

Compositional Taylor expansion

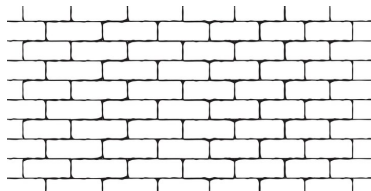
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IRIF

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Compositionality

*"Composing the
meaning of parts
into the meaning of
the whole."
(Milner)*



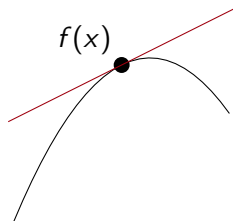
This talk

Differential calculus + Compositionality

Differential calculus

A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is derivable at $x \in \mathbb{R}$ if

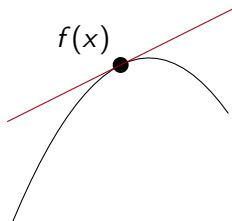
$$f(x + u) = f(x) + f'(x) \cdot u + O(u^2)$$



Differential calculus

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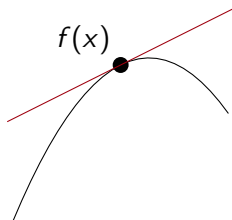
It is two time derivable at x if

$$f(x + u) = f(x) + f'(x) \cdot u + \frac{1}{2}f^{(2)}(x) \cdot u^2 + O(u^3)$$

Differential calculus

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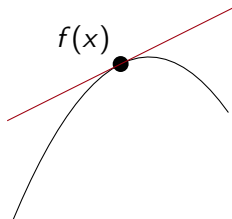
Order n Taylor expansion.

$$f(x + u) = \sum_{k=0}^n \frac{1}{k!} f^{(k)}(x) \cdot u^k + O(u^{n+1})$$

Differential calculus

A function $f : E \rightarrow F$ is derivable at $x \in E$ if

$$f(x + u) = f(x) + f'(x) \cdot u + O(\|u\|^2)$$



It is two time derivable at x if

$$f(x + u) = f(x) + f'(x) \cdot u + \frac{1}{2}f^{(2)}(x) \cdot (u, u) + o(\|u\|^3)$$

Order n Taylor expansion.

$$f(x + u) = \sum_{k=0}^n \frac{1}{k!} f^{(k)}(x) \cdot \underbrace{(u, \dots, u)}_{k \text{ times}} + O(\|u\|^{n+1})$$

Why differential calculus and compositionality matters

- ▶ Automated differentiation
- ▶ Differential λ -calculus and differential Linear Logics
- ▶ Categorical differentiation

Why differential calculus and compositionality matters

- ▶ **Automated differentiation**
- ▶ Differential λ -calculus and differential Linear Logics
- ▶ Categorical differentiation

Automated differentiation:

Compute derivative of programs $P : \mathbb{R}^k \rightarrow \mathbb{R}^l$

- ▶ Very large programs;
- ▶ Allow to perform gradient descent;
- ▶ Used in probabilistic programming.

Why differential calculus and compositionality matters

- ▶ Automated differentiation
- ▶ **Differential λ -calculus and differential Linear Logics**
- ▶ Categorical differentiation

Quantitative properties of programs

- ▶ linear: uses the input exactly once
- ▶ n -linear: uses the input exactly n -times

Taylor Expansion

$$(\lambda x. P)Q \rightsquigarrow \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\partial^n P}{\partial x^n} \cdot \underbrace{(Q, \dots, Q)}_{n \text{ times}} \right) [0/x]$$

Why differential calculus and compositionality matters

- ▶ Automated differentiation
- ▶ Differential λ -calculus and differential Linear Logics
- ▶ **Categorical differentiation**

Categorical differentiation

- ▶ Axiomatization of a derivative in a category
- ▶ At first: models of the differential λ -calculus
- ▶ Became a field on its own

Also: Proof of correctness of AD based on category theory, see Mazza and Pagani 2021; Huot et al. 2023

Choose your fighter

Analysis

- ▶ X, Y, Z : Vector spaces $\mathbb{R}^n$
- ▶ $f, g : X \rightarrow Y$: smooth functions
- ▶ $f'(x) \cdot u$: derivative

Categories

- ▶ X, Y, Z : Objects
- ▶ $f, g : X \rightarrow Y$: Morphisms
- ▶ $f'(x) \cdot u$: derivative, Blute, Cockett, and Seely 2009

Very few category theory will appear in this talk.

