Automatic Differentiation With Higher Infinitesimals

or: Computational Smooth Infinitesimal Analysis in Weil Algebra

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Slides available at: https://bit.ly/casc-smooth

Repository: github.com/konn/smooth

Today's Topic in short:

To Implement computational Higher Infinitesimal Analysis, utilising the connection between **Automatic Differentiation** and **Nilpotent Infinitesimal Analysis**, applying Gröbner basis technique

So what?

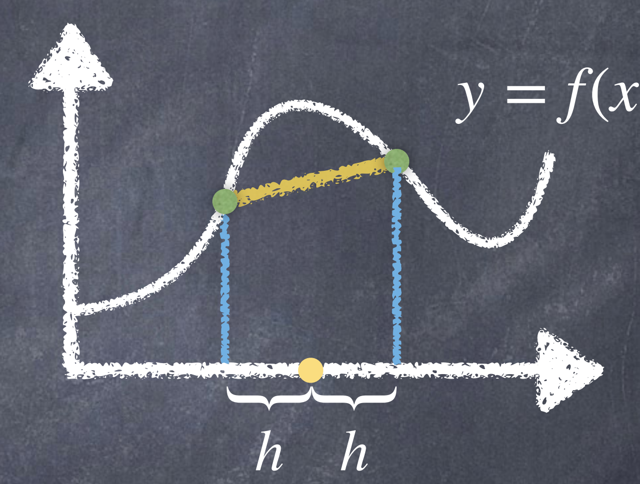
- **Automatic Differentiation** is a collection of methods to efficiently compute higher derivatives of the given function exploiting Chain Rule.
- **Nilpotent Infinitesimal Analysis:** an analysis using nilpotent infinitesimal such that $d^2 = 0$, $d \neq 0$. (Analysis in the era of Newton or Gauß)
  - Although such an infinitesimal real contradicts classically, it can be justified with topos theory and used to develop differential geometry (cf: **Synthetic Differential Geometry** by Lawvere et al.).
  - Such infinitesimals can be algebraically formulated as **Weil algebras.**
- Our Result:Combining Gröbner basis and Automatic Differentiation, we propose an algorithm to achieve infinitesimal analysis with general, higher infinitesimals associated with Weil algebras.
- We first explore the exact connection b/w AD and Nilpotent Analysis.

Automatic Differentiation (Forward-mode)

Three ways of differentiation

- **Automatic Differentiation** calculates differential coefficients efficiently and precisely, using Chain Rule.
- **Numerical Differentiation** replaces limits with small reals (e.g. Euler method)
  - Efficient, but only an approximation.
- **Symbolic Differentiation** expresses functions as symbolic ASTs and then differentiate them symbolically.
  - Exact, but easy to explode exponentially.

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



$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Automatic Differentiation (Forward mode)

A coefficient ring $\mathbb{R}$ value diff. coeff.

```
data AD a = AD { real :: a, inifinitesimal :: a }

AD f f' + AD g g' = AD (f + g) (f' + g')
AD f f' * AD g g' = AD (f * g) (f' * g + f * g')
sin (AD f f') = AD (sin f) (f' * cos f)
```

Linearity

Leibniz Rule

Chain Rule

- Basic Idea: Storing the value and differential coefficient simultaneously.
  - We use a shorthand: $\mathrm{AD}\ x\ y = x + y\mathrm{d}$.
- For $F: \mathbb{R} \to \mathbb{R}$, its AD version $\hat{F}: \mathrm{AD}_{\mathbb{R}} \to \mathrm{AD}_{\mathbb{R}}$ returns $F(f(x)) + \dfrac{\mathrm{d}}{\mathrm{d}x}F(f(x))\mathrm{d}$, regarding inputs as of form $f(x) + f'(x)\mathrm{d}$ for some function f.
- The differential of F at $x = a$ will be the coefficient of d in $\hat{F}(a + \mathrm{d})$.
  - $a + d$ corresp. to the differential at $x = a$ of identity function $f(x) = x$.

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Why does this work?

We can justify with this
with the concepts of
C^∞-ring and Weil algebra!

Justification

- Forward Mode AD corresponds to the dual number ring $\mathbb{R}[d] = \mathbb{R}[X]/(X^2)$, which has the canonical C^∞-ring structure
  - The law $d^2 = 0$ characterises the AD!

Def. (Lawvere)

A C^∞-ring is a commutative ring where the product-preserving map $A(f): A^n \to A$ is defined for any C^∞-function $f: \mathbb{R}^n \to \mathbb{R}$.

"Smooth multivariate function naturally lifts to A"

➡ More Rigorous Def

- Example: the ring $C^\infty(M)$ of real-valued smooth func. on a manifold M.
- Specifically, $\mathbb{R}[d]$ is an instance of Weil algebras, which is the speciall class of C^∞-rings with a nilpotent infinitesimal structure!

