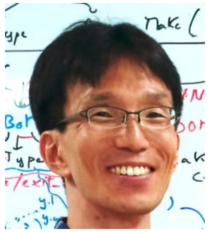
On Correctness of Automatic Differentiation for Non-Differentiable Functions*



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Autodiff: Theory

<u>Problem</u> For $h : \mathbb{R}^N \to \mathbb{R}$ given by $h(x) = (h_L \circ \cdots \circ h_1)(x)$,

how to compute $\nabla h(x)$ correctly and efficiently?

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<u>Chain Rule</u> For $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^l$ differentiable everywhere,

$D(g \circ f)(x) = Dg\big(f(x)\big) \cdot Df(x)$ for every $x \in \mathbb{R}^n$.

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Autodiff $\approx$ efficient way of applying the chain rule.

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Autodiff: Practice

What about in practice?

?

<u>Theorem</u> h_l's are differentiable everywhere $\Longrightarrow$ autodiff correctly computes $\nabla h(x)$.

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Discrepancy between theory and practice.

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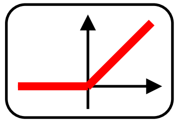
e.g., $\mathrm{ReLU}(x) = \texttt{if } x \geq 0 \texttt{ then } x \texttt{ else } 0 =$ 

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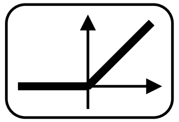
e.g., $\mathrm{ReLU}(x) = \texttt{if}\ x \geq 0\ \texttt{then}\ x\ \texttt{else}\ 0 =$ 

non-differentiable on a measure-zero set

measure = generalization of length, area, …

Autodiff: Practice

Belief: Measure-zero non-differentiability would not matter.

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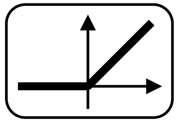
e.g., $\mathrm{ReLU}(x) = \texttt{if}\ x \geq 0\ \texttt{then}\ x\ \texttt{else}\ 0 =$ 

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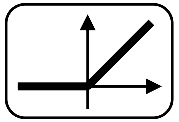
e.g., $\mathrm{ReLU}(x) = \mathtt{if}\ x \geq 0\ \mathtt{then}\ x\ \mathtt{else}\ 0 =$ 

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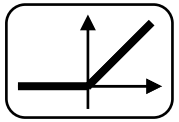
<u>Theorem</u> h_l's are differentiable $\underbrace{\text{everywhere}}_{\text{almost-}}$ $\overset{?}{\Longrightarrow}$ $\underbrace{\text{autodiff correctly computes } \nabla h(x)}_{\text{almost-everywhere}}$.

e.g., $\mathrm{ReLU}(x) = \texttt{if}\ x \geq 0\ \texttt{then}\ x\ \texttt{else}\ 0 =$ 

non-differentiable on a measure-zero set

almost-everywhere = except for a measure-zero set.

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Belief: Measure-zero non-differentiability would not matter.

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<u>Theorem</u> h_l's are differentiable $\underbrace{\text{everywhere}}_{\text{almost-}}$ $\boxed{\Longrightarrow}$ autodiff correctly computes $\underbrace{\nabla h(x)}_{\text{almost-everywhere}}$.

<u>Chain Rule</u> For $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^l$ differentiable $\overbrace{\text{everywhere}}^{\text{almost-}}$,

$\boxed{D(g \circ f)(x) \overset{?}{=} Dg\big(f(x)\big) \cdot Df(x)}$ for $\underbrace{\text{every}}_{\text{almost-}}$ $x \in \mathbb{R}^n$.

Our Results: Part 1

Measure-zero non-differentiabilities do matter!

Theorem h_l's are differentiable everywhere $\cancel{\implies}$ autodiff correctly computes $\nabla h(x)$.

almost-

almost-everywhere

almost-

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almost-

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<u>Theorem</u> h_l's are differentiable everywhere $\cancel{\implies}$ autodiff correctly computes $\nabla h(x)$.

almost-

almost-everywhere

<u>Our Result</u> This and related claims are false!

almost-

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almost-

Subtlety 1

<u>Claim 1</u> For any $f, g : \mathbb{R} \to \mathbb{R}$,

f, g : a.e.-differentiable and continuous

$\boxed{\Longrightarrow}$? $\quad (g \circ f)'(x) = g'\big(f(x)\big) \cdot f'(x)$ for a.e. $x \in \mathbb{R}$.

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well-defined?

