

The Faà di Bruno construction

R.A.G. Seely

John Abbott College
& McGill University

(Joint work with J.R.B. Cockett)

Francesco Faà di Bruno (1825-1888) was an Italian of noble birth, a soldier, a mathematician, and a priest. In 1988 he was beatified by Pope John Paul II for his charitable work teaching young women mathematics. As a mathematician he studied with Cauchy in Paris. He was a tall man with a solitary disposition who spoke seldom and, when teaching class, not always successfully. Perhaps his most significant mathematical contribution concerned the combinatorics of the higher-order chain rules. These results were the cornerstone of “combinatorial analysis”: a subject which never really took off. It is the combinatorics underlying the higher-order chain rule which is of interest to us here.

According to a paper by Craik in the American Mathematical Monthly 2005, the Faà di Bruno formula was known and published 50 years before Faà di Bruno, by the French mathematician Arbogast. But following modern tradition, we shall continue to refer to it by the name of our mathematical saint.

Outline

- Differential and Cartesian differential categories
- The bundle fibration
- The Faà di Bruno construction
- The comonad
- The coalgebras

Theorem *Cartesian differential categories are exactly coalgebras of the Faà di Bruno comonad.*

Prehistory: Differential categories

(Inspired by Ehrhard & Regnier; particularly a talk by E at U Ottawa 2002)

Context: a category of both smooth and linear maps; this might be thought of as a **category** (of **linear maps**) and its **coKleisli category** (of free coalgebras) (whose maps are **smooth**), for a “good” comonad. Then a differential operator takes a **smooth** map to a **smooth** family of **linear** maps (for each point, the Jacobian at that point defines a linear map):

$$\frac{f: !A \longrightarrow B}{D[f]: A \otimes !A \longrightarrow B}$$

Think $D(f): !A \longrightarrow (A \multimap B)$, but we do not want to assume monoidal closed structure.

Consider a simple example: $f(x, y, z) = \langle x^2 + xyz, z^3 - xy \rangle$. This is a **smooth** function from \mathcal{R}^3 to \mathcal{R}^2 . Its Jacobian is

$$\begin{pmatrix} 2x + yz & xz & xy \\ -y & -x & 3z^2 \end{pmatrix}$$

Given a choice of x, y and z , *i.e.* a point of \mathcal{R}^3 , we obtain a **linear** map from \mathcal{R}^3 to \mathcal{R}^2 . But the assignment of the linear map for a point is **smooth**.

So, given a smooth map $f: A \subseteq \mathcal{R}^n \rightarrow \mathcal{R}^m$, one gets a smooth map $D(f): A \rightarrow L(A, \mathcal{R}^m)$: for a point $x \in A$: $D(f)$ is given by the Jacobian of f at x .

There is some key structure on the ambient category needed to make this work. Certainly we expect some **additive structure**: we assume that the category is commutative monoid enriched. We also put some conditions on the comonad $(!, \delta, \epsilon)$, viz that each object $!X$ comes equipped with **natural coalgebra structure**

$$\Delta: !X \longrightarrow !X \otimes !X \qquad e: !X \longrightarrow \top$$

satisfying some “obvious” coherence conditions, viz that $(!X, \Delta, e)$ **is a comonoid** and δ **is a morphism of comonoids**.

A differential combinator D (as before) is supposed to be **additive**, to “preserve” commutativity of diagrams (this is just the property of being a **combinator**)

$$\begin{array}{ccc}
 !A & \xrightarrow{f} & B \\
 !u \downarrow & & \downarrow v \\
 !C & \xrightarrow{g} & D
 \end{array}
 \iff
 \begin{array}{ccc}
 A \otimes !A & \xrightarrow{D[f]} & B \\
 u \otimes !u \downarrow & & \downarrow v \\
 C \otimes !C & \xrightarrow{D[g]} & D
 \end{array}$$

and to satisfy the following “obvious” properties of a differential:

[D.1] Constant maps:

$$D[e_A] = 0$$

[D.2] Product rule:

$$D[\Delta(f \otimes g)] = (1 \otimes \Delta)a_{\otimes}^{-1}(D[f] \otimes g) + (1 \otimes \Delta)a_{\otimes}^{-1}(c_{\otimes} \otimes 1)a_{\otimes}(f \otimes D[g])$$

where $f: !A \rightarrow B$, $g: !A \rightarrow C$, and a_{\otimes}, c_{\otimes} are the associativity and commutativity isomorphisms

[D.3] Linear maps:

$$D[\epsilon_A f] = (1 \otimes e_A)u_{\otimes} f$$

where $f: A \rightarrow B$ and u_{\otimes} is the unit isomorphism

[D.4] The chain rule:

$$D[\delta !f g] = (1 \otimes \Delta)a_{\otimes}^{-1}(D[f] \otimes \delta !f)D[g]$$

where $!A \xrightarrow{f} B$ and $!B \xrightarrow{g} C$

This work (Blute, Cockett, Seely, “Differential categories”, MSCS 2006) gave a good categorical semantics for Ehrhard’s calculus, had some very natural models, and seemed quite satisfactory, until (provoked by conversations with Nicola Gambino!) we thought of reversing the perspective, and focus instead on the coalgebra category of smooth maps (with linear maps being “carved out” inside it). This led to the notion of a Cartesian differential category.

Key structure:

$$\frac{X \xrightarrow{f} Y: x \mapsto f(x)}{X \times X \xrightarrow{D[f]} Y: \langle a, s \rangle \mapsto \frac{df}{dx}(s) \cdot a}$$

(linear in a but not in s)

Example, revisited:

$$\text{If } f: \langle x, y, z \rangle \mapsto \langle x^2 + xyz, z^3 - xy \rangle$$

$$\text{then: } \frac{d\langle x^2 + xyz, z^3 - xy \rangle}{d\langle x, y, z \rangle} = \begin{pmatrix} 2x + yz & xz & xy \\ -y & -x & 3z^2 \end{pmatrix}$$

$$\text{and } \frac{d\langle x^2 + xyz, z^3 - xy \rangle}{d\langle x, y, z \rangle}(\langle r, s, t \rangle) = \begin{pmatrix} 2r + st & rt & rs \\ -s & -r & 3t^2 \end{pmatrix}$$

$$\text{and } \frac{d\langle x^2 + xyz, z^3 - xy \rangle}{d\langle x, y, z \rangle}(\langle r, s, t \rangle) \cdot \langle a, b, c \rangle = \langle (2r + st)a + rtb + rsc, -sa - rb + 3t^2c \rangle$$

Cartesian Differential Categories

1. Category \mathbb{X} , **Cartesian left additive**[†]: hom-sets are commutative monoids & $f(g + h) = (fg) + (fh)$, $f0 = 0$.
(h is **additive** if also $(f + g)h = (fh) + (gh)$ and $0h = 0$.)
'Well-behaved' products: π_0, π_1, Δ additive
 f, g additive $\Rightarrow f \times g$ additive.