Power serieses form a C^∞-ring

Thm 2 (Lawvere)

The ring of multivariate formal power series $\mathbb{R}[[\mathbb{X}]]$ has the structure of C^∞-ring via Taylor expansion.

Idea

For $f : \mathbb{R}^n \xrightarrow{C^\infty} \mathbb{R}$, $g_1, \ldots, g_n \in \mathbb{R}[[\mathbb{X}]]$, we let:

$$\mathbb{R}[[\mathbb{X}]](f)(\overrightarrow{g}) := \sum_{\alpha \in \mathbb{N}^n} \frac{X^{\alpha}}{\alpha!} \mathrm{D}^{\alpha}(f \circ \langle g_1, \ldots, g_n \rangle)(\mathbf{0}).$$

Weil algebra

Def.

$\mathbb{R}$-vector space W is called a Weil algebra if there exists an ideal $I \subseteq \mathbb{R}[X_1, \ldots, X_n]$ such that

$W \cong \mathbb{R}[\mathbb{X}]/I$, and $(X_1, \ldots, X_n)^k \subseteq I$ for some k.

- Intuition: a real line augmented with nilpotent infinitesimals.
- Each variable X_i corresponds to an infinitesimal.
  - X_i is nilpotent in the quotient ring $\mathbb{R}[\mathbb{X}]/I$.
  - Specifically, it is finite dimensional as a vector-space; hence I is zero-dimensional ideal!

Weil ring is a C^∞-ring

Thm (Lawvere)

Any Weil algebra $W = \mathbb{R}[\mathbb{X}]/I$ has the canonical C^∞-structure.

This follows from the following lemma:

Lem 1

For any ring-theoretic ideal I on a C^∞-ring A, A/I has the canonical C^∞-structure induced by the quotient map:

$$(A/I)(f)([x_1]_I, \ldots, [x_m]_I) := \left[A(f)(x_1, \ldots, x_m)\right]_I$$

- Since I is zero-dimensional, $\mathbb{R}[\![X]\!]/I \cong \mathbb{R}[X]/I$ is a C^∞-ring.
- In particular, dual number ring $\mathbb{R}[d] \cong \mathbb{R}[X]/(X^2)$ is also a C^∞-ring!

The C^∞-structure of $\mathbb{R}[d]$

- We let $f(a + b\mathrm{d}) = f(a) + bf'(a)\mathrm{d}$ for the univariate case.
- What about multivariate case $f : \mathbb{R}^n \xrightarrow{C^\infty} \mathbb{R}$?
  - This can be calculated from the C^∞-structure of the univariate formal power series ring by cutting-off the terms at the degree 1 and replacing X with d.

The C^∞-structure of $\mathbb{R}[d]$

Letting $g_i = a_i + b_i X$ $(i = 1,\ldots,n)$,

$$\begin{aligned}
&\mathbb{R}[\![X]\!](f)(\overrightarrow{g}) \\
&= f(\overrightarrow{g}(0)) + \frac{\mathrm{d}}{\mathrm{d}x}(f \circ \langle g_1, \ldots, g_n \rangle)(0)X + \ldots \\
&= f(a_1, \ldots, a_n) + (g_1'(0) + \ldots g_n'(0)) \cdot f'(g_1(0), \ldots, g_n(0))\ X + \ldots \\
&= f(a_1, \ldots, a_n) + (b_1 + \ldots + b_n) \cdot f'(a_1, \ldots, a_n)\ X + \ldots
\end{aligned}$$

Hence, by quotienting by $I = (X^2)$, we have

$$\mathbb{R}[d](f)(a_1 + b_1 d, \ldots, a_n + b_n d) = f(\overrightarrow{a}) + (b_1 + \ldots + b_n) f'(\overrightarrow{a}) \cdot d\,.$$

This coincides with the definition of AD when $n = 1$!

Summary

- (Forward Mode) Automatic Differentiation is a method to compute differentials of composite functions of smooth maps efficiently and precisely by storing the direct value and differential coefficient at some point simultaneously.
- This can be viewed as utilising the structure of C^∞-ring of the dual number ring $\mathbb{R}[d] = \mathbb{R}[X]/(X^2)$.
- The dual number ring is an instance of Weil algebra which axiomatises the real line with nilpotent infinitesimal.

Dual Number Ring and Smooth Infinitesimal Analysis

Why Weil algebras?

Q. Why we have referred to Weil algebra and C^∞-rings, instead of just saying "Forward-mode AD can be justified by Taylor expansion of smooth maps"?