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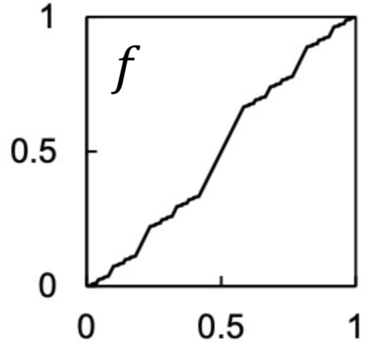
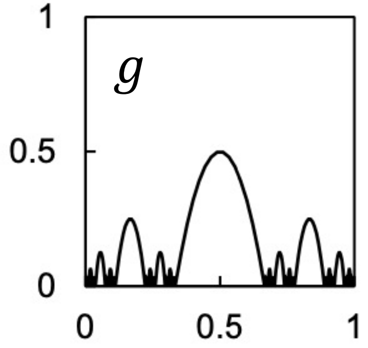
Counterexample Involves the Cantor function.





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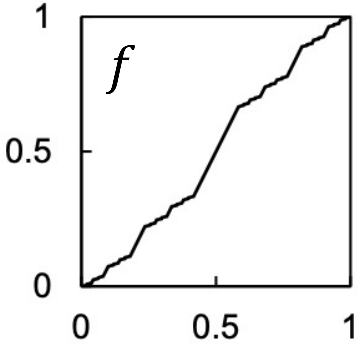
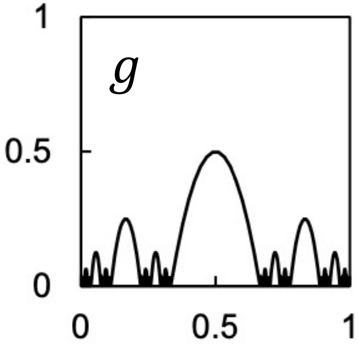
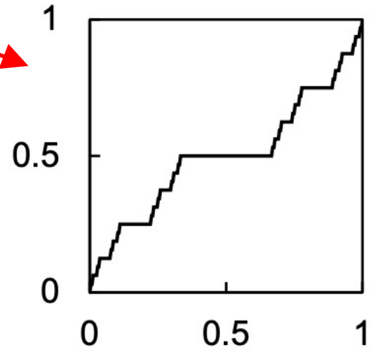




has pathological properties



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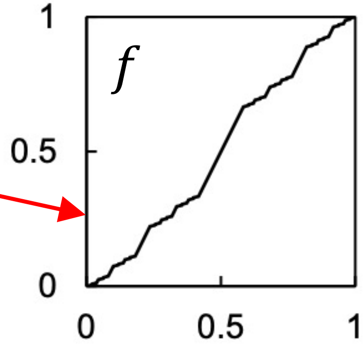
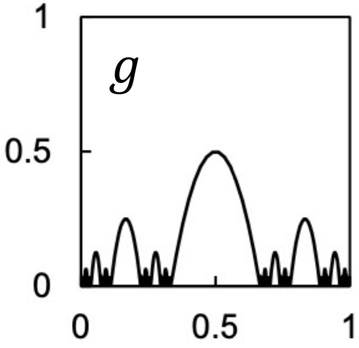
<u>Counterexample</u> Involves the Cantor function.

f is a bijection:

- continuous, a.e.-diff'l.
- positive-measure set $\rightleftarrows$ measure-zero set.





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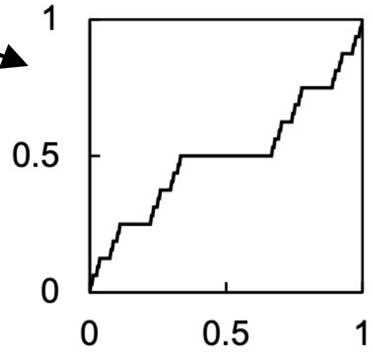

Subtlety 2

<u>Claim 2</u> For any $f, g : \mathbb{R} \to \mathbb{R}$,

$\overbrace{f, g}^{\text{and } g \circ f}$: a.e.-differentiable and continuous

$\boxed{\Longrightarrow}$? $\quad (g \circ f)'(x) = g'\big(f(x)\big) \cdot f'(x) \quad$ for a.e. $x \in \mathbb{R}$.

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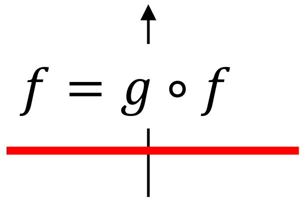
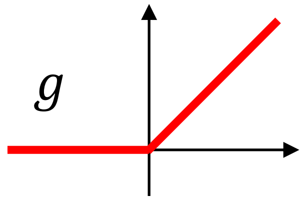
?

well-defined?