How do we make derivative
compositional ?

Fixing the chain rule

$$(g \circ f)'(x) = g'(f(x)) \circ f'(x)$$



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Tangent bundle

$$\frac{f : X \rightarrow Y}{Tf : X \times X \rightarrow Y \times Y}$$

$$Tf(x, u) = (f(x), f'(x) \cdot u)$$

$$T(g \circ f) = Tg \circ Tf$$



Fixing the chain rule

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Dual number intuition

$$(x, u) \in TX \iff \text{polynomial } x + u\varepsilon \text{ with } \varepsilon^2 = 0$$

$$f(x + u\varepsilon) = f(x) + \varepsilon f'(x) \cdot u + O(\varepsilon^2)$$

Fixing the chain rule

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$Tf(x, u)$: the **push forward** above

Fixing the higher order chain rule

Faà di Bruno formula: **bad** (and terrifying)



$$(g \circ f)^{(n)}(x) = \sum_{\{l_1, \dots, l_k\} \text{ partition of } \llbracket 1, n \rrbracket} g^{(k)}\left(\cancel{f(x)}, \cancel{f^{(l_1)}(x)}, \dots, f^{(l_k)}(x)\right)$$

with $f^{(\{i_1, \dots, i_l\})}(x) : (u_1, \dots, u_n) \mapsto \cancel{f^{(l)}(x)}(u_{i_1}, \dots, u_{i_l})$

Fixing the higher order chain rule

Faà di Bruno formula: **bad** (and terrifying)



$$(g \circ f)^{(n)}(x) = \sum_{\{l_1, \dots, l_k\} \text{ partition of } \llbracket 1, n \rrbracket} g^{(k)}(f(x), f^{(l_1)}(x), \dots, f^{(l_k)}(x))$$

with $f^{(\{i_1, \dots, i_l\})}(x) : (u_1, \dots, u_n) \mapsto f^{(l)}(x)(u_{i_1}, \dots, u_{i_l})$

Iterated tangent bundle

$$T^n(g \circ f) = T^n g \circ T^n f$$



What hides in the iterated tangent bundle ?

$$a \in T^n X \iff a(\varepsilon_1, \dots, \varepsilon_n) \text{ polynomial with } \varepsilon_i^2 = 0$$

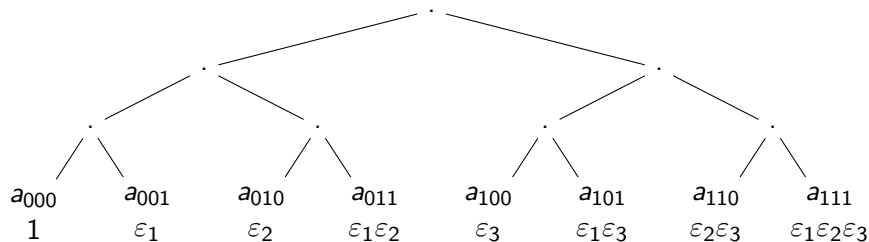


Figure: Graphical representation of an element of $T^3 X$

$T^n f : T^n X \rightarrow T^n Y$: **pushes forward** polynomials

What do I mean by pushes forward ?

$$a(\varepsilon_1, \varepsilon_2) = x + u\varepsilon_1 + v\varepsilon_2 + w\varepsilon_1\varepsilon_2 \in T^2X$$

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Computation of $T^2f(a)$

Let $b = a - x$. By Taylor expansion,

$$f(a) = f(x) + f'(x) \cdot b + \frac{1}{2}f^{(2)}(x) \cdot (b, b) + \cancel{O(b^3)}$$

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- ▶ Develop by linearity and bilinearity
- ▶ Simplify by $\varepsilon_1^2 = \varepsilon_2^2 = 0$.

