A few calculus rules for chain differentials

Article · June 2015

Source: arXiv

3 authors:

Daniel Clark
Institut Mines-Télécom

Jeremie Houssineau
The University of Warwick

Emmanuel Delande
Heriot-Watt University

A few calculus rules for chain differentials

D. E. Clark, J. Houssineau, E. D. Delande

Abstract

This paper summarizes the core definitions and results regarding the chain differential for functions in locally convex topological vector spaces. In addition, it provides a few elementary calculus rules of practical interest, notably for the differentiation of characteristic functionals in various domains of physical science and engineering.

1 Functional differentiation

In this section we discuss two different forms of differential, the Gâteaux differential [5] and the chain differential [2]. The chain differential, which is similar to the epiderivative [1], is adopted since it is possible to determine a chain rule, yet is not as restrictive as the Fréchet derivative.

Results are stated for *locally convex topological vector spaces* which include Banach spaces such as Hilbert and Euclidean spaces, e.g., $\mathbb{R}^n$, as well as spaces of test functions for the study of distributions. This type of space is therefore sufficiently general for most practical applications.

1.1 Gâteaux differential

Definition 1 (Gâteaux differential)**.** *Let X and Y be locally convex topological vector spaces, and let Ω be an open subset of X and let $f : \Omega \to Y$. The Gâteaux differential at $x \in \Omega$ in the direction $\eta \in X$ is*

$$\delta f(x;\eta) := \lim_{\epsilon \to 0} \frac{1}{\epsilon}\big(f(x+\epsilon\eta) - f(x)\big) \tag{1}$$

when the limit exists. If $\delta f(x;\eta)$ exists for all $\eta \in X$ then f is Gâteaux differentiable at x. The Gâteaux differential is homogeneous of degree one in η, so that for all real numbers α, $\delta f(x;\alpha\eta) = \alpha\delta f(x;\eta)$.

In Definition 1, the space X might be a function space. In this case, functions on X can be referred to as *functionals*.

1.2 Chain differential

Due to the lack of continuity properties of the Gâteaux differential, further constraints are required in order to derive a chain rule. Bernhard [2] proposed a new form of Gâteaux differential defined with sequences, which he called the chain differential. It is not as restrictive as the Fréchet derivative though it is still possible to find a chain rule that maintains the general structure.

Definition 2 (Chain differential)**.** *The function $f : X \to Y$, where X and Y are locally convex topological vector spaces, has a* chain differential *$\delta f(x;\eta)$ at point $x \in X$ in the direction $\eta \in X$ if, for any sequence $\eta_m \to \eta \in X$, and any sequence of real numbers $\theta_m \to 0$, it holds that the following limit exists*

$$\delta f(x;\eta) := \lim_{m\to\infty} \frac{1}{\theta_m}\big(f(x+\theta_m\eta_m) - f(x)\big). \tag{2}$$

If $X = X_1 \times \ldots \times X_n$, where $\{X_i\}_{i=1}^n$ are locally convex topological vector spaces, $\boldsymbol{x} := (x_1,\ldots,x_n) \in X$, and $\boldsymbol{\eta} := (\eta_1,\ldots,\eta_n) \in X$, the chain differential $\delta f(\boldsymbol{x};\boldsymbol{\eta})$, if it exists, is also called the total chain differential *of f at point $\boldsymbol{x}$ in the direction $\boldsymbol{\eta}$.*

Definition 3 (n^{th}-order chain differential)**.** *The* n^{th}-order chain differential *of f at point x in the sequence of directions $(\eta_i)_{i=1}^n$, is defined recursively with*

$$\delta^n f\big(x; (\eta_i)_{i=1}^n\big) := \delta\big(y \mapsto \delta^{n-1} f(y; (\eta_i)_{i=1}^{n-1})\big)(x; \eta_n). \tag{3}$$

For the sake of simplicity, when there is no ambiguity on the point at which the chain differential is evaluated, the chain differential $\delta f(x;\eta)$ may also be written as $\delta(f(x);\eta)$. The n^{th}-order chain differential (3) then takes the more compact form

$$\delta^n f\big(x; (\eta_i)_{i=1}^n\big) := \delta\big(\delta^{n-1} f(x; (\eta_i)_{i=1}^{n-1}); \eta_n\big). \tag{4}$$

Similarly to the notion of partial derivatives, the notion of chain differential can be defined for appropriate multivariate functions.