A. To generalise Forward Mode AD to multivariate / higher-order differentials and higher-order nilpotent infinitesimals.

Higher-order diff. with Weil algebras

- A tensor of the dual number rings can be used to compute higher derivatives. Let:

$$\mathbb{R}[d_1, \ldots, d_n] = \mathbb{R}[X_1, \ldots, X_n]/(X_i^2 \mid i \leq n) \cong \underbrace{\mathbb{R}[d] \otimes_{\mathbb{R}} \ldots \otimes_{\mathbb{R}} \mathbb{R}[d]}_{n\text{-copies}}$$

- Then, by an easy induction, we have:

$$\mathbb{R}[\overrightarrow{d}](f)(x + d_1 + \ldots + d_n) = \sum_{0 \leq i \leq n} f^{(i)}(x)\sigma_n^i(\overrightarrow{d}),$$

where σ_k^i is the k-variate elementary symmetric expr. of degree i.

- In particular, we can get k-th derivative of f by looking at the coefficient of $d_1 \ldots d_k$ of $\mathbb{R}[\overrightarrow{d}](f)(x + d_1 + \ldots + d_n)$!
  - It has all the information of derivatives up to nth
- Likewise, higher derivatives of multivariate functions can be computed by a finite tensor products of the dual number rings.

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Our Contribution

Further Generalisation

- The structure of a Weil algebra $W = \mathbb{R}[\mathbb{X}]/I$ is determined by an ideal I with $(X_1, \ldots, X_n) \subseteq \sqrt{I}$.
- W is a finite-dimensional vector space; i.e, I is zero-dimensional.
  - We can employ Gröbner basis algorithms to compute their $\mathbb{R}$-algebra structure.
- For C^∞-structures of infinitesimal, we can first calculate in the formal power series ring, cutoff at the appropriate degree and take the quotient map.
  - In this way, we can do the calculation in the space with general nilpotent infinitesimals on computers!

Weil algebra Test

Algorithm 1 (WeilTest)

- Input: a polynomial ideal $I \subseteq \mathbb{R}[\mathbf{X}]$
- Is $I \subseteq \mathbb{R}[\mathbb{X}]$ a zerodimensional ideal? No → Not a Weil algebra
- Computer the Gröbner basis of $\sqrt{I}$ with Gröbner algorithms
- $X_1, \ldots, X_n \overset{?}{\in} \sqrt{I}$
    - No → Not a Weil algebra
    - Yes → Returns monomial basis, an upper bound of multidegree, and the multiplication table ([6])

- With these information, algebraic operations on Weil algebra W is easy.
- In our paper, we also returns the expression of nontrivial monomials as the linear combination of basis for the sake of efficiency.

C^∞-structure of Weil algebra

- Lem 1: the C^∞-structu.re of a Weil algebra is given by the quotienting that of $\mathbb{R}[\![X]\!]$.
- By Thm. 2, the C^∞-structure of $\mathbb{R}[\![X]\!]$ is given by:

$$\mathbb{R}[\![\mathbf{X}]\!](f)(g_1, \ldots, g_m) = \sum_{\alpha \in \mathbb{N}^n} \frac{\mathbf{X}^\alpha}{\alpha!} D^\alpha \left(f \circ \langle g_1, \ldots, g_m \rangle\right)(\mathbf{0})\,.$$

- We need an arbitrary partial derivatives of composite functions.
    - In general, AD calculating higher-order derivatives of multivariate functions is called Tower-mode AD.
    - Tower-mode AD and $\mathbb{R}[\![\mathbf{X}]\!]$ coincides modulo the factor of $\alpha! = \alpha_1! \cdot \cdots \cdot \alpha_m!$.
- Here, we think about C^∞-maps, derivatives are commutative.
    - We proposed, in [9], a variant of Tower AD optimised for this case (Appendix)

Computing C^∞-structure of Weil algebra

Algorithm 2 (LiftWeil)

- Input: $f : \mathbb{R}^n \xrightarrow{C^\infty} \mathbb{R}$ a smooth map admitting Tower AD,
  Information of Weil algebra $W = \mathbb{R}[X_1, \ldots, X_n]/I$ given by Alg. 1 (Especially, monomial basis $\left\{\boldsymbol{X}^{\boldsymbol{\beta}_1}, \ldots, \boldsymbol{X}^{\boldsymbol{\beta}_k}\right\}$ and multidegree upper bound $\boldsymbol{\alpha}$ of W), and an element $\overrightarrow{w} = (w_1, \ldots, w_n) \in W^n$.
- Output: $W(f)(\overrightarrow{w}) \in W$: given by C^∞-structure of W.

1. Take the representative polynomials $\overrightarrow{g}$ of $\overrightarrow{w}$.
2. Calculate $h \in \mathbb{R}[X]$ given by cutting off $\mathbb{R}[\![\mathbf{X}]\!](f)(\overrightarrow{g})$ at the upper bound $\boldsymbol{\alpha}$ (Using Tower AD and multiply by factorial).
3. Calculates $\bar{h}^G = \sum_{i \leq k} c_k \boldsymbol{X}^{\boldsymbol{\beta}_k}$ and return $(c_1, \ldots, c_k)$.