The resulting polynomial is $T^2f(a)$

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$$f(x) + \varepsilon_1 f'(x) \cdot u + \varepsilon_2 f'(x) \cdot v + \varepsilon_1 \varepsilon_2 \left(f^{(2)}(x) \cdot (u, v) + f'(x) \cdot w \right)$$

$Tf(x, u) = (f(x), f'(x) \cdot u)$: order 1 Taylor expansion

Let us do the same
for Taylor expansion

A compositional Taylor expansion

Tangent bundle

$$TX = X \times X \qquad \frac{f : X \rightarrow Y}{Tf : TX \rightarrow TY}$$

A compositional Taylor expansion

Taylor bundle

$$T_n X = X \times X^n$$

$$\frac{f : X \rightarrow Y}{T_n f : T_n X \rightarrow T_n Y}$$

A compositional Taylor expansion

Taylor bundle

$$T_n X = X \times X^n \qquad \frac{f : X \rightarrow Y}{T_n f : T_n X \rightarrow T_n Y}$$

Higher order dual numbers intuition

$$(x, u, v) \in T_2 X \iff \text{polynomial } x + u\varepsilon + v\varepsilon^2 \text{ with } \varepsilon^3 = 0$$

$T_2 f(x, u, v)$: **push forward** of polynomial.

A compositional Taylor expansion

Taylor bundle

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$T_2 f(x, u, v)$: **push forward** of polynomial.

$$f(x + u\varepsilon + v\varepsilon^2) = f(x) + f'(x) \cdot (u\varepsilon + v\varepsilon^2) + \frac{1}{2}f^{(2)}(x) \cdot (u\varepsilon + v\varepsilon^2, u\varepsilon + v\varepsilon^2)$$

$$T_2 f(x, u, v) = \left(f(x), f'(x) \cdot u, \frac{1}{2}f^{(2)}(x) \cdot (u, u) + f'(x) \cdot v \right)$$

A compositional Taylor expansion

Taylor bundle

$$T_n X = X \times X^n \qquad \frac{f : X \rightarrow Y}{T_n f : T_n X \rightarrow T_n Y}$$

Higher order dual numbers intuition

$$a \in T_n X \iff \text{polynomial } \sum_{k=0}^n a_k \varepsilon^k \text{ with } \varepsilon^{n+1} = 0$$

$T_n f(a)$: **push forward** of polynomial a , computed as follows

- ▶ Order n Taylor expansion of $f \left(a_0 + \sum_{k=1}^n a_k \varepsilon^k \right)$ at a_0
- ▶ Develop by multilinearity
- ▶ Simplify by $\varepsilon^{n+1} = 0$.

A compositional Taylor expansion

$$\pi_i(\mathsf{T}_n f(x, u_1, \dots, u_n)) = \sum_{k=1}^j \sum_{\substack{i_1, \dots, i_k \text{ s.t.} \\ i_1 + \dots + i_k = j}} \frac{1}{k!} f^{(k)} \circ (x, u_{i_1}, \dots, u_{i_k}) \quad (1)$$

A compositional Taylor expansion

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Generalizes Taylor expansion

$$\mathsf{T}_n f(x, u, 0, \dots, 0) = \left(\frac{1}{k!} f^{(k)}(x) \cdot (u, \dots, u) \right)_{k=0}^n$$

Is compositional

$$\mathsf{T}_n(g \circ f) = \mathsf{T}_n g \circ \mathsf{T}_n f$$

Proof: by... equation 1 ?