Counterexample $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

$\Longrightarrow$ easy to check that $(*)$ holds.





Subtlety 2: Undefined g'

<u>Claim 2</u> For any $f, g : \mathbb{R} \to \mathbb{R}$,

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$\Longrightarrow$ $g'\big(f(x)\big)$

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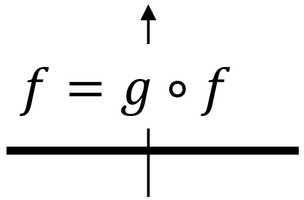

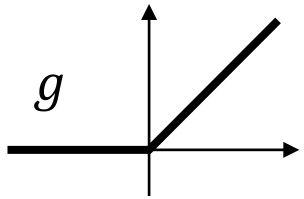

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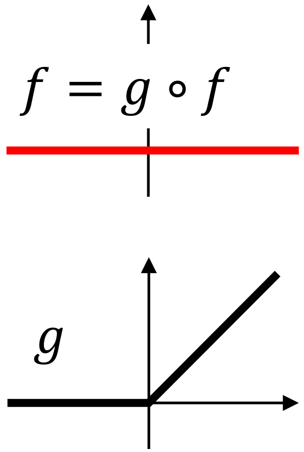
<u>Counterexample</u> $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

$\Longrightarrow$ $(g \circ f)'(x)$ $\quad g'(f(x))$ $\quad f'(x)$

$= 0$ $\quad = g'(0)$ $\quad = 0$

$=$ undefined for all x



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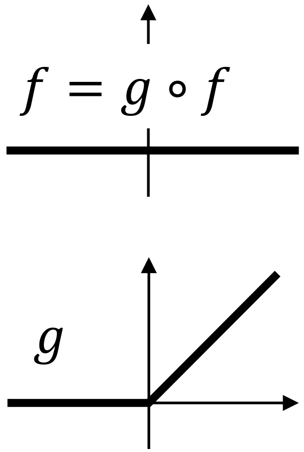
Counterexample $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

$\Longrightarrow \quad \underset{= 0}{(g \circ f)'(x)} \quad dg\big(f(x)\big) \quad \underset{= 0}{f'(x)}$

$$dg(y) = \begin{cases} 7 & \text{for } y = 0 \\ g'(y) & \text{for } y \neq 0 \end{cases}$$



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<u>Counterexample</u> $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

$$\Longrightarrow \quad \boxed{\underbrace{(g \circ f)'(x)}_{=\,0} = dg(f(x)) \times \underbrace{f'(x)}_{=\,0}} \quad \text{for all } x \in \mathbb{R}.$$

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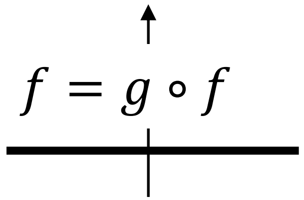

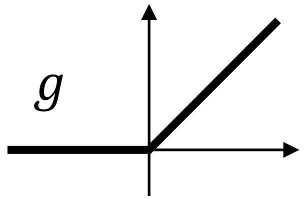

Subtlety 3

Claim 3 For any $f, g : \mathbb{R} \to \mathbb{R}$,

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$\boxed{\Longrightarrow}$?

$$\underbrace{(g \circ f)'(x) = dg\big(f(x)\big) \cdot df(x)}_{\exists\, df, dg \,:\, \mathbb{R} \to \mathbb{R} \text{ such that } df \overset{\text{a.e.}}{=} f',\ dg \overset{\text{a.e.}}{=} g',\text{ and}}$$ for a.e. $x \in \mathbb{R}$.

Subtlety 3

<u>Claim 3</u> For any $f, g : \mathbb{R} \to \mathbb{R}$,

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well-defined!

$\Longrightarrow$?

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$\overset{?}{\Longrightarrow}$ $\underbrace{(g \circ f)'(x) \overset{?}{=} dg\big(f(x)\big) \cdot df(x)}$ for a.e. $x \in \mathbb{R}$.