Application 1: More efficient higher derivatives

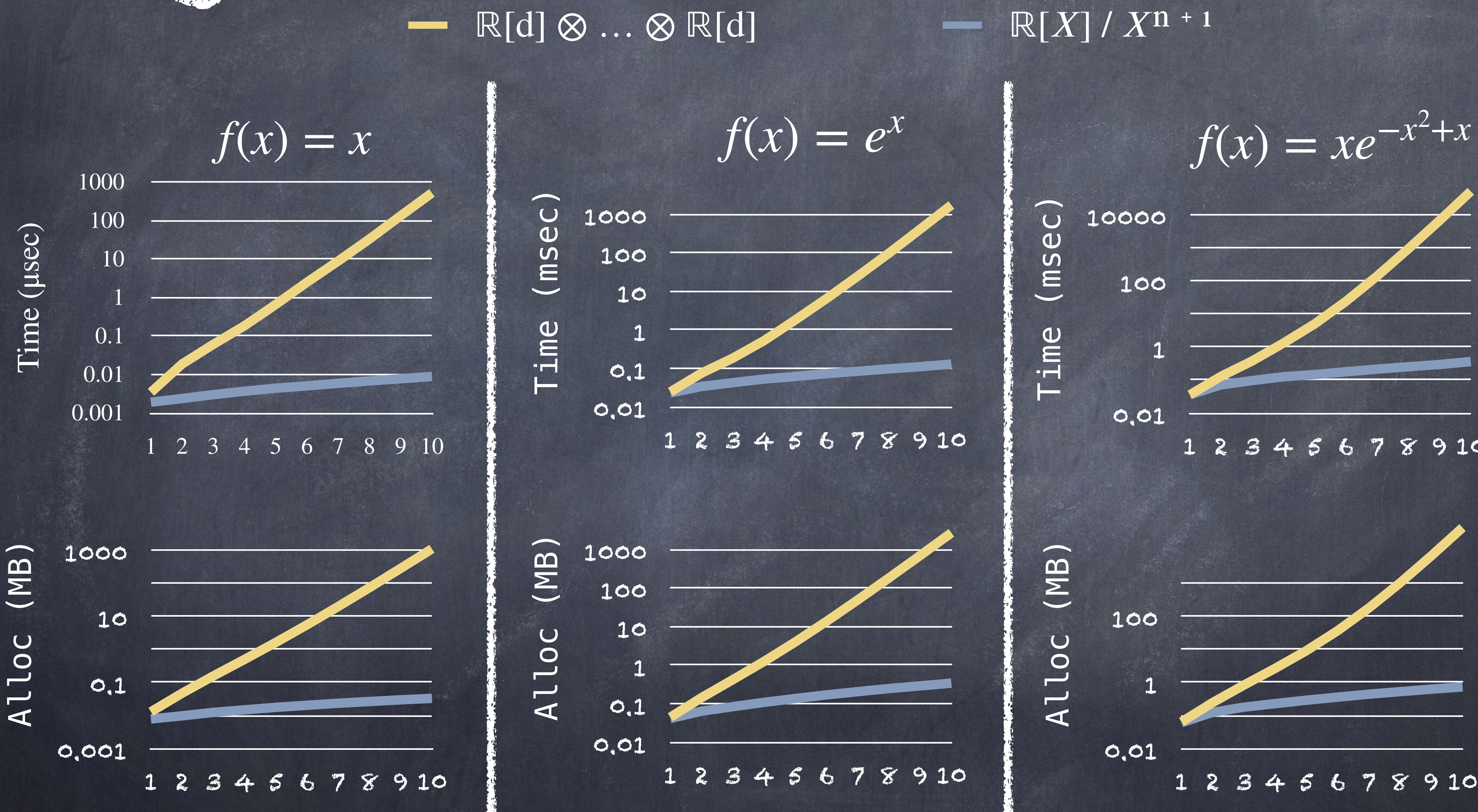
- "Tensor of dual numbers" approach needs n-many variables to calculate nth derivative.
    - The result much duplicate and redundant informations.
    - In particular, # of terms explodes to 2^n to calculate up to nth!
- We can save space and time using the following lemma:

Lem

For $\varepsilon = (X) \in \mathbb{R}[X]/X^n$ and smooth $f : \mathbb{R} \to \mathbb{R}$, we have:

$$\mathbb{R}[\varepsilon](f)(x + \varepsilon) = \sum_{0 \leq i < n} \frac{1}{i!} f^{(i)}(x) \varepsilon^i$$

Higher derivatives: bench



Environment: virtual Linux environment on GitHub Actions (Standard_DS2_v2 Azure instance) with two Intel Xeon Platinum 8171M virtual CPUs (2.60GHz) and 7 GiB of RAM.