2. Differential operator D :

$$\frac{X \xrightarrow{f} Y}{X \times X \xrightarrow{D[f]} Y}$$

(Ref: [Blute-Cockett-Seely] TAC 2009)

[†]**Eg** (of "left additive"): the category of commutative monoids & **set** maps is left additive; the additive maps are homomorphisms.

Satisfying:

$$\mathbf{[CD.1]} \quad D[f + g] = D[f] + D[g] \text{ and } D[0] = 0$$

$$\mathbf{[CD.2]} \quad \langle h + k, v \rangle D[f] = \langle h, v \rangle D[f] + \langle k, v \rangle D[f] \text{ and } \langle 0, v \rangle D_{\times}[f] = 0$$

$$\mathbf{[CD.3]} \quad D[1] = \pi_0, \quad D[\pi_0] = \pi_0\pi_0 \text{ and } D[\pi_1] = \pi_0\pi_1$$

$$\mathbf{[CD.4]} \quad D[\langle f, g \rangle] = \langle D[f], D[g] \rangle$$

$$\mathbf{[CD.5]} \quad D[fg] = \langle D[f], \pi_1 f \rangle D[g]$$

$$\mathbf{[CD.6]} \quad \langle \langle g, 0 \rangle, \langle h, k \rangle \rangle D[D[f]] = \langle g, k \rangle D[f]$$

$$\mathbf{[CD.7]} \quad \langle \langle 0, h \rangle, \langle g, k \rangle \rangle D[D[f]] = \langle \langle 0, g \rangle, \langle h, k \rangle \rangle D[D[f]]$$

$$\text{[Dt.1]} \quad \frac{d(f_1 + f_2)}{dp}(s) \cdot a = \frac{df_1}{dp}(s) \cdot a + \frac{df_2}{dp}(s) \cdot a \quad \text{and} \quad \frac{d0}{dp}(s) \cdot a = 0;$$

$$\text{[Dt.2]} \quad \frac{df}{dp}(s) \cdot (a_1 + a_2) = \frac{df}{dp}(s) \cdot a_1 + \frac{df}{dp}(s) \cdot a_2 \quad \text{and} \quad \frac{df}{dp}(s) \cdot 0 = 0;$$

$$\text{[Dt.3]} \quad \frac{dx}{dx}(s) \cdot a = a, \quad \frac{df}{d(p, p')}(s, s') \cdot (a, 0) = \frac{df[s'/p']}{dp}(s) \cdot a$$

$$\quad \text{and} \quad \frac{df}{d(p, p')}(s, s') \cdot (0, a') = \frac{df[s/p]}{dp'}(s') \cdot a';$$

$$\text{[Dt.4]} \quad \frac{d(f_1, f_2)}{dp}(s) \cdot a = \left(\frac{df_1}{dp}(s) \cdot a, \frac{df_2}{dp}(s) \cdot a \right);$$

$$\text{[Dt.5]} \quad \frac{dg[f/p']}{dp}(s) \cdot a = \frac{dg}{dp'}(f[s/p]) \cdot \left(\frac{df}{dp}(s) \cdot a \right) \quad (\text{no variable of } p \text{ may occur in } f);$$

$$\text{[Dt.6]} \quad \frac{d\frac{df}{dp}(s) \cdot p'}{dp'}(r) \cdot a = \frac{df}{dp}(s) \cdot a.$$

$$\text{[Dt.7]} \quad \frac{d\frac{df}{dp_1}(s_1) \cdot a_1}{dp_2}(s_2) \cdot a_2 = \frac{d\frac{df}{dp_2}(s_2) \cdot a_2}{dp_1}(s_1) \cdot a_1$$

The Chain Rule

$$D[fg] = \langle D[f], \pi_1 f \rangle D[g]$$

$$\frac{dg[f/x']}{dx}(s) \cdot a = \frac{dg}{dx'}(f[s/x]) \cdot \left(\frac{df}{dx}(s) \cdot a \right)$$

$$(fg)^{(1)}(s) \cdot a = g^{(1)}(f) \cdot (f^{(1)}(s) \cdot a)$$



Bun(\mathbb{X}), the Bundle Fibration over \mathbb{X}

Objects: (A, X) (pairs of objects of \mathbb{X})

Morphisms: $(f_*, f_1): (A, X) \rightarrow (B, Y): f_*: X \rightarrow Y$ in \mathbb{X} ;
 $f_1: A \times X \rightarrow B$ in \mathbb{X} , additive in its first argument.

Composition: $(f_*, f_1)(g_*, g_1) = (f_*g_*, \langle f_1, \pi_1 f_* \rangle g_1)$
(Think $f_1 = D(f_*)$)

Some Properties:

- Additive structure: defined “component-wise”
- $p: \text{Bun}(\mathbb{X}) \rightarrow \mathbb{X}: (A, X) \mapsto A; (f_*, f_1) \mapsto f_*$ is a fibration
- If \mathbb{X} is Cartesian left additive, so are the fibres, and so is the total category. Furthermore, p is a Cartesian left additive functor.

Suppose $p: \text{Bun}(\mathbb{X}) \rightarrow \mathbb{X}$ has a left additive section $\mathcal{D}: \mathbb{X} \rightarrow \text{Bun}(\mathbb{X})$. Some interesting consequences follow (motivation for (some of) the axioms of a Cartesian differential operator?).

Notation: write $\mathcal{D}(A) = (A, d_0(A))$ and $\mathcal{D}(f) = (f, D[f])$.
(\mathcal{D} a section \Rightarrow first component as given)

Note then that $D[f]: A \times d_0(A) \rightarrow d_0(B)$ is additive in its first argument.

Also, \mathcal{D} a functor forces the following equation:

$$\langle D[f], \pi_1 f \rangle D[g] = D[fg]$$

(since the lefthand side is the second component of $\mathcal{D}(f)\mathcal{D}(g)$ and the righthand side is the second component of $\mathcal{D}(fg)$)

So $\text{Bun}(\mathbb{X})$ captures differential structure of \mathbb{X} , where composition in $\text{Bun}(\mathbb{X})$ is governed by the chain rule.

In addition, \mathcal{D} preserves identities, so $1 = (\pi_0, 1) = (D[1], 1)$, so:

$$D[1] = \pi_0$$

Also $\mathcal{D}(\pi_0) = (\pi_0, \pi_0\pi_0)$, so:

$$D[\pi_0] = \pi_0\pi_0$$

Similarly

$$D[\pi_1] = \pi_0\pi_1$$

\mathcal{D} preserves $+$: $\mathcal{D}(f + g) = \mathcal{D}(f) + \mathcal{D}(g)$, and so

$$D[f + g] = D[f] + D[g]$$

In short, the first 5 axioms of a Cartesian differential operator D follow from the existence of a left additive section \mathcal{D} to p .