Definition 4 (Partial chain differential)**.** *Let $\{X_i\}_{i=1}^n$ and Y be locally convex topological vector spaces. The function $f : X_1 \times \ldots \times X_n \to Y$ has a* partial chain differential $\delta_i f(\boldsymbol{x};\eta)$ *with respect to the i^{th} variable, at point $\boldsymbol{x} = (x_1, \ldots, x_n) \in X_1 \times \ldots \times X_n$ in the direction $\eta \in X_i$ if, for any sequence $\eta_m \to \eta \in X_i$, and any sequence of real numbers $\theta_m \to 0$, it holds that the following limit exists*

$$\delta_i f(\boldsymbol{x};\eta) := \lim_{m\to\infty} \frac{1}{\theta_m}\big(f(x_1, \ldots, x_i + \theta_m \eta_m, \ldots, x_n) - f(\boldsymbol{x})\big). \tag{5}$$

2 Core calculus rules for the chain differential

This section summarises the core derivation rules for the chain differential. Note that they all have a counterpart defined for the usual derivative.

Lemma 1 (Chain rule, from [2], Theorem 1)**.** *Let X, Y and Z be locally convex topological vector spaces, $f : Y \to Z$, $g : X \to Y$ and g and f have chain differentials at x in the direction η and at $g(x)$ in the direction $\delta g(x;\eta)$ respectively. Then the composition $f \circ g$ has a chain differential at point x in the direction η, given by the chain rule*

$$\delta(f \circ g)(x;\eta) = \delta f\big(g(x); \delta g(x;\eta)\big). \tag{6}$$

Note that, unlike its counterpart for the usual derivative, the chain differential of a composition $f \circ g$ does *not* reduce to the product of a chain differential of f and a chain differential of g. This key difference has important implications on the structure of the general higher-order chain rule in Theorem 2.

Similarly to the usual derivatives, the total chain differential of a multivariate function (see Definition 2) can be constructed, in certain conditions defined in the theorem below, as a sum involving its partial chain differentials (see Definition 4).

Theorem 1 (Total chain differential, from [3], Theorem 1)**.** *Let $\{X_i\}_{i=1}^n$ and Y be locally convex topological vector spaces, $f : X_1 \times \ldots \times X_n \to Y$, $\boldsymbol{x} \in X_1 \times \ldots \times X_n$ and $\boldsymbol{\eta} := (\eta_1, \ldots, \eta_n) \in X_1 \times \ldots \times X_n$. If, for $1 \le i \le n$, it holds that*

1. *the partial chain differential $\delta_i f$ exists in a neighbourhood $\Omega \subseteq X_1 \times \ldots \times X_n$ of $\boldsymbol{x}$, and,*
2. *the function $(x,\eta) \mapsto \delta_i f(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n; \eta)$ is continuous over $\Omega \times X_i$,*

then f has a total chain differential at point $\boldsymbol{x}$ in the direction $\boldsymbol{\eta}$, and it is given by

$$\delta f(\boldsymbol{x};\boldsymbol{\eta}) = \sum_{i=1}^{n} \delta_i f(\boldsymbol{x};\eta_i). \tag{7}$$

The proof is given in appendix in Section A.1. This intermediary result is an important component in the construction of the general higher-order chain rule in Theorem 2.

Theorem 2 (General higher-order chain rule, from [3], Theorem 2)**.** *Let X, Y and Z be locally convex topological vector spaces, and $f : Y \to Z$. Assume that $g : X \to Y$ has higher order chain differentials at point x in all the sequences of directions $(\eta_i)_{i\in I}$, $I \subseteq \{1,\dots,n\}$. Assume additionally that there exists an open subset $\Omega \subseteq Y$ such that $g(x) \in \Omega$ and $\delta^{|I|}g(x;(\eta_i)_{i\in I}) \in \Omega$, $I \subseteq \{1,\dots,n\}$. If, for every point $y \in \Omega$ and every sequence $(\xi_i)_{i=1}^m \in \Omega^m$, $1 \leq m \leq n$, it holds that*

1. *f has a m^{th}-order chain differential at point y in the sequence of directions $(\xi_i)_{i=1}^m$, and,*
2. *the conditions of Theorem 1 hold for the function $(y,\xi_1,\dots,\xi_m) \mapsto \delta^m f(y;(\xi_i)_{i=1}^m)$,*
3. *the functions $\xi_j \mapsto \delta^m f(y;(\xi_i)_{i=1}^m)$, $1 \leq j \leq m$, are linear and continuous on Ω,*

then the n^{th}-order chain differential of the composition $f \circ g$ at point x in the sequence of directions $(\eta_i)_{i=1}^n$ is given by

$$\delta^n(f\circ g)(x;(\eta_i)_{i=1}^n) = \sum_{\pi\in\Pi_n} \delta^{|\pi|} f\Big(g(x);\big(\delta^{|\omega|}g(x;(\eta_i)_{i\in\omega})\big)_{\omega\in\pi}\Big), \tag{8}$$

where $\Pi_n := \Pi(\{1,\dots,n\})$ denotes the set of the partitions of the index set $\{1,\dots,n\}$, and $|\pi|$ denotes the cardinality of the set π.