Application 2: Tensors

- The tensor $W_1 \otimes_{\mathbb{R}} W_2$ of Weil algebras W_1, W_2 is again a Weil (Lem 4):

$$\mathbb{R}[\![X]\!]/I \otimes_{\mathbb{R}} \mathbb{R}[\![Y]\!]/J \cong \mathbb{R}[\![X, Y]\!]/\langle I, J\rangle$$

- The structure of tensors can be calculated with convolution (Alg. 4).
  - Using tensors we can combine arbitrary, multiple Weil algebras.
  - In particular, we can "package" higher-order ADs as Weil algebras, and "compose" them with tensors!

Ex.

Letting $\mathbb{R}[\varepsilon] = \mathbb{R}[x]/(x^{n+1}), \mathbb{R}[\delta] = \mathbb{R}[y]/(y^{m+1})$,

$$(\mathbb{R}[\varepsilon] \otimes_{\mathbb{R}} \mathbb{R}[\delta])(f)(x+\varepsilon, y+\delta) = \sum_{\substack{0 \leq i \leq n \\ 0 \leq j \leq m}} \frac{1}{i!j!} \partial x^i \partial y^j f(x, y).$$

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Summary

- Forward Mode Automatic Differentiation corresponds to the nilpotent infinitesimal analysis of second-order.
  - Justified by the theory of C^∞-rings by Lawvere et al.
  - In particular, Forward AD is an instance of Weil algebra which has nilpotent infinitesimals.
  - These concepts came from Synthetic Differential Geometry.
- Our Result: Combining AD and algorithms for zero-dimensional ideals, we achieved computational infinitesimal analysis with higher-order nilpotent infinitesimals on computers.
- Future Works: Optimisation, Synthetic treatment of Differential Geometry on Computers

Existing Works

- Nishimura and Osoekawa (2007) applies zero-dimensional algorithms to calculate the fundamental relation of generators of limit of Weil algebras.
    - They focus on the utility application to develop the theory of Weil algebra in SDG and not interested in computing differentials of smooth functions.
- Our interest is other direction - our central concern is computational infinitesimal analysis and smooth-ring computation.
    - Our contribution clarifies the connection of ADs and SIAs, which has been already pointed out but not discussed thoroughly, and implement it on the computer.

Future Works

- Develop Synthetic Differential Geometry (by Lawvere et al.) on computers using higher infinitesimals.
  - In SDG, general Weil algebras such as $\mathbb{R}[d_1, \ldots, d_n] = \mathbb{R}[x_1, \ldots, x_n]/(d_i d_j \mid i, j \leq n)$ are used to develop theory.
  - This opens a door to synthetic treatment of differential-geometric objects on computer.
    - Challenge: although $C^\infty(M)$ is finitely-presented as a C^∞-ring but, not so as an $\mathbb{R}$-algebra!
- Investigate the connection with other flavours of ADs, such as Reverse-Mode.

References

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Thank you!

Any Questions?

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  - Justified by the theory of C^∞-rings by Lawvere et al.
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- Our Result: Combining AD and algorithms for zero-dimensional ideals, we achieved computational infinitesimal analysis with higher-order nilpotent infinitesimals on computers.
- Future Works: Optimisation, Synthetic treatment of Differential Geometry on Computers