The point of the rest of the talk is to generalise this fibration to include higher order differentiation so as to “justify” the remaining two axioms.

(Actually, all we need is second-order differentiation, but once one goes beyond 1 it's hard to stop ...)

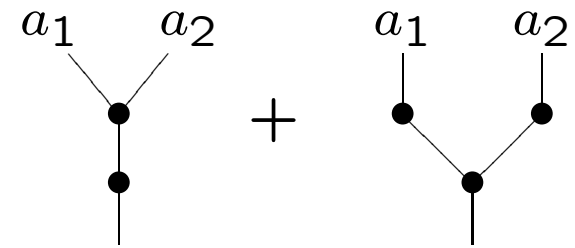
So: let's look at the 2nd order chain rule (an excellent high-school exercise, if you've never done it).

2nd Order Chain Rule

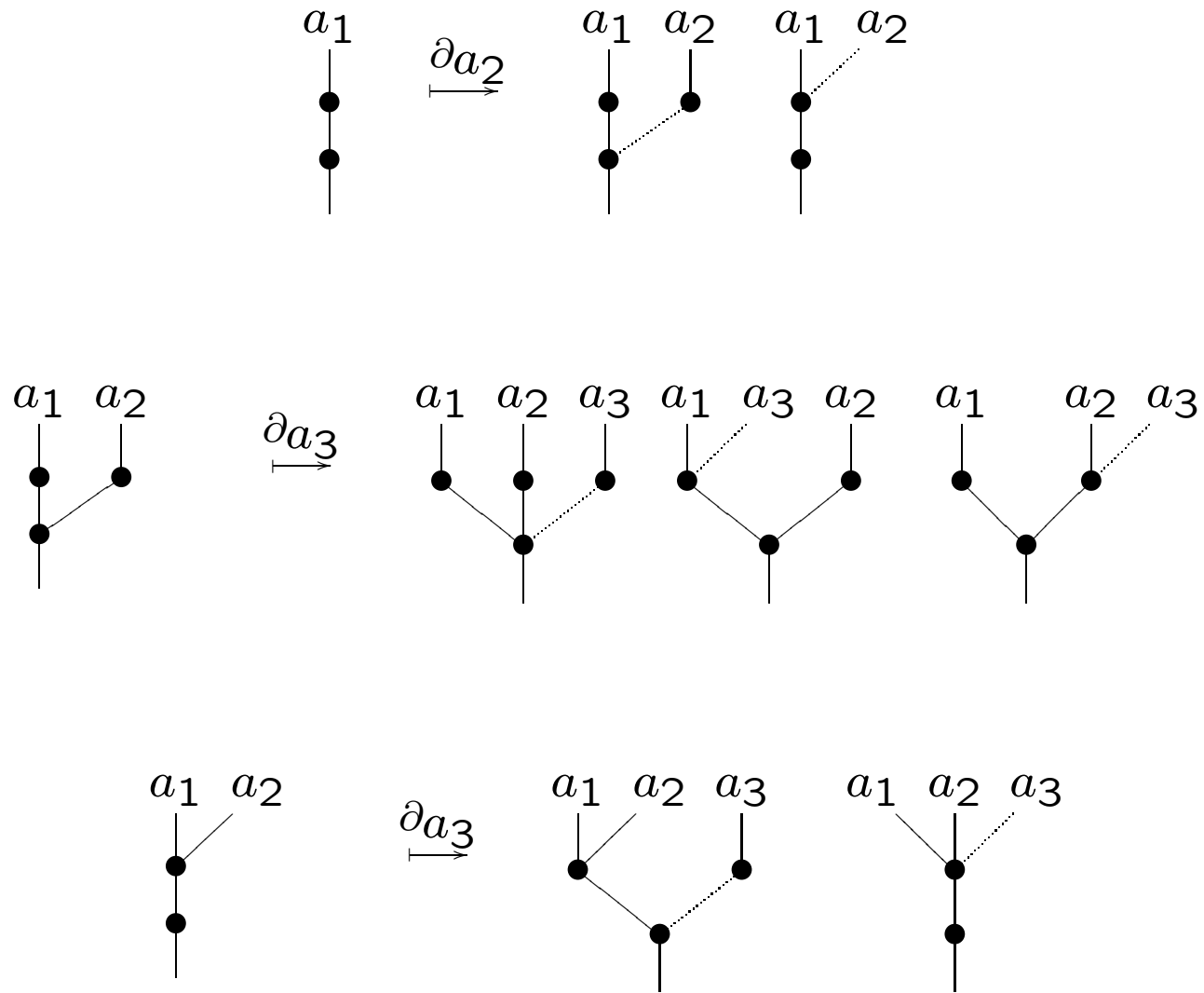
$$\begin{aligned} & \frac{d^{(2)}g(f(x))}{dx} (s) \cdot a_1 \cdot a_2 \\ &= \frac{dg}{dx} (f(s)) \cdot \left(\frac{d^{(2)}f}{dx} (s) \cdot a_1 \cdot a_2 \right) \\ &+ \frac{d^{(2)}g}{dx} (f(s)) \cdot \left(\frac{df}{dx} (s) \cdot a_1 \right) \cdot \left(\frac{df}{dx} (s) \cdot a_2 \right) \end{aligned}$$

i.e.

$$\begin{aligned} & (fg)^{(2)}(s) \cdot a_1 \cdot a_2 \\ &= g^{(1)}(f(s)) \cdot (f^{(2)}(s) \cdot a_1 \cdot a_2) \\ &+ g^{(2)}(f(s)) \cdot (f^{(1)}(s) \cdot a_1) \cdot (f^{(1)}(s) \cdot a_2) \end{aligned}$$



The differential of a symmetric tree



Faà(\mathbb{X}), the Fàa di Bruno Fibration over \mathbb{X}

Objects: (A, A) (pairs of objects of \mathbb{X})

(for “pedegogical reasons” we shall write such pairs as (A, X) , with the unstated assumption that $A = X$)

Morphisms: $f = (f_*, f_1, f_2, \dots): (A, X) \longrightarrow (B, Y)$, where:

$f_*: X \longrightarrow Y$ in \mathbb{X} ;

for $r > 0$: $f_r: \underbrace{A \times \dots \times A}_r \times X \longrightarrow B$ a “symmetric form” (i.e. additive and symmetric in the first r arguments)

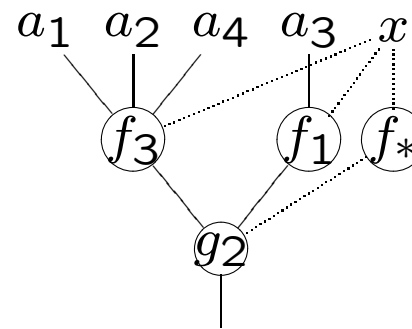
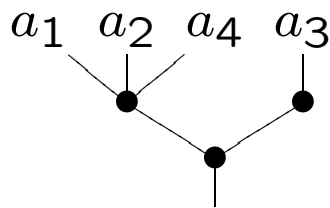
(think $f_r: A^{\otimes r}/r! \times X \longrightarrow B$, even though \mathbb{X} need not have \otimes)

Composition? This is where the higher order chain rules come in ...

