$$= \left. \frac{\partial f}{\partial y_1}(y_1, z_z + h) \right|_{y_1=z_1+h_1} \quad (33)$$

and similarly

$$\frac{\partial R_{00}}{\partial h_2} = \left. \frac{\partial f}{\partial y_2}(z_1 + h_1, y_2) \right|_{y_2=z_2+h_2} \quad (34)$$

Consequently,

$$\begin{aligned} \left(\frac{\partial}{\partial h_1} \right)^{k_1} \left(\frac{\partial}{\partial h_2} \right)^{k_2} R_{00} &= \left(\frac{\partial}{\partial h_1} \right)^{k_1} \left(\frac{\partial}{\partial h_2} \right)^{k_2} f(z_1 + h_1, z_2 + h_2) \\ &= \left(\frac{\partial}{\partial h_1} \right)^{k_1} \left(\frac{\partial}{\partial h_2} \right)^{k_2} f(y_1, y_2) \Big|_{y_1=z_1+h_1, y_2=z_2+h_2} \end{aligned} \quad (35)$$

if $k_1 + k_2 > 0$, and the requisite derivatives exist finitely. It follows that $f(z_1 + h_1, z_2 + h_2) = f(z_1, z_2) + R_{00}$ as hoped. Taking this as the starting point of a double induction, whose inductive hypothesis is the validity of (30) for a general f such that $\frac{\partial^{q_1+1+q_2+1} f}{\partial z_1^{q_1+1} \partial z_2^{q_2+1}}$ is jointly continuous, application of (30) to $\frac{\partial f}{\partial z_1}$, $\frac{\partial f}{\partial z_2}$, and $\frac{\partial^2 f}{\partial z_1 \partial z_2}$ yields (30) for f with orders $(q_1 + 1, q_2)$, $(q_1, q_2 + 1)$, and $(q_1 + 1, q_2 + 1)$. This establishes the desired double induction on f , and with it a Taylor series integral remainder formula for functions of two variables which the writers have not seen elsewhere. Application of $\left(\frac{\partial}{\partial h_1} \right)^{p_1} \left(\frac{\partial}{\partial h_2} \right)^{p_2}$ to LR_{q_1, q_2} for $p_1 \leq q_1$, $p_2 \leq q_2$ and fairly general L shows as in Section 2 that

$$\lim_{h_1 \rightarrow 0, h_2 \rightarrow 0} \left(\frac{\partial}{\partial h_1} \right)^{p_1} \left(\frac{\partial}{\partial h_2} \right)^{p_2} LR_{q_1, q_2} = 0 \quad (36)$$

This is applicable to remainders of $F(u_1, u_2)$ and of $u_1(z_1, z_2)$ and $u_2(z_1, z_2)$, provided that $\frac{\partial^{q_1+q_2+2} F(u_1, u_2)}{\partial u_1^{q_1+1} \partial u_2^{q_2+1}}$ and $\frac{\partial^{q_1+q_2+2} u_i(z_1, z_2)}{\partial z_1^{q_1+1} \partial z_2^{q_2+1}}$ are jointly continuous functions of their two arguments. Having gained the desired integral remainder theorems, the rest of the proof is straight forward.

Suppose $F(u_1, u_2)$, $u_1(z_1, z_2)$, and $u_2(z_1, z_2)$ are approximated to order (q_1, q_2) . Then if $j_s = u_s(\vec{z} + \vec{h}) - u_s(\vec{z})$ for $s = 1, 2$, and ${}_F R_{q_1, q_2}$ and ${}_{u_s} R_{q_1, q_2}$ are the ‘‘integral remainders’’ exhibited in (30) for $f = F, u_1, u_2$.

$$\begin{aligned} F(\vec{u} + \vec{j}) &= F(u_1(z_1 + h_1, z_2 + h_2), u_2(z_1 + h_1, z_2 + h_2)) \\ &= \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{j_1^{m_1} j_2^{m_2}}{m_1! m_2!} D_{\vec{u}}^{\vec{m}} F + {}_F R_{q_1, q_2}(\vec{u}, \vec{j}) \\ &= \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{D_{\vec{u}}^{\vec{m}} F}{m_1! m_2!} \left(\sum_{n_1=1}^{q_1} \sum_{n_2=1}^{q_2} \frac{h_1^{n_1} h_2^{n_2}}{n_1! n_2!} D_{\vec{z}}^{\vec{n}} u_1 + u_1 R_{q_1, q_2}(\vec{z}, \vec{h}) \right)^{m_1} \\ &\quad \cdot \left(\sum_{n_1=1}^{q_1} \sum_{n_2=1}^{q_2} \frac{h_1^{n_1} h_2^{n_2}}{n_1! n_2!} D_{\vec{z}}^{\vec{n}'} u_2 + u_2 R_{q_1, q_2}(\vec{z}, \vec{h}) \right)^{m_2} + {}_F R_{q_1, q_2}(\vec{u}, \vec{j}) \end{aligned} \quad (37)$$