The proof is given in appendix in Section A.2. The counterpart for usual derivatives is known as Fàa di Bruno's rule [4].

Theorem 3 (General higher-order product rule)**.** *Let X and Y be locally convex topological vector spaces and let $g : X \to Y$ and $z : X \to Y$. Assuming that f and g have higher order chain differentials at point x in all the sequences of directions $(\eta_i)_{i\in I}$, $I \subseteq \{1,\dots,n\}$, then the product $f \cdot g$ has a n^{th}-order chain differential at point x in the sequence of directions $(\eta_i)_{i=1}^n$, and it is given by*

$$\delta^n(f\cdot g)(x;(\eta_i)_{i=1}^n) = \sum_{\pi\subseteq\{1,\dots,n\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-|\pi|}g(x;(\eta_i)_{i\in\pi^c}) \tag{9}$$

where $\pi^c := \{1,\dots,n\}\setminus\pi$ denotes the complement of π in $\{1,\dots,n\}$.

The proof is given in appendix in Section A.3. The counterpart for usual derivatives is known as Leibniz' rule.

3 Practical derivations for the chain rule

This section provides specific applications of the chain rule given in Lemma 1 in which the outer function of the composition $f \circ g$ assumes a specific form, commonly encountered in practical derivations.

Theorem 4 (Practical derivations for the chain rule)**.** *Let X, Y and Z be locally convex topological vector spaces, $f : Y \to Z$, $g : X \to Y$. Assume additionally that g has a chain differential at some point x in some direction η. Then:*

a) if f is a continuous linear function ℓ, then the composition $f \circ g$ has a chain differential at point x in the direction η, and it is given by

$$\delta(\ell \circ g)(x;\eta) = \ell\big(\delta g(x;\eta)\big). \tag{10}$$

Leibniz' rule

b) if f is the k^{th} power function $y \mapsto y^k$, $k > 0$, then the composition $f \circ g$ has a chain differential at point x in the direction η, and it is given by

$$\delta\big((y \mapsto y^k) \circ g\big)(x;\eta) = k\big(g(x)\big)^{k-1}\delta g(x;\eta). \tag{11}$$

c) if f is the exponential function exp*, then the composition $f \circ g$ has a chain differential at point x in the direction η, and it is given by*

$$\delta(\exp \circ g)(x;\eta) = \exp\big(g(x)\big)\delta g(x;\eta). \tag{12}$$

The proof is given in appendix in Section A.4.

Appendix A Proofs

A.1 Total chain differential (Theorem 1)

Proof. The result is proved in the case $n = 2$ from which the general case can be straightforwardly deduced. Let us fix a point $\boldsymbol{x} = (x, y) \in X_1 \times X_2$ and a direction $\boldsymbol{\eta} = (\eta, \xi) \in X_1 \times X_2$, such that f has partial chain differentials $\delta_1 f(\boldsymbol{x};\eta)$ and $\delta_2 f(\boldsymbol{x};\xi)$. Let us then fix arbitrary sequences of directions $\eta_m \to \eta \in X_1$, $\xi_m \to \xi \in X_2$, and an arbitrary sequence of real numbers $\theta_m \to 0$. For $m \leq 0$ we can write

$$\begin{aligned}\theta_m^{-1}\big[f(\boldsymbol{x} + \theta_m\boldsymbol{\eta}) - f(\boldsymbol{x})\big] &= \theta_m^{-1}\big[f(x + \theta_m\eta_m, y + \theta_m\xi_m) - f(x,y)\big] && (13a)\\ &= \theta_m^{-1}\big[g_1(y + \theta_m\xi_m) - g_1(y)\big] + \theta_m^{-1}\big[g_2(x + \theta_m\eta_m) - g_2(x)\big], && (13b)\end{aligned}$$

where we define $g_1(y)$ and $g_2(x)$ as follows:

$$\begin{cases} g_1(y) &= f(x + \theta_m\eta_m, y),\\ g_2(x) &= f(x,y). \end{cases} \tag{14}$$