Faà di Bruno convolution

τ : a symmetric tree of height 2, width r , on variables $\{a_1, \dots, a_r\}$;
 $(A, X) \xrightarrow{f} (B, Y) \xrightarrow{g} (C, Z)$ in $\text{Faà}(\mathbb{X})$.

Then $(f \star g)_\tau: \underbrace{A \times \dots \times A}_r \times X \rightarrow C$ is defined thus (for example):
 for τ the tree on the left, interpret it as the tree on the right:



$$(f \star g)_\tau = g_2(f_*(x), f_1(a_3, x), f_3(a_1, a_2, a_4, x)): A \times A \times A \times A \times X \rightarrow C$$

NB: $(f \star g)_\tau$ is additive in each argument except the last whenever the components of f and g have this property.

$\iota_2^{a_1}$ is the (unique) height 2 width 1 tree (with variable a_1)

$$\mathcal{T}_2^{a_1, \dots, a_r} = \partial_{a_2, \dots, a_r}(\iota_2^{a_1}),$$

i.e. the bag of trees obtained by “deriving” $\iota_2^{a_1}$ r -times with respect to the given variables. (This is the set of all symmetric trees of height 2 and width r .)

The Faà di Bruno convolution (composition in $\text{Faà}(\mathbb{X})$) of f and g is given by setting $(fg)_* = f_*g_*$, and for $r > 0$

$$(fg)_r = (f \star g)_{\mathcal{T}_2^{a_1, \dots, a_r}} = \sum_{n \cdot \tau \in \mathcal{T}_2^{a_1, \dots, a_r}} n \cdot (f \star g)_\tau$$

(This is well-defined: permuting the variables of any $\tau \in \mathcal{T}_2^{a_1, \dots, a_r}$ either leaves τ fixed or produces a new tree in $\mathcal{T}_2^{a_1, \dots, a_r}$.)

Proposition For any Cartesian left additive category \mathbb{X} , $\text{Faà}(\mathbb{X})$ is a Cartesian left additive category.

$\text{Fa}\grave{\text{a}}: \text{CLAdd} \longrightarrow \text{CLAdd}$ is a functor:

$$\mathbb{X} \mapsto \text{Fa}\grave{\text{a}}(\mathbb{X}) ; (f_*, f_1, \dots) \mapsto (F(f_*), F(f_1), \dots)$$

$\epsilon: \text{Fa}\grave{\text{a}}(\mathbb{X}) \longrightarrow \mathbb{X}: (A, X) \mapsto X, (f_*, f_1, \dots) \mapsto f$ is a fibration.
(and a natural transformation)

There is a functor (indeed, a natural transformation)

$\delta: \text{Fa}\grave{\text{a}}(\mathbb{X}) \longrightarrow \text{Fa}\grave{\text{a}}(\text{Fa}\grave{\text{a}}(\mathbb{X}))$ so that $(\text{Fa}\grave{\text{a}}, \epsilon, \delta)$ is a comonad on CLAdd .

On objects: $\delta: (A, X) \mapsto ((A, A), A, X)$

On morphisms, things are a bit “complicated”. Some notation:
we write $f = (f_*, f_1, f_2, \dots): (A, X) \longrightarrow (B, Y)$ as follows

$$\begin{aligned} f_*: X &\longrightarrow Y & : & x \mapsto f_*(x) \\ f_n: A^n \times X &\longrightarrow B & : & (a_{*1}, \dots, a_{*n}, x) \mapsto f_n(x) \cdot a_{*1} \cdot \dots \cdot a_{*n} \end{aligned}$$

We then define $\delta: \text{Fa}\grave{\text{a}}(\mathbb{X}) \longrightarrow \text{Fa}\grave{\text{a}}(\text{Fa}\grave{\text{a}}(\mathbb{X}))$ as follows:

on objects, δ takes (A, X) to $((A, A), A, X)$.

On arrows, $f \mapsto \delta(f) = (f, f^{[1]}, f^{[2]}, \dots)$ by setting

$$f_*^{[n]}: A^n \times X \longrightarrow B: (a_{*1}, \dots, a_{*n}, x) \mapsto f_n(x) \cdot a_{*1} \cdot \dots \cdot a_{*n}$$

$$f_r^{[n]}: (A^n \times A)^r \times (A^n \times X) \longrightarrow B:$$

$$\left(\begin{array}{c|c} a_{11} \dots a_{1n} & a_{1*} \\ \vdots & \vdots \\ a_{r1} \dots a_{rn} & a_{r*} \\ \hline a_{*1} \dots a_{*n} & x \end{array} \right) \mapsto \sum_{\substack{s \leq n \ \& \ s \leq r \\ \& \text{ramp}_{r,n}^s(\alpha | \gamma)}} f_{r+n-s}(x) \cdot a_{\alpha_1 1} \cdot \dots \cdot a_{\alpha_n n} \cdot a_{\gamma_1 * } \cdot \dots \cdot a_{\gamma_{r-s} * }$$

where the “ramp” condition amounts to choosing (for each $s \leq \min(r, n)$) s elements from $(a_{ij})_{i \leq r, j \leq n}$, at most one from each row and column, (this amounts to choosing a partial isomorphism) and constructing the function term as follows (for example,):

If σ is the following partial iso (here $n = 4$, $r = 5$, and $s = 3$):

$$\left(\begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & a_{14} & a_{1*} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{2*} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{3*} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{4*} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{5*} \\ \hline a_{*1} & a_{*2} & a_{*3} & a_{*4} & x \end{array} \right) \rightsquigarrow \left(\begin{array}{cccc|c} \boxed{a_{11}} & a_{12} & a_{13} & a_{14} & a_{1*} \\ a_{21} & a_{22} & a_{23} & a_{24} & \color{green}a_{2*} \\ a_{31} & a_{32} & a_{33} & \boxed{a_{34}} & a_{3*} \\ a_{41} & a_{42} & a_{43} & a_{44} & \color{green}a_{4*} \\ a_{51} & \boxed{a_{52}} & a_{53} & a_{54} & a_{5*} \\ \hline a_{*1} & a_{*2} & \color{green}a_{*3} & a_{*4} & x \end{array} \right)$$