A simpler proof by abstract nonsense

$$\mathsf{T}^2 f(x, u, v, w) = \left(f(x), f'(x) \cdot u, f'(x) \cdot v, f^{(2)}(x) \cdot (u, v) + f'(x) \cdot w \right)$$

$$\mathsf{T}_2 f(x, u, v) = \left(f(x), f'(x) \cdot u, \frac{1}{2} f^{(2)}(x) \cdot (u, u) + f'(x) \cdot v \right)$$

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A natural transformation

$$\text{injection } L_n : T_n \rightarrow T^n X \quad (T_n X = X \times X^n \quad T^n X = X^{2^n})$$

$$T^n f \circ L_n = L_n \circ T_n f \quad \text{☺}$$

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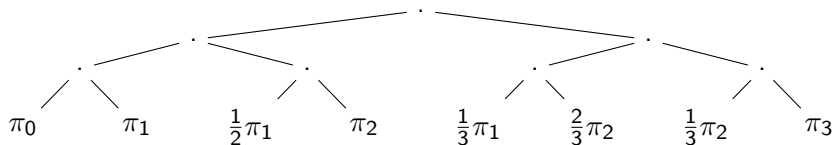


Figure: Graphical representation of L_3

A simpler proof by abstract nonsense

$$L_n \circ T_n(g \circ f) = T^n(g \circ f) \circ L_n = T^n g \circ T^n f \circ L_n = L_n \circ T_n g \circ T_n f$$

A natural transformation

injection $L_n : T_n \rightarrow T^n X$ ($T_n X = X \times X^n$ $T^n X = X^{2^n}$)

$$T^n f \circ L_n = L_n \circ T_n f \quad \text{☺}$$

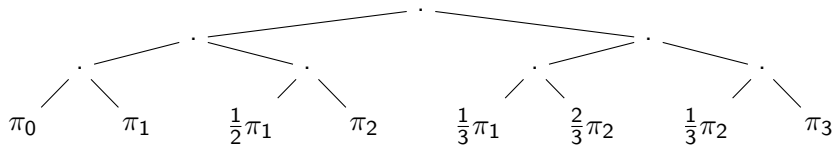


Figure: Graphical representation of L_3

- ▶ $T_n(g \circ f) = T_n g \circ T_n f$: functoriality equation
- ▶ $L_n : T_n X \rightarrow T^n X$: naturality equation

Category theory

Compute on Taylor expansions
without writing them down

The monad T

What is a monad ?

Monads: a way to produce effect

- ▶ $V : X \rightarrow Y$: pure computation
- ▶ $C : X \rightarrow \mathbf{T}Y$: **effectful** computation

The monad T

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Monads: a way to produce effect

- ▶ $V : X \rightarrow Y$: pure computation
 - ▶ $C : X \rightarrow \mathbf{T}Y$: **effectful** computation
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- ▶ $\mathbf{T}Y = Y \cup \{\text{fail}\}$: option monad.

The monad T

What is a monad ?

Monads: a way to produce effect

- ▶ $V : X \rightarrow Y$: pure computation
 - ▶ $C : X \rightarrow TY$: **effectful** computation
-
- ▶ $TY = Y \cup \{\text{fail}\}$: option monad.
 - ▶ $TY = Y \times \Sigma^*$: output monad

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Monads: a way to produce effect

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Two main ingredients

Return : $\text{return} : X \rightarrow TX$

The monad T

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Monads: a way to produce effect

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 - ▶ $C : X \rightarrow \mathbf{T}Y$: **effectful** computation
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Two main ingredients

Return : $\text{return} : X \rightarrow TX$

Bind : $\text{bind} : (X \rightarrow TY) \rightarrow (Y \rightarrow TZ) \rightarrow (X \rightarrow TZ)$

The monad T

What is a monad ?