$\exists\, df, dg : \mathbb{R} \to \mathbb{R}$ such that $df \overset{\text{a.e.}}{=} f'$, $dg \overset{\text{a.e.}}{=} g'$, and

Subtlety 3: Wrong Equation for $(g \circ f)'$

<u>Claim 3</u> For any $f, g : \mathbb{R} \to \mathbb{R}$,

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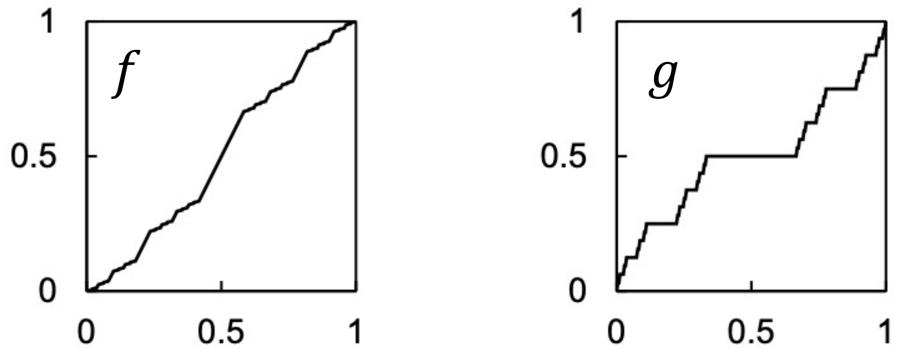
$$\cancel{\implies} \quad \underbrace{(g \circ f)'(x) \cancel{=} dg(f(x)) \cdot df(x)}_{\exists\, df, dg : \mathbb{R} \to \mathbb{R} \text{ such that } df \overset{\text{a.e.}}{=} f',\ dg \overset{\text{a.e.}}{=} g', \text{ and}} \quad \text{for a.e. } x \in \mathbb{R}.$$

<u>Counterexample</u> Involves the Cantor function again.



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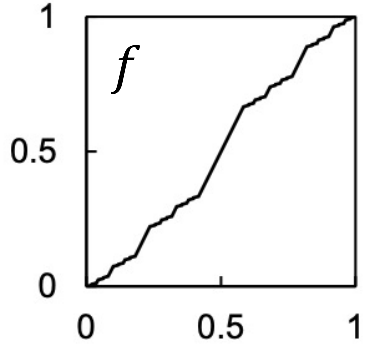
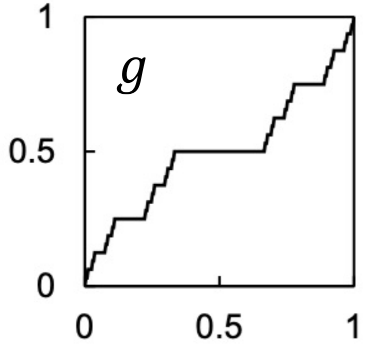
$$\cancel{\Longrightarrow} \quad \boxed{(g \circ f)'(x)} \cancel{=} dg(f(x)) \cdot \boxed{df(x)} \qquad \text{for a.e. } x \in \mathbb{R}.$$

Show $\boxed{(g \circ f)'(x) \neq 0}$ and $\boxed{f'(x) = 0}$ for positive-measure x.

Counterexample Involves the Cantor function again.





Our Results: Part 1

Theorem h_l's are differentiable $\underbrace{\text{everywhere}}_{\text{almost-}}$ $\cancel{\implies}$ autodiff correctly computes $\underbrace{\nabla h(x)}_{\text{almost-everywhere}}$.

Our Result This and related claims are false!

Chain Rule For $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^l$ differentiable $\overbrace{\text{everywhere}}^{\text{almost-}}$,

$\cancel{D(g \circ f)(x) = Dg(f(x)) \cdot Df(x)}$ for $\underbrace{\text{every}}_{\text{almost-}}$ $x \in \mathbb{R}^n$.

Our Results: Part 1

Our Result Autodiff has been used without correctness guarantee!

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✓

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Chain Rule For $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^l$, differentiable $\overbrace{\text{everywhere}}^{\text{almost-}}$,

$$\cancel{D(g \circ f)(x) = Dg(f(x)) \cdot Df(x)} \quad \text{for } \underbrace{\text{every}}_{\text{almost-}}\ x \in \mathbb{R}^n.$$

Our Questions: Part 2

Can we recover the correctness theorem?

Theorem h_l's are differentiable $\underbrace{\text{everywhere}}_{\text{almost-}}$ $\cancel{\Rightarrow}$ $\underbrace{\text{autodiff correctly computes } \nabla h(x)}_{\text{almost-everywhere}}$.