Then construct

$$f^\sigma = f_6(x) \cdot \color{red}a_{11} \cdot \color{red}a_{52} \cdot \color{green}a_{*3} \cdot \color{red}a_{34} \cdot \color{green}a_{2*} \cdot \color{green}a_{4*}$$

f_6 since we need $n + r - s = 6$ linear arguments. The linear arguments of f are determined by putting in the selected arguments and arguments from the bottom row and rightmost column corresponding to the rows and columns **not** containing a selected argument. Then we set $f_r^{[n]}$ to be the sum of all such expressions:

$$f_r^{[n]} = \sum_{\sigma \in \text{ParIso}(r,n)} f^\sigma$$

Let's explicitly develop some of these terms. First $f^{[0]}$, which is just f :

$$\begin{aligned}(\overline{x}) &\mapsto f_*(x) \\ \left(\frac{a_{1*}}{x}\right) &\mapsto f_1(x) \cdot a_{1*} \\ \left(\frac{a_{1*}}{a_{2*}}\right) &\mapsto f_2(x) \cdot a_{1*} \cdot a_{2*} \\ &\vdots\end{aligned}$$

Next $f^{[1]}$:

$$\begin{aligned} \left(\overline{a_{*1} \mid x} \right) &\mapsto f_1(x) \cdot a_{*1} \\ \left(\begin{array}{c|c} a_{11} & a_{1*} \\ \hline a_{*1} & x \end{array} \right) &\mapsto f_2(x) \cdot a_{*1} \cdot a_{1*} \\ &\quad + f_1(x) \cdot a_{11} \\ \left(\begin{array}{c|c} a_{11} & a_{1*} \\ a_{21} & a_{2*} \\ \hline a_{*1} & x \end{array} \right) &\mapsto f_3(x) \cdot a_{*1} \cdot a_{1*} \cdot a_{2*} \\ &\quad + f_2(x) \cdot a_{21} \cdot a_{1*} \\ &\quad + f_1(x) \cdot a_{11} \cdot a_{2*} \\ &\quad \vdots \end{aligned}$$

Here are the first few terms of $f^{[2]}$:

$$\left(\overline{a_{*1} \ a_{*2} \mid x} \right) \mapsto f_2(x) \cdot a_{*1} \cdot a_{*2}$$

$$\left(\begin{array}{cc|c} a_{11} & a_{12} & a_{1*} \\ \hline a_{*1} & a_{*2} & x \end{array} \right) \mapsto \begin{aligned} & f_3(x) \cdot a_{*1} \cdot a_{*2} \cdot a_{1*} \\ & + f_2(x) \cdot a_{11} \cdot a_{*2} \\ & + f_2(x) \cdot a_{*1} \cdot a_{12} \end{aligned}$$

$$\left(\begin{array}{cc|c} a_{11} & a_{12} & a_{1*} \\ a_{21} & a_{22} & a_{2*} \\ \hline a_{*1} & a_{*2} & x \end{array} \right) \mapsto \begin{aligned} & f_4(x) \cdot a_{*1} \cdot a_{*2} \cdot a_{1*} \cdot a_{2*} \\ & + f_3(x) \cdot a_{21} \cdot a_{*2} \cdot a_{1*} \\ & + f_3(x) \cdot a_{*1} \cdot a_{22} \cdot a_{1*} \\ & + f_3(x) \cdot a_{11} \cdot a_{*2} \cdot a_{2*} \\ & + f_3(x) \cdot a_{*1} \cdot a_{12} \cdot a_{2*} \\ & + f_2(x) \cdot a_{11} \cdot a_{22} \\ & + f_2(x) \cdot a_{21} \cdot a_{12} \end{aligned}$$

⋮

Remark: The intended interpretation of $f_r^{[n]}$ is the r^{th} higher order differential term

$$\frac{d^r f(x) \cdot a_1 \cdots a_n}{d(x, a_1, \dots, a_n)} (x, a_1, \dots, a_n) \cdot (a_1, a_{11}, \dots, a_{1n}) \cdots (a_r, a_{r1}, \dots, a_{rn})$$

Properties: $f_r^{[n]}$ is additive, symmetric in its first r arguments.

$$(f + g)_r^{[n]} = f_r^{[n]} + g_r^{[n]}$$

If F is Cartesian left additive, $\text{Fa}\grave{\text{a}}(F)(f^{[n]}) = (\text{Fa}\grave{\text{a}}(F)(f))^{[n]}$

$\delta: \text{Fa}\grave{\text{a}}(\mathbb{X}) \rightarrow \text{Fa}\grave{\text{a}}(\text{Fa}\grave{\text{a}}(\mathbb{X}))$ is a functor, and is natural (as a natural transformation).

$(\text{Fa}\grave{\text{a}}, \epsilon, \delta)$ is a comonad on CLAdd.

An example of the proofs:

Let's show that $\delta(f)\delta(g) = \delta(fg)$:

For the most part (as seen in the sequence of equations on the next slide) this involves expanding the definitions, followed by several applications of additivity; only the last step requires comment, as it involves a combinatorial argument.

(There's a sense in which this result is "obvious" — each side is just a sum of the "natural" chain-rule-type terms — but verifying the details didn't seem so "obvious" to us at first ... still doesn't!)

$$\begin{aligned}
\delta(f)\delta(g) &= \sum_{\tau_1, \tau_2} (\delta(f) \star \delta(g))_{\tau_1 \times \tau_2} \\
&= \sum_{\tau_1, \tau_2} \left(\left(\sum_{\sigma: i \rightarrow j} f^\sigma \right)_{ij} \star \left(\sum_{\sigma': k \rightarrow l} g^{\sigma'} \right)_{kl} \right)_{\tau_1 \times \tau_2} \\
&= \sum_{\tau_1, \tau_2} \left(\sum_{\sigma'} g^{\sigma'} \right) \left(\sum_{\sigma_{ij}: \alpha_i \rightarrow \beta_j} f^{\sigma_{ij}} \right)_{ij} \\
&= \sum_{\tau_1, \tau_2} \sum_{\sigma'} g^{\sigma'} \left(\sum_{\sigma_{ij}} f^{\sigma_{ij}} \right)_{ij} \\
&= \sum_{\tau_1, \tau_2} \sum_{\sigma'} g^{\sigma'} \left(\sum_{\sigma_{ij}} f^{\sigma_{ij}} \right)_{ij \in \sigma'} \\
&= \sum_{\tau_1, \tau_2} \sum_{\sigma', \sigma_{ij}, ij \in \sigma'} g^\sigma(\dots, f^{\sigma_{ij}}, \dots) \\
&= \sum_{\sigma: n \rightarrow m} \sum_{\tau \in \mathcal{T}_{|\sigma^*|}} (f \star g)_\tau^\sigma = \delta(fg)
\end{aligned}$$

The key combinatorial lemma is the equivalence of the following data:

- Partitions $\tau_1 = (\alpha_1, \dots, \alpha_k), \tau_2 = (\beta_1, \dots, \beta_l)$ and partial isomorphisms $\sigma': k \rightarrow l$ and $\sigma_{ij}: \alpha_i \rightarrow \beta_j$ for $(i, j) \in \sigma'$
- Partial isomorphism $\sigma: n \rightarrow m$ and partition τ of σ_* .

where n is the set partitioned by τ_1 , m the set partitioned by τ_2 , σ is the union of the σ_{ij} , and

$$\sigma_* = \sigma \cup \{(x, *) \mid x \in n \setminus \pi_1 \sigma\} \cup \{(*, y) \mid y \in m \setminus \pi_2 \sigma\}$$

Notice that $|\sigma_*| = n + m - |\sigma|$.