Appendices

Categorically Rigorous

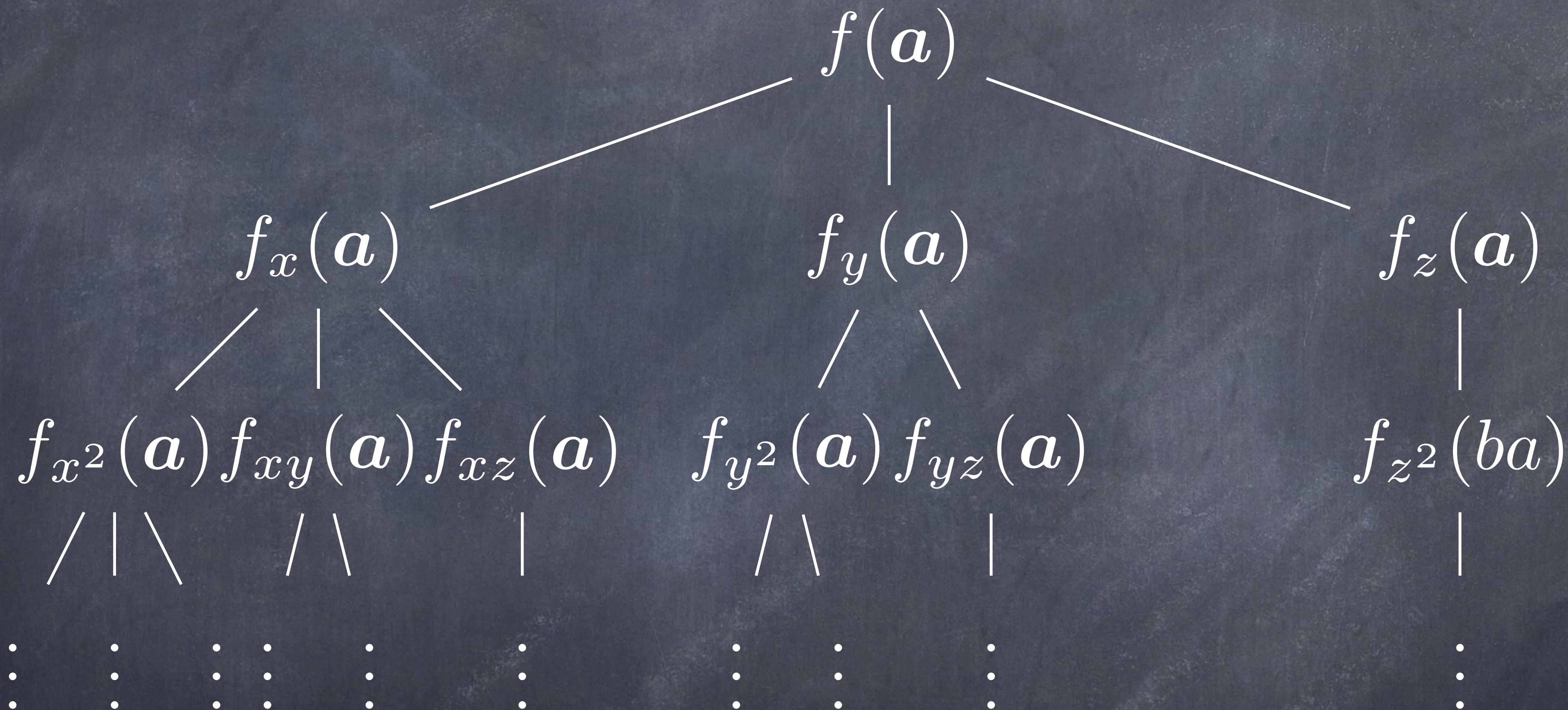
Definition of smooth rings

Def. (Lawvere)

Let $\mathbf{CartSp}$ be the category of all finite-dimensional