Given $\theta_m \neq 0$, define $h : \mathbb{R} \to \mathbb{R}$ as $h(t) = g_1(y + t\xi_m)$. From the mean value theorem for real-valued functions, there exists $c_y \in [0, \theta_m]$ such that

$$\begin{aligned}\theta_m^{-1}\big[h(\theta_m) - h(0)\big] &= \left.\frac{\mathrm{d}h}{\mathrm{d}t}\right|_{t=c_y} && (15a)\\ &= \delta h(c_y; 1), && (15b)\end{aligned}$$

which, when replacing $h(t)$ by $g_1(y + t\xi_m)$, can be rewritten

$$\begin{aligned}\theta_m^{-1}\big[g_1(y + \theta_m\xi_m) - g_1(y)\big] &= \delta\big(g_1(y + c_y\xi_m); 1\big) && (16a)\\ &= \delta g_1(y + c_y\xi_m; \xi_m), && (16b)\end{aligned}$$

where Lemma 1 has been used to obtain the last equality. Similarly for $g_2(x)$, there exists $c_x \in [0, \theta_m]$ such that

$$\theta_m^{-1}\left[g_2(x + \theta_m\eta_m) - g_2(x)\right] = \delta g_2(x + c_x\eta_m; \eta_m). \tag{17}$$

Let us now prove that the limit of the term

$$\Big|\theta_m^{-1}\big[f(\boldsymbol{x} + \theta_m\boldsymbol{\eta}) - f(\boldsymbol{x})\big] - \delta_1 f(\boldsymbol{x};\eta_m) - \delta_2 f(\boldsymbol{x};\xi_m)\Big| \tag{18}$$

is equal to 0 when $r \to \infty$. Substituting (16b) and (17) into (13b), (18) becomes

$$\big|\delta g_2(x + c_x\eta_m; \eta_m) + \delta g_1(y + c_y\xi_m; \xi_m) - \delta_1 f(\boldsymbol{x}; \eta_m) - \delta_2 f(\boldsymbol{x}; \xi_m)\big|. \tag{19}$$

By the triangle inequality, (19) is bounded above by the following summation

$$\big|\delta g_2(x + c_x\eta_m; \eta_m) - \delta_1 f(\boldsymbol{x}; \eta_m)\big| + \big|\delta g_1(y + c_y\xi_m; \xi_m) - \delta_2 f(\boldsymbol{x}; \xi_m)\big|. \tag{20}$$

Substituting g_1 and g_2 with f, the bound (20) becomes

$$\big|\delta_1 f(x + c_x\eta_m, y; \eta_m) - \delta_1 f(\boldsymbol{x}; \eta_m)\big| + \big|\delta_2 f(x, y + c_y\xi_m; \xi_m) - \delta_2 f(\boldsymbol{x}; \xi_m)\big|, \tag{21}$$

which tends to 0 when $m \to \infty$ because of the continuity of the functions $(z, \nu) \mapsto \delta_1 f(z, y; \nu)$ and $(z, \nu) \mapsto \delta_2 f(x, z; \nu)$. Thus, it holds that

$$\lim_{m\to\infty} \Big|\theta_m^{-1}\big[f(\boldsymbol{x} + \theta_m\boldsymbol{\eta}) - f(\boldsymbol{x})\big] - \delta_1 f(\boldsymbol{x}; \eta_m) - \delta_2 f(\boldsymbol{x}; \xi_m)\Big| = 0, \tag{22}$$

that is, f has a total chain differential in point $\boldsymbol{x}$ in direction $\boldsymbol{\eta}$, and it is such that

$$\delta f(\boldsymbol{x}; \boldsymbol{\eta}) = \delta_1 f(\boldsymbol{x}; \eta) + \delta_2 f(\boldsymbol{x}; \xi), \tag{23}$$

which is equivalent to the Proposition 3 in [2]. □

A.2 General higher-order chain rule (Theorem 2)

Proof. The proof is constructed by induction on the number of directions n. Lemma 1 gives the base case $n = 1$. For the induction step, we apply the differential operator to the case n to give the case $n + 1$ and show that it involves a summation over partitions of elements $\eta_1, \ldots, \eta_{n+1}$ in the following way

$$\delta^{n+1}(f \circ g)(x; (\eta_i)_{i=1}^{n+1}) = \sum_{\pi\in\Pi_n} \delta\Big(u \mapsto \delta^{|\pi|} f\Big(g(u); \big(\delta^{|\omega|} g(u; (\eta_j)_{j\in\omega})\big)_{\omega\in\pi}\Big)\Big)(x; \eta_{n+1}). \tag{24}$$

The main objective in this proof is to calculate a term of the summation on the right-hand side of (24), of the form

$$\delta\Big(u \mapsto \delta^k f\big(g(u); (h_i(u))_{i=1}^k\big)\Big)(x; \eta). \tag{25}$$