We sketch the proof, with an example as illustration.

We shall frequently identify an integer n with the set of integers from 1 to n , unless otherwise stated. We shall represent a partial isomorphism as the set of pairs (i, j) where $i \mapsto j$.

More notation: write $\sigma_i = \bigcup_j \sigma_{ij}$ and $\sigma_j = \bigcup_i \sigma_{ij}$ (and similarly for σ_{i*}, σ_{j*}).

Suppose we are given partitions $\tau_1 = (\alpha_1, \dots, \alpha_k), \tau_2 = (\beta_1, \dots, \beta_l)$ and partial isomorphisms $\sigma': k \rightarrow l$ and $\sigma_{ij}: \alpha_i \rightarrow \beta_j$ for $(i, j) \in \sigma'$

We define a partition τ on σ_* as $\tau :=$

$$\begin{aligned} \{\sigma_{ij*}\}_{(i,j) \in \sigma'} \cup & \{((\alpha_i \setminus \pi_1 \sigma_i) \times \{*\}) \setminus \sigma_{i*}\}_{i \in k} \\ & \cup \{(\{*\} \times (\beta_j \setminus \pi_2 \sigma_j)) \setminus \sigma_{j*}\}_{j \in l} \end{aligned}$$

This means that pairs from the same σ_{ij*} end up in the same partition, and pairs with a $*$ end up in the same partition if the “other” elements come from the same α_i or β_j (and aren't already in some σ_{ij*}).

Consider the following example:

$$\tau_1 = ((1, 3), (2, 5), (4, 6))$$

$$\tau_2 = ((1, 2, 4), (3), (5)) \quad (\text{so } k = l = 3)$$

$$\sigma': 3 \rightarrow 3 = \{(1, 3), (3, 1)\} \quad (\text{so e.g. } (2, 2) \text{ is not in } \sigma)$$

$$\sigma_{13}: \{1, 3\} \rightarrow \{5\} = \{(3, 5)\}$$

$$\sigma_{31}: \{4, 6\} \rightarrow \{1, 2, 4\} = \{(4, 4), (6, 1)\}$$

Then $\sigma = \bigcup_{ij} \sigma_{ij}: 6 \rightarrow 5 = \{(3, 5), (4, 4), (6, 1)\}$ and

$$n = 6, m = 5, |\sigma| = 3$$

$$\sigma_* = \{(3, 5), (4, 4), (6, 1), (1, *), (2, *), (5, *), (*, 2), (*, 3)\}$$

$$\sigma_{13*} = \{(3, 5), (1, *)\}$$

$$\sigma_{31*} = \{(4, 4), (6, 1), (*, 2)\}$$

And so we get

$$\tau = (((4, 4), (6, 1), (*, 2)), ((3, 5), (1, *)), ((2, *), (5, *)), ((*, 3)))$$

(This completes one direction of the equivalence)

What's going on?

The given partitions and partial isos amount to this selection from a variable base:

$$\left(\begin{array}{c} \left(\begin{array}{ccc} a_{1,1} & a_{1,2} & a_{1,4} \\ a_{3,1} & a_{3,2} & a_{3,4} \end{array} \right) & \left(\begin{array}{c} a_{1,3} \\ a_{3,3} \end{array} \right) & \left(\begin{array}{c} a_{1,5} \\ a_{3,5} \end{array} \right) \\ \left(\begin{array}{ccc} a_{2,1} & a_{2,2} & a_{2,4} \\ a_{5,1} & a_{5,2} & a_{5,4} \end{array} \right) & \left(\begin{array}{c} a_{2,3} \\ a_{5,3} \end{array} \right) & \left(\begin{array}{c} a_{2,5} \\ a_{5,5} \end{array} \right) \\ \left(\begin{array}{ccc} a_{4,1} & a_{4,2} & a_{4,4} \\ a_{6,1} & a_{6,2} & a_{6,4} \end{array} \right) & \left(\begin{array}{c} a_{4,3} \\ a_{6,3} \end{array} \right) & \left(\begin{array}{c} a_{4,5} \\ a_{6,5} \end{array} \right) \end{array} \right)$$

and it's clear that what both sets of data are defining is the following term from the sums that define $\delta(f)\delta(g)$ and $\delta(fg)$:

$$g_4(x) \cdot (f_3(x) \cdot a_{44} \cdot a_{61} \cdot a_{*2}) \cdot (f_2(x) \cdot a_{35} \cdot a_{1*}) \cdot (f_2(x) \cdot a_{2*} \cdot a_{5*}) \cdot (f_1(x) \cdot a_{*3})$$

The other direction:

Suppose we are given a partial isomorphism $\sigma: n \rightarrow m$ and a partition τ of σ_* .

We must construct partitions $\tau_1 = (\alpha_1, \dots, \alpha_k)$, $\tau_2 = (\beta_1, \dots, \beta_l)$ and partial isomorphisms $\sigma': k \rightarrow l$ and $\sigma_{ij}: \alpha_i \rightarrow \beta_j$ for $(i, j) \in \sigma'$, of appropriate sizes.

Since τ is a partition of a matrix, we easily obtain partitions τ_1, τ_2 of the rows and columns: define $\pi'_i \gamma = \pi_i \gamma \setminus \{*\}$, and let $\hat{\tau} = (\gamma_1, \dots, \gamma_p)$; then define $\tau_1 = (\pi'_1 \gamma_i)_i$ and $\tau_2 = (\pi'_2 \gamma_i)_i$

We can also construct partial isomorphisms from τ , by ignoring the pairs with *s, and taking the remaining pairs from each partition: let $\tau_1 = (\alpha_1, \dots, \alpha_k)$ and $\tau_2 = (\beta_1, \dots, \beta_l)$ and then define $\sigma' = \{(i, j) \mid (\alpha_i \times \beta_j) \cap \sigma_* \neq \emptyset\}$ and, for $(i, j) \in \sigma'$, define $\sigma_{ij} = (\alpha_i \times \beta_j) \cap \sigma_*$. Note that by this construction, σ is the union of these partial isomorphisms, as required.