Monads: a way to produce effect

- ▶ $V : X \rightarrow Y$: pure computation
 - ▶ $C : X \rightarrow \mathbf{T}Y$: **effectful** computation
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- ▶ $TY = Y \cup \{\text{fail}\}$: option monad.
 - ▶ $TY = Y \times \Sigma^*$: output monad

Two main ingredients

Return : $\text{return} : X \rightarrow TX$

Bind : $\text{bind} : (X \rightarrow TY) \rightarrow (Y \rightarrow TZ) \rightarrow (X \rightarrow TZ)$

Subject to 3 equations.

$$\text{bind}(\text{bind}(f, g), h) = \text{bind}(f, \text{bind}(g, h))$$

The monad T

$$f : X \rightarrow TY$$

$$f = f_0 + \varepsilon f_1 \quad f(x) = f_0(x) + f_1(x)\varepsilon$$

The monad T

$$f : X \rightarrow TY$$

$$f = f_0 + \varepsilon f_1 \quad f(x) = f_0(x) + f_1(x)\varepsilon$$

The return

$$\text{return} : X \rightarrow TX$$

$$\text{return}(x) = x$$

The monad T

$$f : X \rightarrow TY$$

$$f = f_0 + \varepsilon f_1 \quad f(x) = f_0(x) + f_1(x)\varepsilon$$

The return

$$\text{return} : X \rightarrow TX$$

$$\text{return}(x) = x$$

The bind

$$f = f_0 + \varepsilon f_1 : X \rightarrow TY \quad g = g_0 + \varepsilon g_1 : Y \rightarrow TZ$$

$$\text{binf}(f, g)(x) : X \rightarrow TZ$$

$$\text{bind}(f, g)(x) = g_0(f_0(x)) + \varepsilon(g'_0(f_0(x)) \cdot f_1(x) + g_1(f_0(x)))$$

The monad T_n

$$f : X \rightarrow T_n Y$$

$$f = f_0 + \varepsilon f_1 + \cdots + \varepsilon^n f_n \quad f(x) = f_0(x) + f_1(x) \varepsilon + \cdots + f_n(x) \varepsilon^n$$

The monad T_n

$$f : X \rightarrow T_n Y$$

$$f = f_0 + \varepsilon f_1 + \cdots + \varepsilon^n f_n \quad f(x) = f_0(x) + f_1(x) \varepsilon + \cdots + f_n(x) \varepsilon^n$$

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The monad T_n

$$f : X \rightarrow T_n Y$$

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The return

$$\text{return} : X \rightarrow T_n X$$

$$\text{return}(x) = x$$

The bind

$$f : X \rightarrow T_n Y \quad g : Y \rightarrow T_n Z$$

$$\text{bind}(f, g)(x) : X \rightarrow T_n Z$$

- ▶ Taylor expansion of each g_i at $f_0(x)$
- ▶ Develop by multilinearity and simplify by $\varepsilon^{n+1} = 0$
- ▶ Return the resulting polynomial

The bind

$$f : X \rightarrow T_n Y \quad g : Y \rightarrow T_n Z$$

$$\text{bind}(f, g)(x) : X \rightarrow T_n Z$$

- ▶ Taylor expansion of each g_i at $f_0(x)$
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The bind equation

$$\text{bind}(\text{bind}(f, g), h) = \text{bind}(f, \text{bind}(g, h))$$

Do we really want to prove the equation above directly ? ☹️

Category saves the day

- ▶ **T is a monad**
- ▶ T^n is a monad
- ▶ $L_n : T^n X \rightarrow T^n X$ strikes again

Easy

Category saves the day

- ▶ T is a monad
- ▶ T^n **is a monad**
- ▶ $L_n : T^n X \rightarrow T^n X$ strikes again

Category theory tools
No computations, all induction

Distributive law $c : TT \Rightarrow TT$
and the Yang-Baxter equation

Category saves the day

- ▶ T is a monad
- ▶ T^n is a monad
- ▶ $L_n : T^n X \rightarrow T^n X$ **strikes again**

Same as the proof of $T_n(g \circ f) = T_n g \circ T_n f$

$L_n : T^n X \rightarrow T^n X$ becomes a **monad transformer**

Monad strengths:

$$\begin{aligned}\phi_1 : T_n X \times Y &\rightarrow T_n(X \times Y) \\ \phi_1 \left(\sum_{i=0}^n x_i \varepsilon^i, y \right) &= (x_0, y) + \sum_{i=1}^n (x_i, 0) \varepsilon^i\end{aligned}$$