Euclidean spaces and C^∞-maps between them.

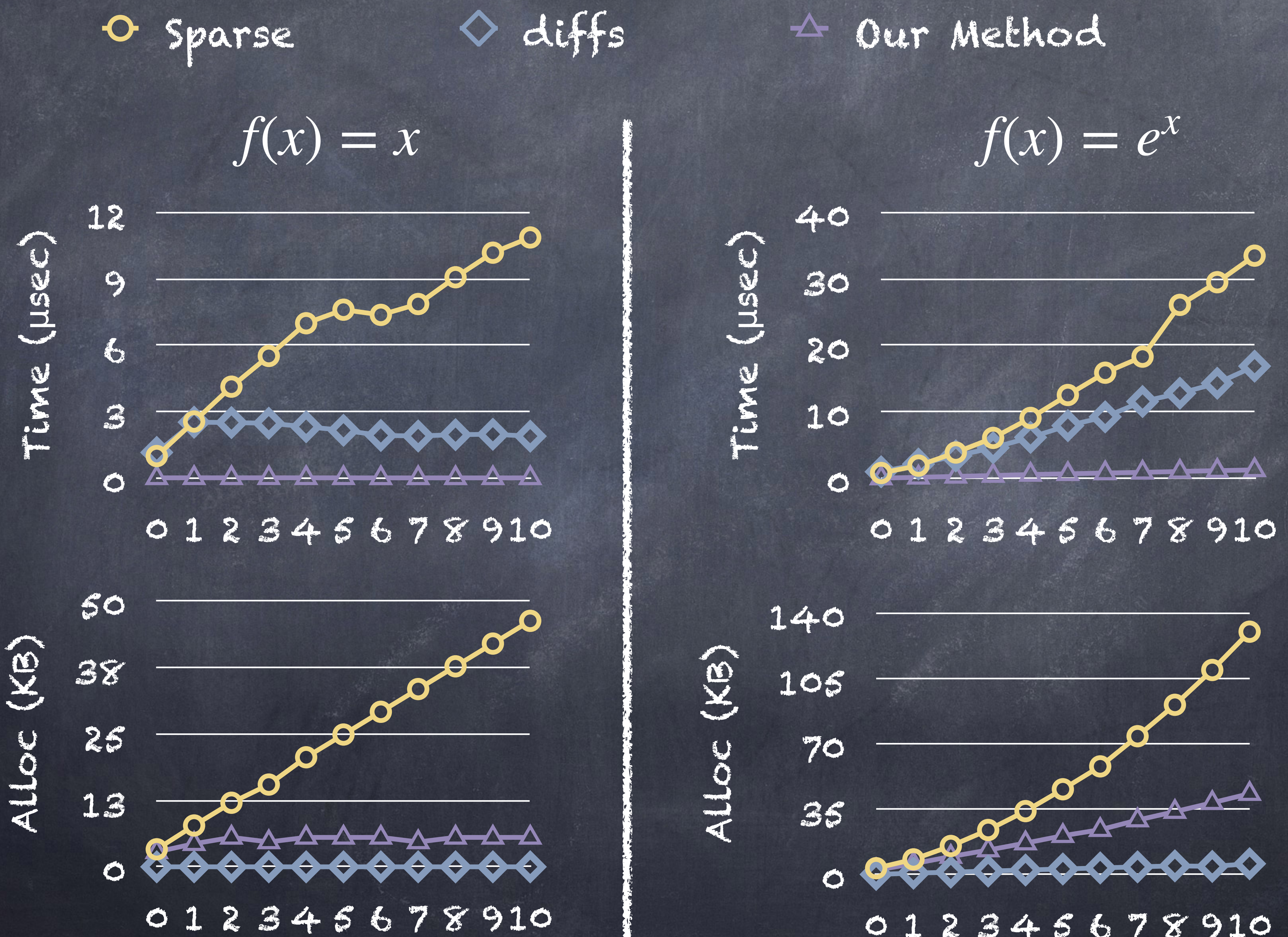
A C^∞-ring is a product-preserving functor $A : \mathbf{CartSp} \to \mathbf{Sets}$.