Example: Let's take the σ of the previous example, with a new τ :

$$\sigma: 6 \longrightarrow 5 = \{(3, 5), (4, 4), (6, 1)\}$$

$$\text{so } \sigma_* = \{(3, 5), (4, 4), (6, 1), (1, *), (2, *), (5, *), (*, 2), (*, 3)\}$$

$$\tau = (((3, 5)), ((4, 4), (6, 1)), ((1, *), (2, *), (*, 3)), ((5, *), (*, 2)))$$

Then we obtain

$$\tau_1 = ((3), (4, 6), (1, 2), (5)) \quad \text{and} \quad \tau_2 = ((5), (4, 1), (3), (2))$$

(note $k = l = 4$, and $n = 6$, $m = 5$ as required).

Then

$$\sigma' = \{(1, 1), (2, 2)\}$$

(since $\{(3, 5)\}$ is a pair from σ_* coming from the first partition in τ_1 and the first partition in τ_2 , and $\{(4, 4), (6, 1)\}$ are pairs in σ_* coming from the second partition in τ_1 and the second partition in τ_2).

Also

$$\sigma_{11} = \{(6, 1)\} \quad \text{and} \quad \sigma_{22} = \{(4, 4), (3, 5)\}$$

whose union is the $\sigma: 6 \rightarrow 5 = \{(3, 5), (4, 4), (6, 1)\}$ we started with.

And this completes the construction. (That these processes are inverse we leave as homework!)

What's going on?

This time we have the following selection from the variable base:

$$\left(\begin{array}{cc} \left(\boxed{a_{3,5}} \right) & \left(a_{3,4} \ a_{6,3} \right) & \left(a_{3,3} \right) & \left(a_{3,2} \right) \\ \left(\begin{array}{cc} \boxed{a_{4,4}} & a_{4,1} \\ a_{6,4} & \boxed{a_{6,1}} \end{array} \right) & & \left(a_{4,3} \right) & \left(a_{4,2} \right) \\ \left(a_{4,5} \right) & & \left(a_{6,3} \right) & \left(a_{6,2} \right) \\ \left(a_{6,5} \right) & & & \\ \left(a_{1,5} \right) & \left(a_{1,4} \ a_{1,1} \right) & \left(a_{1,3} \right) & \left(a_{1,2} \right) \\ \left(a_{2,5} \right) & \left(a_{2,4} \ a_{2,1} \right) & \left(a_{2,3} \right) & \left(a_{2,2} \right) \\ \left(a_{5,5} \right) & \left(a_{5,4} \ a_{5,1} \right) & \left(a_{5,3} \right) & \left(a_{5,2} \right) \end{array} \right)$$

and the common function term corresponding to this is

$$g_6(x) \cdot (f_1(x) \cdot a_{35}) \cdot (f_2(x) \cdot a_{44} \cdot a_{61}) \cdot (f_2(x) \cdot a_{1*} \cdot a_{2*}) \cdot (f_1(x) \cdot a_{5*}) \cdot (f_1(x) \cdot a_{*3}) \cdot (f_1(x) \cdot a_{*2})$$

Coalgebras

Suppose \mathbb{X} , $\mathcal{D}: \mathbb{X} \rightarrow \text{Faà}(\mathbb{X})$ is a coalgebra (so $\epsilon\mathcal{D} = 1$, $\mathcal{D}\text{Faà}(\mathcal{D}) = \mathcal{D}\delta$).

What is the effect of \mathcal{D} on objects?

Let $\mathcal{D}(X) = (\mathcal{D}_0(X), \mathcal{D}_1(X))$; then

$X = \epsilon(\mathcal{D}(X)) = \epsilon(\mathcal{D}_0(X), \mathcal{D}_1(X)) = \mathcal{D}_1(X)$ so $\mathcal{D}_1(X) = X$.

Also

$$\begin{aligned} (\mathcal{D}\text{Faà}(\mathcal{D}))(X) &= \text{Faà}(\mathcal{D})(\mathcal{D}(X)) = \\ & \text{Faà}(\mathcal{D})(\mathcal{D}_0(X), X) = ((\mathcal{D}_0(\mathcal{D}_0(X)), \mathcal{D}_0(X))(\mathcal{D}_0(X), X)) \end{aligned}$$

And

$$(\mathcal{D}\delta)(X) = \delta(\mathcal{D}_0(X), X) = ((\mathcal{D}_0(X), \mathcal{D}_0(X)), (\mathcal{D}_0(X), X))$$

so $\mathcal{D}_0(\mathcal{D}_0(X)) = \mathcal{D}_0(X)$, *i.e.* \mathcal{D}_0 is an idempotent. But since $\mathcal{D}_0(X) = \mathcal{D}_1(X) = X$, in fact \mathcal{D}_0 is identity on objects.

Since the bundle fibration is included in the Faà di Bruno fibration, we know (BCS, TAC2009) \mathcal{D} induces a differential structure satisfying [CD.1]–[CD.5]:

The differential combinator $D[f]$ is the second component $f^{(1)}$ of $\mathcal{D}(f) := (f, f^{(1)}, f^{(2)}, \dots)$.

But [CD.6], [CD.7] ... ?

For that we consider the effect of \mathcal{D} on morphisms.

On morphisms: Write $\mathcal{D}(f) = (f, f^{(1)}, f^{(2)}, \dots)$. The coalgebra equation for δ tells us these are equal:

$$\text{Faà}(\mathcal{D})(\mathcal{D}(f)) = \begin{pmatrix} f & f^{(1)} & f^{(2)} & f^{(3)} & f^{(4)} & \dots \\ f^{(1)} & (f^{(1)})^{(1)} & (f^{(2)})^{(1)} & (f^{(3)})^{(1)} & (f^{(4)})^{(1)} & \dots \\ f^{(2)} & (f^{(1)})^{(2)} & (f^{(2)})^{(2)} & (f^{(3)})^{(2)} & (f^{(4)})^{(2)} & \dots \\ f^{(3)} & (f^{(1)})^{(3)} & (f^{(2)})^{(3)} & (f^{(3)})^{(3)} & (f^{(4)})^{(3)} & \dots \\ f^{(4)} & (f^{(1)})^{(4)} & (f^{(2)})^{(4)} & (f^{(3)})^{(4)} & (f^{(4)})^{(4)} & \dots \\ \dots & & & & & \dots \end{pmatrix}$$

$$\delta(\mathcal{D}(f)) = \begin{pmatrix} f & \mathcal{D}(f)_*^{[1]} & \mathcal{D}(f)_*^{[2]} & \mathcal{D}(f)_*^{[3]} & \mathcal{D}(f)_*^{[4]} & \dots \\ f^{(1)} & \mathcal{D}(f)_1^{[1]} & \mathcal{D}(f)_1^{[2]} & \mathcal{D}(f)_1^{[3]} & \mathcal{D}(f)_1^{[4]} & \dots \\ f^{(2)} & \mathcal{D}(f)_2^{[1]} & \mathcal{D}(f)_2^{[2]} & \mathcal{D}(f)_2^{[3]} & \mathcal{D}(f)_2^{[4]} & \dots \\ f^{(3)} & \mathcal{D}(f)_3^{[1]} & \mathcal{D}(f)_3^{[2]} & \mathcal{D}(f)_3^{[3]} & \mathcal{D}(f)_3^{[4]} & \dots \\ f^{(4)} & \mathcal{D}(f)_4^{[1]} & \mathcal{D}(f)_4^{[2]} & \mathcal{D}(f)_4^{[3]} & \mathcal{D}(f)_4^{[4]} & \dots \\ \dots & & & & & \dots \end{pmatrix}$$