The additional differentiation with respect to η applies to every function on X, i.e. to the function g and to the functions h_i, $1 \le i \le k$. To highlight the structure of this result, we can define a multi-variate function F such that

$$\begin{aligned} F: \quad & Y^{k+1} \to Z \\ (y_0, \ldots, y_k) & \mapsto \delta^k f(y_0; (y_i)_{i=1}^k) \end{aligned}, \tag{26}$$

so that (25) can be rewritten as $\delta\Big(F \circ \Big(u \mapsto \big(g(u), h_1(u), \ldots, h_k(u)\big)\Big)\Big)(x; \eta)$, which is equal to

$$\delta F\Big(g(x), h_1(x), \ldots, h_k(x); \delta\Big(u \mapsto \big(g(u), h_1(u), \ldots, h_k(u)\big)\Big)(x; \eta)\Big), \tag{27}$$

using Lemma 1. Let us focus on the direction $\delta\Big(u \mapsto \big(g(u), h_1(u), \ldots, h_k(u)\big)\Big)(x; \eta)$ in (27). Let us define a sequence $\eta_m \to \eta \in X$ and a sequence of real numbers $\theta_m \to 0$. Using the definition of the chain differential (2), we can write

$$\begin{aligned} &\delta\Big(u \mapsto \big(g(u), h_1(u), \ldots, h_k(u)\big)\Big)(x; \eta) \\ &= \lim_{m\to\infty} \theta_m^{-1}\Big[\big(g(x + \theta_m\eta_m), h_1(x + \theta_m\eta_m), \ldots, h_k(x + \theta_m\eta_m)\big) - \big(g(x), h_1(x), \ldots, h_k(x)\big)\Big] && \text{(28a)} \\ &= \big(\delta g(x; \eta), \delta h_1(x; \eta), \ldots, \delta h_k(x; \eta)\big), && \text{(28b)} \end{aligned}$$

where the last equality is given by the definition of the chain differential (2) applied to the functions g and h_i, $1 \leq i \leq k$. Substituting (28b) into (27) and applying Theorem 1, (25) becomes

$$\delta_1 F\big(g(x), h_1(x), \ldots, h_k(x); \delta g(x;\eta)\big) + \sum_{i=1}^{k} \delta_{i+1} F\big(g(x), h_1(x), \ldots, h_k(x); \delta h_i(x;\eta)\big). \tag{29}$$

- Consider the first term of the summation in (29):

$$\delta_1 F\big(g(x), h_1(x), \ldots, h_k(x); \delta g(x;\eta)\big). \tag{30}$$

  Using the definition of F, it can be written as $\delta\Big(y \mapsto \delta^k f\big(y; (h_i(x))_{i=1}^k\big)\Big)\big(g(x); \delta g(x;\eta)\big)$, which is equal to

$$\delta^{k+1} f\big(g(x); h_1(x), \ldots, h_k(x), \delta g(x;\eta)\big), \tag{31}$$

  by definition of the $(k+1)^{th}$-order chain differential.

- Now consider any other term in (29):

$$\delta_{i+1} F\big(g(x), h_1(x), \ldots, h_k(x); \delta h_i(x;\eta)\big). \tag{32}$$

  Using the definition of F, it can be written as

$$\delta\Big(y \mapsto \delta^k f\big(g(x); h_1(x), \ldots, y, \ldots, h_k(x)\big)\Big)\big(h_i(x); \delta h_i(x;\eta)\big). \tag{33}$$

  Let us define a sequence $\nu_m \to \delta h_i(x;\eta) \in Y$ and a sequence of real numbers $\theta_m \to 0$. Using the definition of the chain differential (2), (33) becomes

$$\lim_{m\to\infty} \theta_m^{-1}\Big[\delta^k f\big(g(x); h_1(x), \ldots, h_i(x) + \theta_m \nu_m, \ldots, h_1(x)\big) - \delta^k f\big(g(x); h_1(x), \ldots, h_i(x), \ldots, h_1(x)\big)\Big]$$
$$= \lim_{m\to\infty} \delta^k f\big(g(x); h_1(x), \ldots, \nu_m, \ldots, h_1(x)\big) \tag{34a}$$
$$= \delta^k f\big(g(x); h_1(x), \ldots, \delta h_i(x;\eta), \ldots, h_1(x)\big), \tag{34b}$$

  while the first equality exploits the linearity of the function $y \mapsto \delta^k f\big(g(x); h_1(x), \ldots, y, \ldots, h_k(x)\big)$, and the second equality its continuity on Ω.