Succinct Tower AD



- Stores differentials as an infinite tree with decaying branching.
- Goes right if no further differentiation will be taken for preceding variables.

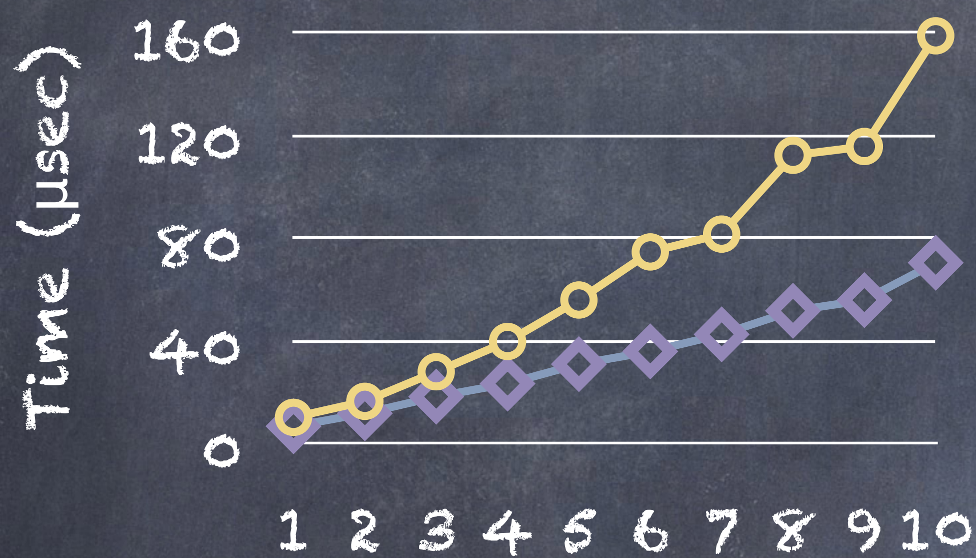
Tower bench: Univariate

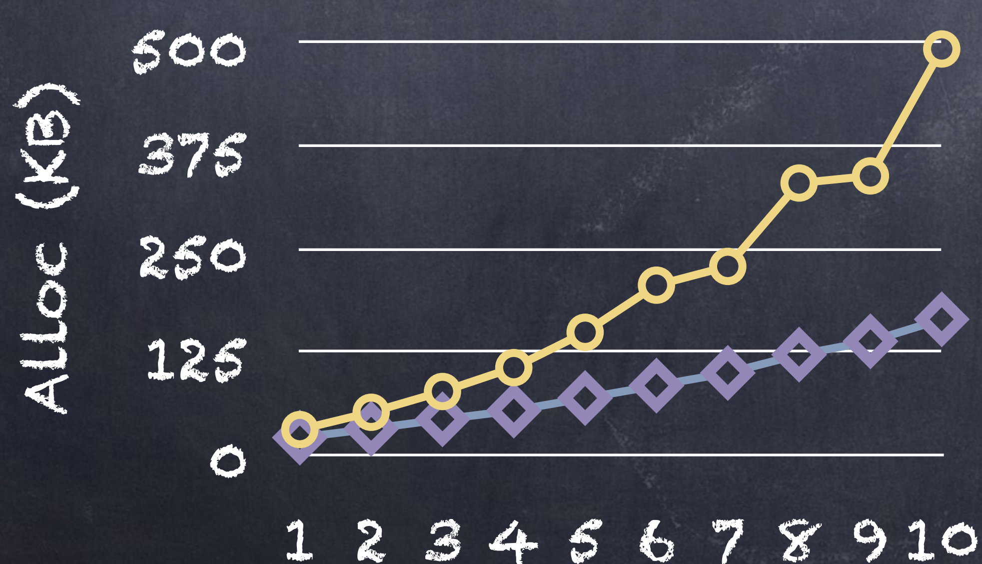


Tower bench: Multivariate

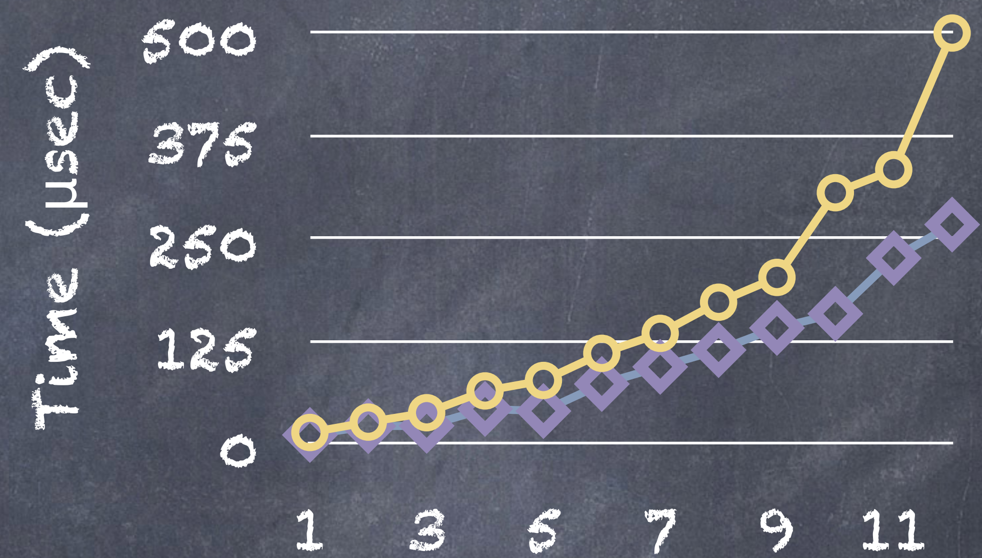
○ Sparse ◇ Our Method

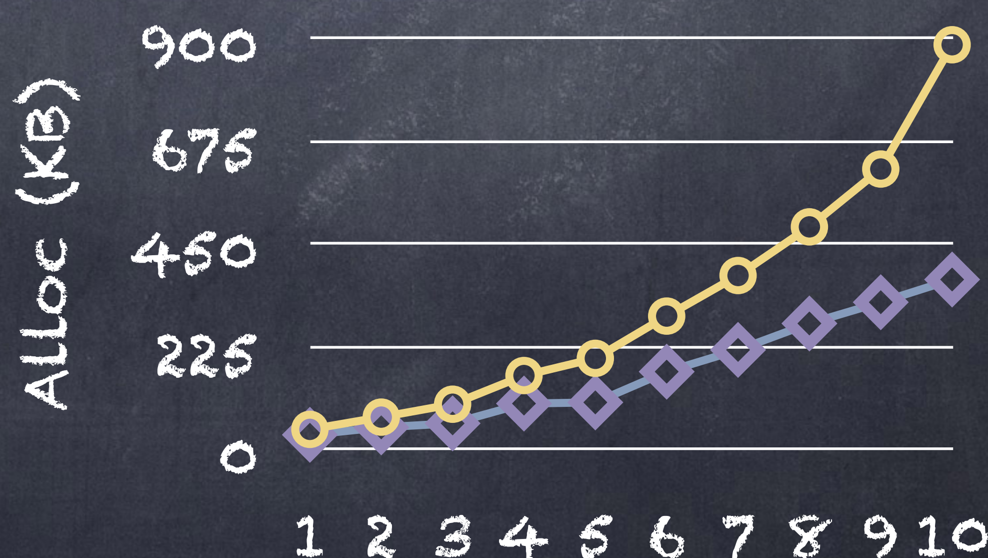
$$f(x, y) = \sin x \cdot e^{y^2}$$





$$f(x, y, z) = \sin x \cdot e^{y^2+z}$$





Tower bench: $\mathbb{R}[x,y]/(x^3 - y^2, y^3)$