(which is enough to guarantee [CD.6] & [CD.7]):

(Why?)

$$\begin{aligned} \text{Since } (f^{(1)})^{(1)} &= \mathcal{D}(f)_1^{[1]}, \\ \left(\begin{array}{c|c} a_{1,1} & x_1 \\ a_{*,1} & x \end{array} \right) &\mapsto (f^{(1)})^{(1)} \begin{pmatrix} x_1 \\ x \end{pmatrix} \cdot \begin{pmatrix} a_{1,1} \\ a_{*,1} \end{pmatrix} \\ &= f^{(2)}(x) \cdot a_{*,1} \cdot x_1 + f^{(1)}(x) \cdot a_{1,1} \end{aligned}$$

Setting $a_{*,1} = 0$ which yields **[CD.6]**:

$$(f^{(1)})^{(1)} \begin{pmatrix} x_1 \\ x \end{pmatrix} \cdot \begin{pmatrix} a_{1,1} \\ 0 \end{pmatrix} = f^{(1)}(x) \cdot a_{1,1}$$

and setting $a_{1,1} = 0$ yields **[CD.7]**:

$$\begin{aligned} &(f^{(1)})^{(1)} \begin{pmatrix} x_1 \\ x \end{pmatrix} \cdot \begin{pmatrix} 0 \\ a_{*,1} \end{pmatrix} \\ &= f^{(2)}(x) \cdot a_{*,1} \cdot x_1 \\ &= f^{(2)}(x) \cdot x_1 \cdot a_{*,1} \\ &= (f^{(1)})^{(1)} \begin{pmatrix} a_{*,1} \\ x \end{pmatrix} \cdot \begin{pmatrix} 0 \\ x_1 \end{pmatrix} \end{aligned}$$

It is worth noticing that we have in fact proved more: the coalgebra is in the following sense determined by the differential combinator of the Cartesian differential category: each $f^{(n)}$ is in fact determined by $D[f] = f^{(1)}$.

For, as we have just seen,

$$\begin{aligned}
 \mathcal{D}(f)_1^{[1]} \left(\begin{array}{c|c} 0 & a_1 \\ \hline a_{*1} & x \end{array} \right) &= (f^{(1)})^{(1)} \left(\begin{array}{c} a_{1*} \\ x \end{array} \right) \cdot \left(\begin{array}{c} 0 \\ a_{*1} \end{array} \right) \\
 &= f^{(2)}(x) \cdot a_{*1} \cdot a_{1*} + f^{(1)}(x) \cdot 0 \\
 &= f^{(2)}(x) \cdot a_{*1} \cdot a_{1*} + 0 \\
 &= f^{(2)}(x) \cdot a_{*1} \cdot a_{1*}
 \end{aligned}$$

In this manner, we can reconstruct $f^{(2)}$ from $(f^{(1)})^{(1)}$, and similarly (by induction) $f^{(n+1)}$ from $(f^{(n)})^{(1)}$.

So we have proved

Proposition *Every coalgebra of the Faà di Bruno comonad is a Cartesian differential category. And moreover, the coalgebra structure is determined by the induced differential operator.*

To prove the converse involves some calculations using the term calculus of Cartesian differential categories. Here are some highlights.

Higher order derivatives

Define $\frac{d^{(1)}t}{dx}(s) \cdot a = \frac{dt}{dx}(s) \cdot a$ and

$$\frac{d^{(n)}t}{dx}(s) \cdot a_1 \cdot \dots \cdot a_n = \frac{d \frac{d^{(n-1)}t}{dx}(x) \cdot a_1 \cdot \dots \cdot a_{n-1}}{dx}(s) \cdot a_n$$

Then

$$\frac{dt[x+s/y]}{dx}(0) \cdot a = \frac{dt}{dy}(s) \cdot a \quad (x \text{ not free in } s)$$

$$\frac{d^{(2)}t}{dx}(s) \cdot a_1 \cdot a_2 = \frac{d^{(2)}t}{dx}(s) \cdot a_2 \cdot a_1 \quad (x \text{ not free in } a_1, a_2)$$

$$\frac{d^{(n)}t}{dx}(s) \cdot a_1 \cdot \dots \cdot a_n = \frac{d^{(n)}t}{dx}(s) \cdot a_{\sigma(1)} \cdot \dots \cdot a_{\sigma(n)} \quad (\text{for any } \sigma \in \mathcal{S}_n.)$$

$$\frac{d \frac{d^{(n)}t}{dz}(s) \cdot a_1 \cdot \dots \cdot x \cdot \dots \cdot a_n}{dx}(s') \cdot a_r = \frac{d^{(n)}t}{dz}(s) \cdot a_1 \cdot \dots \cdot a_r \cdot \dots \cdot a_n$$

$$\begin{aligned} \frac{d \frac{dt}{dx}(p) \cdot a}{dy}(p') \cdot a' &= \frac{d^{(2)}t}{dx}(p[p'/y]) \cdot a[p'/y] \cdot \left(\frac{dp}{dy}(p') \cdot a' \right) \\ &\quad + \frac{dt}{dx}(p[p'/y]) \cdot \left(\frac{da}{dy}(p') \cdot a' \right) \quad (\text{for } y \notin t) \end{aligned}$$

Corollary: *In any cartesian differential category:*

$$\frac{d^{(n)}g(f(x))}{dx} (z) \cdot a_1 \cdot \dots \cdot a_n = (f \star g)_{\mathcal{I}_2^{a_1, \dots, a_n}}(z)$$

Furthermore

$$\frac{d^{(m)}f_n(f_{n-1}(\dots(f(x))\dots))}{dx} (z) \cdot a_1 \cdots a_m = (f_1 \star f_2 \star \dots \star f_n)_{\mathcal{I}_n^{a_1, \dots, a_m}}(z)$$

In other words, the higher order derivatives connect with the Faà di Bruno convolution in exactly the right way, ...

... and so (after some technical calculations!):

Theorem *Cartesian differential categories are exactly coalgebras of the Faà di Bruno comonad.*