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- $f(x) = \mathrm{ReLU}(x) - \mathrm{ReLU}(-x)$: $\partial^c f(0) = \{1\} \not\ni 0 = f'(0)$ (by autodiff).

Our Results: Part 2

<u>Theorem</u> h_l's are differentiable everywhere $\not\Longrightarrow$ autodiff correctly computes $\nabla h(x)$.

? almost-

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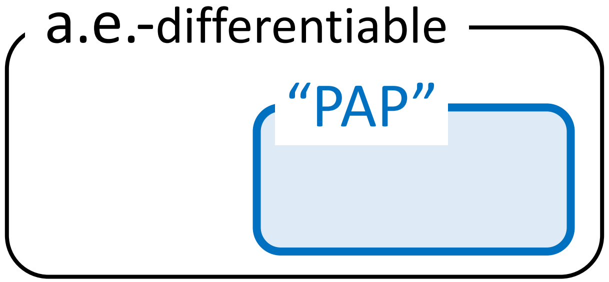

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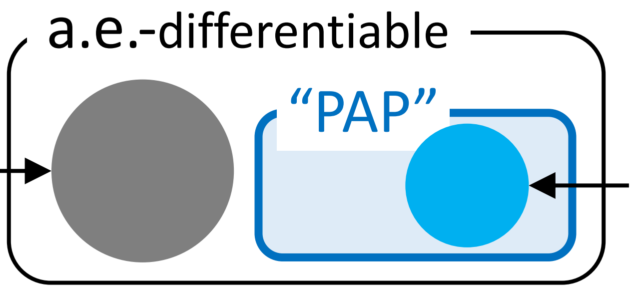
pathological func's
(Cantor func, ⋯)



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Our Results: Part 2

Our Result Prove the claim for PAP functions h_l's.

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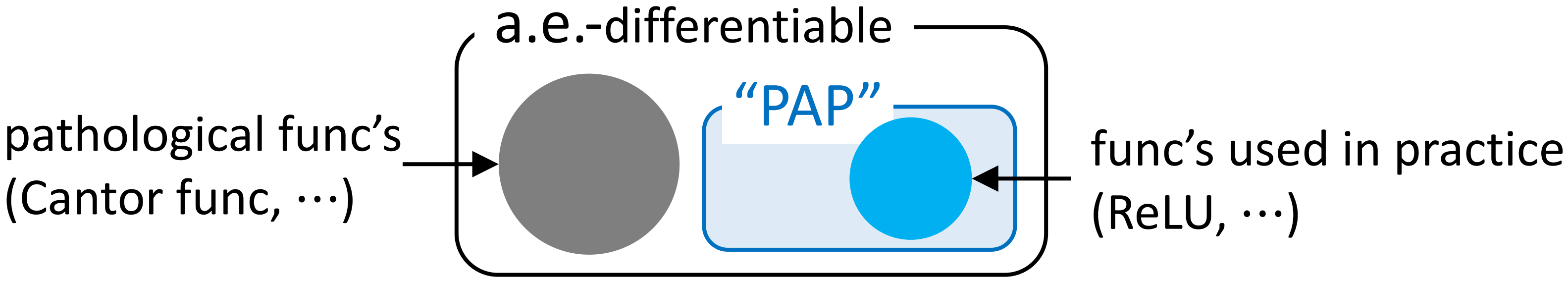

Our Results: Part 2

<u>Our Result</u> Autodiff computes so-called "intensional derivatives" of h.

<u>Our Result</u> Prove the claim for PAP functions h_l's.

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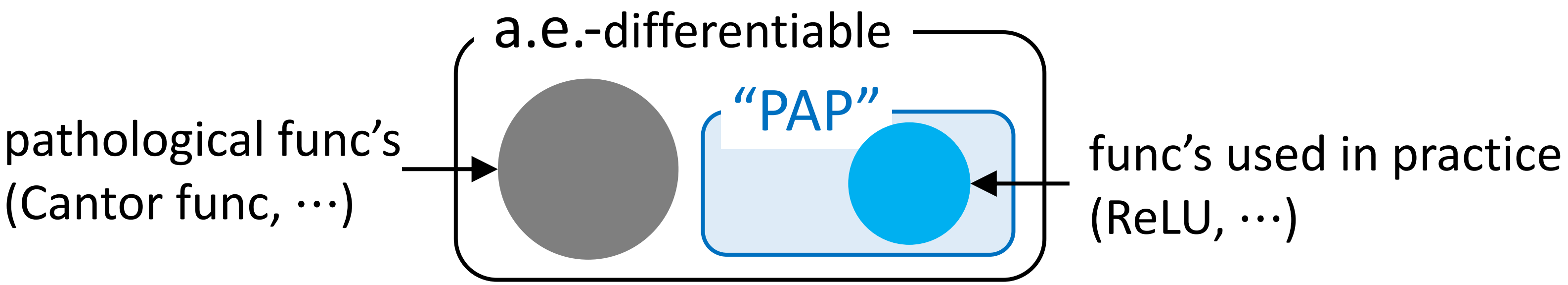