Now,

$$\begin{aligned} &\left(\sum_{n_1=1}^{q_1} \sum_{n_2=1}^{q_2} \frac{h_1^{n_1} h_2^{n_2}}{n_1! n_2!} D_{\vec{z}}^{\vec{n}} u_1 + u_1 R_{q_1, q_2}(\vec{z}, \vec{h}) \right)^{m_1} \\ &= \sum_{t_1=0}^{m_1} \sum_{\substack{\vec{s} \\ \sigma(\vec{s})=m_1-t_1}} \binom{m_1}{\vec{s} \quad t_1} \prod_{n_1=1}^{q_1} \prod_{n_2=1}^{q_2} \left(\frac{h_1^{n_1} h_2^{n_2}}{n_1! n_2!} D_{\vec{z}}^{\vec{n}} u_1 \right)^{s_{\vec{n}}} \left(u_1 R_{q_1, q_2}(\vec{z}, \vec{h}) \right)^{t_1} \end{aligned} \quad (38)$$

where the \vec{s} summation is over double sequences $s_{n_1, n_2} = \vec{s}_{\vec{n}}$, for $n_1 = 1, 2, \dots, q_1$, $n_2 = 1, 2, \dots, q_2$ (since $N = 2$). Thus \vec{s} maps $A_2 = \{1, 2, \dots, q_1\} \times \{1, 2, \dots, q_2\}$ onto $\{0, 1, \dots, m_1\}$, such that $\sigma(\vec{s}) = \sum_{\vec{n}} s_{\vec{n}} = m_1 - t_1$. The symbol $\binom{m_1}{\vec{s}} = \frac{m_1!}{t_1! \prod_{\vec{n} \in A_2} s_{\vec{n}}!}$. A like formula holds for $j_2^{m_2}$. Combining that with (37) and (38) yields

$$F(\vec{u} + \vec{j}) = \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{D_{\vec{u}}^{\vec{m}} F}{m_1! m_2!} \sum_{t_1=0}^{m_1} \sum_{t_2=0}^{m_2} \sum_{\substack{\vec{s} \\ \sigma(\vec{s})=m_1-t_1}} \sum_{\substack{\vec{s}' \\ \sigma(\vec{s}')=m_2-t_2}} \binom{m_1}{\vec{s}} \binom{m_2}{\vec{s}'} h_1^{\tau_1} h_2^{\tau_2} \\ \bullet \prod_{\vec{n} \in A_2} \left(\frac{D_{\vec{z}}^{\vec{n}} u_1}{n_1! n_2!} \right)^{s_{\vec{n}}} \prod_{\vec{n}' \in A_2} \left(\frac{D_{\vec{z}'}^{\vec{n}'} u_2}{n_1'! n_2'!} \right)^{s_{\vec{n}'}} (u_1 R_{q_1, q_2})^{t_1} (u_2 R_{q_1, q_2})^{t_2} + {}_F R_{q_1, q_2} \quad (39)$$

where

$$\tau_j = \tau_j(\vec{s}, \vec{s}') = \sum_{\vec{n} \in A_2} n_j s_{\vec{n}} + \sum_{\vec{n}' \in A_2} n_j' s_{\vec{n}'}, \quad j = 1, 2 \quad (40)$$

and $A_2 = \{0, 1, \dots, q_1\} \times \{0, 1, \dots, q_2\}$ (or a suitable subset of it). On taking

$$\lim_{h_1 \rightarrow 0} \lim_{h_2 \rightarrow 0} \frac{\partial^{p_1+p_2} F(\vec{u} + \vec{j}(\vec{z}, \vec{h}))}{\partial h_1^{p_1} \partial h_2^{p_2}} \quad (41)$$

all terms in (39) with $t_1 > 0$ or $t_2 > 0$ tend to zero, as does ${}_F R_{q_1, q_2}$, by iteration of the calculations (11–20) in Section 2. Also, the entry $m_1 = m_2 = 0$ in (39) does not contribute to this limiting derivative, (41). The remaining terms produce, again as in Section 2,