Partial derivative

Monad strengths:

$$\begin{aligned}\phi_1 : T_n X \times Y &\rightarrow T_n(X \times Y) \\ \phi_1 \left(\sum_{i=0}^n x_i \varepsilon^i, y \right) &= (x_0, y) + \sum_{i=1}^n (x_i, 0) \varepsilon^i\end{aligned}$$

Partial derivatives

$$f : X \times Y \rightarrow Z$$

$$T_n^{\partial_1} f : T_n X \times Y \xrightarrow{\phi_1} T_n(X \times Y) \xrightarrow{T_n f} T_n Z$$

$$T_n^{\partial_2} f : X \times T_n Y \xrightarrow{\phi_2} T_n(X \times Y) \xrightarrow{T_n f} T_n Z$$

Category theory concepts captures Taylor expansion

Differential calculus	Category theory
Faá di Bruno	Functoriality of T_n
Dual numbers	Kleisli category of monad T_n
Schwarz theorem	Distributive law $c : T_n T_n \Rightarrow T_n T_n$
Partial derivatives	Monad strength
Multiple dual numbers $\varepsilon_1, \dots, \varepsilon_I$	Canonical monad $T_{n_1} \cdots T_{n_I}$

All proof on the category theory world: no combinatorics

We can also do
infinitary Taylor expansions

Infinitary Taylor expansion

Taylor functor

$$T_{\omega}X = X \times X \times X \times \dots$$

$$\frac{f : X \rightarrow Y}{T_{\omega}f : T_{\omega}X \rightarrow T_{\omega}Y}$$

Infinitary Taylor expansion

Taylor functor

$$T_{\omega}X = X \times X \times X \times \dots$$

$$\frac{f : X \rightarrow Y}{T_{\omega}f : T_{\omega}X \rightarrow T_{\omega}Y}$$

Higher order dual numbers intuition

$$a \in T_{\omega}X \iff \text{power series } \sum_{k=0}^{\infty} a_k \varepsilon^k$$

$T_n f(a)$: **push forward** of power series a .

- ▶ Taylor expansion of $f \left(a_0 + \sum_{k=1}^n a_k \varepsilon^k \right)$ at a_0
- ▶ Develop by multilinearity

This captures the theory of analytic maps

Analytic map:

$$f(x + u) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x) \cdot \underbrace{(u, \dots, u)}_{k \text{ times}}$$

This captures the theory of analytic maps

Analytic map:

$$f(x + u) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x) \cdot \underbrace{(u, \dots, u)}_{k \text{ times}}$$

A categorical approach to analyticity

Let $\sigma : T_{\omega}X \rightarrow X$ such that $\sigma(x_0, x_1, x_2, \dots) = \sum_{i=0}^{\infty} x_i$.

$$f \text{ analytic} \iff \sigma \circ T_{\omega}f = f \circ \sigma$$

This captures the theory of analytic maps

Analytic map:

$$f(x + u) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x) \cdot \underbrace{(u, \dots, u)}_{k \text{ times}}$$

A categorical approach to analyticity

Let $\sigma : T_{\omega}X \rightarrow X$ such that $\sigma(x_0, x_1, x_2, \dots) = \sum_{i=0}^{\infty} x_i$.

$$f \text{ analytic} \iff \sigma \circ T_{\omega}f = f \circ \sigma$$

Taylor expansion is a bimonad

To conclude

- ▶ A compositional approach to derivatives T
- ▶ A compositional approach to higher derivatives T^n
- ▶ A composition approach to order n Taylor expansion T_n
- ▶ A compositional approach to infinitary Taylor expansion T_ω

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No combinatorics on Taylor series

- ▶ All proof: rely on category theory
- ▶ The monad transformer $L_n : T_n X \rightarrow T^n X$.
- ▶ Categorical notions (Monad, strength, distributive law) correspond to properties of the differential calculus