Substituting (31) and (34b) in (29), (25) becomes

$$\delta^{k+1} f\big(g(x); h_1(x), \ldots, h_k(x), \delta g(x;\eta)\big) + \sum_{i=1}^{k} \delta^k f\big(g(x); h_1(x), \ldots, \delta h_i(x;\eta), \ldots, h_1(x)\big). \tag{35}$$

Considering $\eta := \eta_{n+1}$ and $h_i(x) := \delta^{|\omega_i|} g\big(x; (\eta_j)_{j\in\omega_i}\big)$ and replacing the result (35) into (24), we find

$$\delta^{n+1}(f \circ g)(x; (\eta_i)_{i=1}^{n+1})$$
$$= \sum_{\pi\in\Pi_n} \delta^{|\pi|+1} f\Big(g(x); \big(\delta^{|\omega|} g(x; (\eta_j)_{j\in\omega})\big)_{\omega\in\pi\cup\{\{n+1\}\}}\Big)$$
$$+ \sum_{\pi\in\Pi_n} \sum_{\nu\in\pi} \delta^{|\pi|} f\Big(g(x); \big(\delta^{|\omega|} g(x; (\eta_j)_{j\in\omega})\big)_{\omega\in\pi\setminus\{\nu\}\cup\{\nu\cup\{n+1\}\}}\Big) \tag{36a}$$
$$= \sum_{\pi\in\Pi_{n+1}} \delta^{|\pi|} f\Big(g(x); \big(\delta^{|\omega|} g(x; (\eta_j)_{j\in\omega})\big)_{\omega\in\pi}\Big). \tag{36b}$$

Following a similar argument used for the recursion of Stirling numbers of the second kind and their relation to Bell numbers [9, p74], the result above can be viewed as a means of generating all partitions of $n+1$ elements from all partitions of n elements: The first term in Eq. (36a) corresponds to the creation of a new element to the partition $\pi \in \Pi_n$, containing only $n+1$, and each term in the second summation appends $n+1$ to one of the existing element ν of the partition π. This argument follows similar arguments previously used for ordinary and partial derivatives [6–8]. Hence the result is proved by induction. $\square$

A.3 General higher-order product rule (Theorem 3)

Proof. The proof is constructed by induction on the number of directions n.

a) Case $n = 0$.
We can write immediately

$$\sum_{\pi\subseteq\emptyset} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{0-|\pi|} g(x;(\eta_i)_{i\in\emptyset\setminus\pi}) = \delta^0 f(x)\delta^0 g(x) \tag{37a}$$

$$= f(x)g(x) \tag{37b}$$

$$= (f\cdot g)(x) \tag{37c}$$

$$= \delta^0 (f\cdot g)(x). \tag{37d}$$

b) Case $n = 1$.
Let us fix a point $x \in X$ and a direction $\eta_1 \in X$, such that both f and g have a first-order chain differential at point x in direction η_1. Let us then fix a sequence $\eta_{1,m} \to \eta_1 \in X$, and a sequence of real numbers $\theta_m \to 0$. Since f has a first-order chain differential at point x, it is continuous in x and thus

$$\lim_{m\to\infty} f(x+\theta_m\eta_{1,m}) = f(x). \tag{38}$$

Since both f and g have a first-order chain differential at point x in direction η_1, we have [2]

$$\lim_{m\to\infty} \theta_m^{-1}\big[f(x+\theta_m\eta_{1,m}) - f(x)\big] = \delta f(x;\eta_1), \tag{39}$$

$$\lim_{m\to\infty} \theta_m^{-1}\big[g(x+\theta_m\eta_{1,m}) - g(x)\big] = \delta g(x;\eta_1). \tag{40}$$

From (38), (39), and (40), it holds that

$$\begin{aligned}
&\lim_{m\to\infty} \theta_m^{-1}\big[(f\cdot g)(x+\theta_m\eta_{1,m}) - (f\cdot g)(x)\big]\\
&= \lim_{m\to\infty} \theta_m^{-1}\big[f(x+\theta_m\eta_{1,m})g(x+\theta_m\eta_{1,m}) - f(x+\theta_m\eta_{1,m})g(x) + f(x+\theta_m\eta_{1,m})g(x) - f(x)g(x)\big] && \text{(41a)}\\
&= \lim_{m\to\infty} f(x+\theta_m\eta_{1,m}) \lim_{m\to\infty} \theta_m^{-1}\big[g(x+\theta_m\eta_{1,m}) - g(x)\big]\\
&\qquad + \lim_{m\to\infty} \theta_m^{-1}\big[f(x+\theta_m\eta_{1,m}) - f(x)\big]g(x), && \text{(41b)}\\
&= f(x)\delta g(x;\eta_1) + \delta f(x;\eta_1)g(x). && \text{(41c)}
\end{aligned}$$