$$\frac{\partial^{p_1+p_2} G(\vec{z})}{\partial z_1^{p_1} \partial z_2^{p_2}} = p_1! p_2! \sum_{m_1=0}^{q_1} \sum_{m_2=0}^{q_2} \frac{D_{\vec{u}}^{\vec{m}} F}{m_1! m_2!} \sum_{\vec{s}} \sum_{\vec{s}'} \binom{m_1}{\vec{s}} \binom{m_2}{\vec{s}'} \prod_{\vec{n} \in A_2} \left(\frac{D_{\vec{z}}^{\vec{n}} u_1}{n_1! n_2!} \right)^{s_{\vec{n}}} \prod_{\vec{n}' \in A_2} \left(\frac{D_{\vec{z}'}^{\vec{n}'} u_1}{n_1'! n_2'!} \right)^{s_{\vec{n}'}} \quad (42)$$

with $m_1 \cdot m_2 \neq 0$, $\sigma(\vec{s}) = m_1$, $\sigma(\vec{s}') = m_2$, and where $\tau_1(\vec{s}, \vec{s}') = p_1$, $\tau_2(\vec{s}, \vec{s}') = p_2$ couple the pair of double sequences \vec{s}, \vec{s}' through the definition (40). The only surprise is that both of the τ conditions depend on two sequences jointly, greatly complicating the results. The entry $\vec{m} = (0, 0)$ must be omitted from the summation in (41).

The extension to vector \vec{F} and \vec{G} is as in Section 2. As before, the indices q_1, q_2 can be replaced in (42) in the transition from (21) to (4), by p_1, p_2 , and the domain A_2 of \vec{s} and \vec{s}' is then $\{0, 1, \dots, p_1\} \times \{0, 1, \dots, p_2\}$ instead of $\{0, 1, \dots, q_1\} \times \{0, 1, \dots, q_2\}$, when calculating derivatives of order (p_1, p_2) . From (42) it is easy to guess the correct Bruno formulas for $D_{\vec{z}}^{\vec{p}} G(\vec{z}) = D_{\vec{z}}^{\vec{p}} F(\vec{u}(\vec{z}))$ where $\vec{p} = (p_1, \dots, p_N)$, $\vec{z} = (z_1, \dots, z_N)$, $\vec{u}(\vec{z}) = (u_1(\vec{z}), \dots, u_M(\vec{z}))$, and F, M, N are arbitrary.

Briefly, describing Bruno formulas for functions of, say four variables, there are four single summations and four quadruple summations, limited by eight conditions, four of which are fully cross-coupled. There are Taylor-like terms on the outside function, four generalized binomial coefficients, and four sets of Bruno products, each formed over a quadruple cartesian product of indices. All of this goes to calculate a single partial derivative by the chain rule.

5. Symbolic Computing Aspects

The use of a symbolic manipulator, such as Maple or Macsyma, can easily produce higher-order differential results. However, it achieves these results by recursively applying a chain rule. While this is entirely correct, the outputs are often quite messy and further manipulation is needed to simplify the results. If only a select number of terms are needed, one then has to go back and try to weed out such terms. But utilizing the Bruno formulas, one can easily isolate the needed terms, and they are already simplified.

As an example, a double vector laplacian was performed using the Bruno formulas and again by brute

force (i.e. by recursive application of the chain rule). The Bruno results were fairly clean and organized, while the brute force outputs had to be tediously manipulated to reproduce the same results. An additional advantage is that the Bruno formulas can be written in a clean, closed-form notation that can be partially manipulated before the need to evaluate them.

The double vector laplacian was computed using Macsyma since the functional dependencies can be suppressed (this is only for compactness of notation purposes). Once all the dependencies are set up (using subscripted variables, say (x_1, x_2, x_3) , instead of variables with different labels, say (x, y, z) , of course) it is just a matter of implementing (42). Some care must be taken to make sure the conditions $\sigma(\vec{s}) = m_1$, $\sigma(\vec{s}^{\prime}) = m_2$, $\tau_1(\vec{s}, \vec{s}^{\prime}) = p_1$, and $\tau_2(\vec{s}, \vec{s}^{\prime}) = p_2$ are satisfied. One approach to solve this problem is to sum over all possible indices and introduce coefficients that have the value of one when they are satisfied and zero when the conditions are not satisfied.

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