That is, $f\cdot g$ has a first-order chain differential at point x in direction η_1 and it is such that

$$\delta(f\cdot g)(x;\eta_1) = f(x)\delta g(x;\eta_1) + \delta f(x;\eta_1)g(x). \tag{42}$$

c) Case $n \geq 2$.
Let us fix a point $x \in X$ and a sequence of directions $(\eta_i)_{i=1}^n \in X^n$ such that both f and g have higher order chain differentials at point x in all sequences of directions $(\eta_i)_{i\in I}$, $I \subseteq \{1,\dots,n\}$. We

can then write

$$
\begin{aligned}
&\sum_{\pi\subseteq\{1,\dots,n\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n\}\setminus\pi}) \\
&= \sum_{\pi\subseteq\{1,\dots,n-1\}} \delta^{|\pi|+1} f(x;(\eta_i)_{i\in\pi\cup\{n\}})\delta^{n-1-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi}) \\
&\qquad\qquad + \sum_{\pi\subseteq\{1,\dots,n-1\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-1-|\pi|+1} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi\cup\{n\}}) \qquad (43a) \\
&= \sum_{\pi\subseteq\{1,\dots,n-1\}} \delta\big(\delta^{|\pi|} f(x;(\eta_i)_{i\in\pi});\eta_n\big)\delta^{n-1-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi}) \\
&\qquad\qquad + \sum_{\pi\subseteq\{1,\dots,n-1\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta\big(\delta^{n-1-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi});\eta_n\big) \qquad (43b) \\
&= \sum_{\pi\subseteq\{1,\dots,n-1\}} \delta\big(\delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-1-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi});\eta_n\big) \qquad (43c) \\
&= \delta\Big(\sum_{\pi\subseteq\{1,\dots,n-1\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-1-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n-1\}\setminus\pi});\eta_n\Big) \qquad (43d) \\
&= \delta\big(\delta^{n-1}(f\cdot g)(x;(\eta_i)_{i=1}^{n-1});\eta_n\big), \qquad (43e)
\end{aligned}
$$

where the last equality was obtained by exploiting case $n-1$. Thus, $f\cdot g$ has a n^{th}-order chain differential at point x in directions $\eta_1,\dots,\eta_n$ and it is such that

$$
\delta^n(f\cdot g)(x;(\eta_i)_{i=1}^n) = \sum_{\pi\subseteq\{1,\dots,n\}} \delta^{|\pi|} f(x;(\eta_i)_{i\in\pi})\delta^{n-|\pi|} g(x;(\eta_i)_{i\in\{1,\dots,n\}\setminus\pi}). \qquad (44)
$$

This ends the proof by induction. □

A.4 Practical derivations for the chain rule (Theorem 4)

Proof. Let us fix a point $x\in X$ and a direction $\eta\in X$, such that g has a chain differential at point x in direction η. Let us then fix a sequence $\nu_m\to\delta g(x;\eta)\in Y$, and a sequence of real numbers $\theta_m\to 0$.

a) Let us assume that f is a continuous linear function ℓ. For any $m\geq 0$ we can write

$$
\begin{aligned}
\theta_m^{-1}\big[\ell(g(x)+\theta_m\nu_m)-\ell(g(x))\big] &= \theta_m^{-1}\big[\ell(g(x))+\theta_m\ell(\nu_m)-\ell(g(x))\big] \qquad (45a)\\
&= \ell(\nu_m). \qquad (45b)
\end{aligned}
$$

Thus, it holds that

$$
\begin{aligned}
\lim_{m\to\infty}\theta_m^{-1}\big[\ell(g(x)+\theta_m\nu_m)-\ell(g(x))\big] &= \lim_{m\to\infty}\ell(\nu_m) \qquad (46a)\\
&= \ell\big(\lim_{m\to\infty}\nu_m\big) \qquad (46b)\\
&= \ell(\delta g(x;\eta)). \qquad (46c)
\end{aligned}
$$

Thus, using the definition of the chain differential (2), we have

$$
\delta\ell\big(g(x);\delta g(x;\eta)\big) = \ell\big(\delta g(x;\eta)\big). \qquad (47)
$$

Using the chain rule (6) ends the proof.

b) Let us assume that f is the k^{th}-power function $y \mapsto y^k$ for some $k > 0$. For any $m \geq 0$ we can write

$$
\begin{aligned}
&\theta_m^{-1}\Big[\big(g(x)+\theta_m\nu_m\big)^k - \big(g(x)\big)^k\Big] \\
&= \theta_m^{-1}\Big[\sum_{p=0}^{k}\binom{k}{p}\big(g(x)\big)^p(\theta_m\nu_m)^{k-p} - \big(g(x)\big)^k\Big] && (48a)\\
&= \theta_m^{-1}\Big[\big(g(x)\big)^k + k\big(g(x)\big)^{k-1}\theta_m\nu_m + \sum_{p=0}^{k-2}\binom{k}{p}\big(g(x)\big)^p(\theta_m\nu_m)^{k-p} - \big(g(x)\big)^k\Big] && (48b)\\
&= k\big(g(x)\big)^{k-1}\nu_m + \sum_{p=0}^{k-2}\binom{k}{p}\big(g(x)\big)^p(\theta_m)^{k-p-1}(\nu_m)^{k-p}. && (48c)
\end{aligned}
$$

Thus, it holds that

$$
\begin{aligned}
&\lim_{m\to\infty}\theta_m^{-1}\Big[\big(g(x)+\theta_m\nu_m\big)^k - \big(g(x)\big)^k\Big] \\
&= k\big(g(x)\big)^{k-1}\underbrace{\lim_{m\to\infty}\nu_m}_{=\delta g(x;\eta)} + \sum_{p=0}^{k-2}\binom{k}{p}\big(g(x)\big)^p\underbrace{\lim_{m\to\infty}(\theta_m)^{k-p-1}}_{=0}\underbrace{\lim_{m\to\infty}(\nu_m)^{k-p}}_{=\delta g(x;\eta)^{k-p}} && (49a)\\
&= k\big(g(x)\big)^{k-1}\delta g(x;\eta). && (49b)
\end{aligned}
$$

Thus, using the definition of the chain differential (2), we have

$$
\delta(y\mapsto y^k)\big(g(x);\delta g(x;\eta)\big) = k\big(g(x)\big)^{k-1}\delta g(x;\eta). \tag{50}
$$

Using the chain rule (6) ends the proof.

c) Let us assume that f is the exponential function. For any $m \geq 0$ we can write

$$
\begin{aligned}
\theta_m^{-1}\Big[\exp\big(g(x)+\theta_m\nu_m\big) - \exp\big(g(x)\big)\Big] &= \theta_m^{-1}\exp\big(g(x)\big)\big[\exp(\theta_m\nu_m)-1\big] && (51a)\\
&= \theta_m^{-1}\exp\big(g(x)\big)\big[\theta_m\nu_m + o(\theta_m\nu_m)\big]. && (51b)
\end{aligned}
$$

Thus, it holds that

$$
\begin{aligned}
\lim_{m\to\infty}\theta_m^{-1}\Big[\exp\big(g(x)+\theta_m\nu_m\big) - \exp\big(g(x)\big)\Big] &= \exp\big(g(x)\big)\big[\underbrace{\lim_{m\to\infty}\nu_m}_{=\delta g(x;\eta)} + \underbrace{\lim_{m\to\infty}\theta_m^{-1}\,o(\theta_m\nu_m)}_{=0}\big] && (52a)\\
&= \exp\big(g(x)\big)\delta g(x;\eta). && (52b)
\end{aligned}
$$

Thus, using the definition of the chain differential (2), we have

$$
\delta\exp\big(g(x);\delta g(x;\eta)\big) = \exp\big(g(x)\big)\delta g(x;\eta). \tag{53}
$$

Using the chain rule (6) ends the proof. □

References

[1] J.-P. Aubin and H. Frankowska. *Set Valued Analysis*. Birkhauser, 1990.

[2] P. Bernhard. Chain differentials with an application to the mathematical fear operator. *Nonlinear Analysis*, 62:1225–1233, 2005.

[3] D. E. Clark and J. Houssineau. Faà di Bruno's formula for chain differentials. *arXiv:1310.2833*, 2013.

[4] F. Faà di Bruno. Note sur un nouvelle formule de calcul différentiel. *Quarterly Journal of Pure and Applied Mathematics*, 1:359–360, 1857.

[5] R. Gâteaux. Fonctions d'une infinité de variables indépendantes. *Bulletin de la Société Mathématique de France*, 47:70–96, 1919.

[6] M. Hardy. Combinatorics of partial derivatives. *Electronic Journal of Combinatorics*, 13:R1, 2006.

[7] H.-N. Huang, S. A. M. Marcantognini, and N. J. Young. Chain Rules for Higher Derivatives. *The Mathematical Intelligencer*, 28(2):61–69, 2006.

[8] T.W. Ma. Higher Chain Formula proved by Combinatorics. *Electronic Journal of Combinatorics*, 16:N21, 2009.

[9] R. Stanley. *Enumerative Combinatorics*, volume 1. Cambridge University Press, 2 edition, 2012.