PAP Functions

piecewise analytic under analytic partition

Definition $f : \mathbb{R}^n \to \mathbb{R}^m$ is called PAP if f can be "decomposed" into

$$f_1\big|_{A_1}, f_2\big|_{A_2}, \cdots$$

such that

$$f_i : \mathbb{R}^n \to \mathbb{R}^m \text{ and } A_i \subseteq \mathbb{R}^n \text{ are "analytic".}$$

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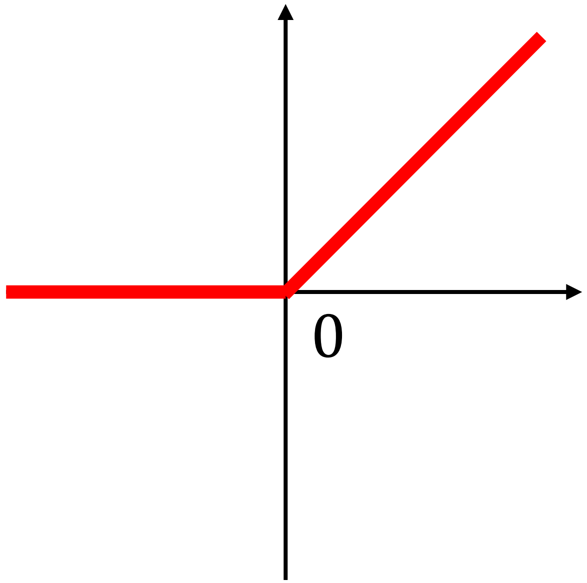

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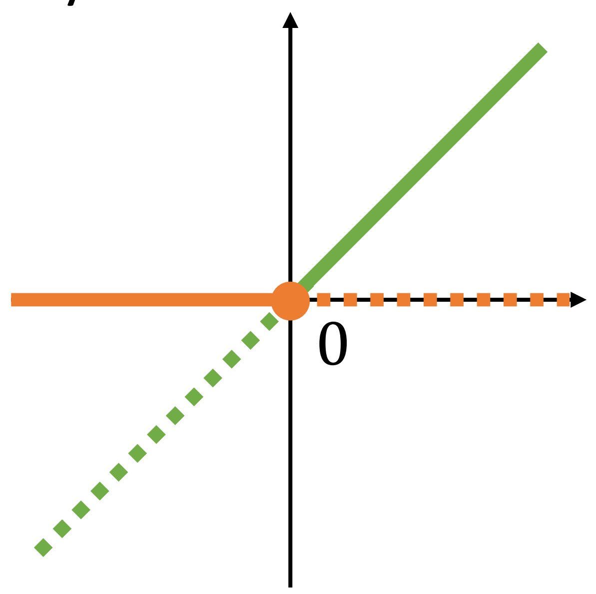

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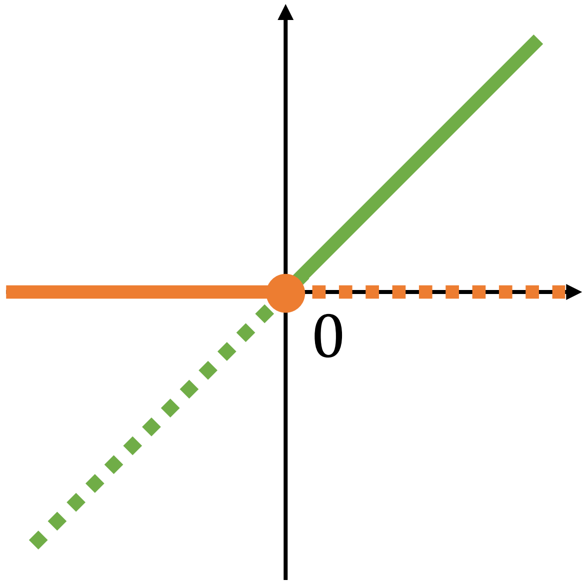

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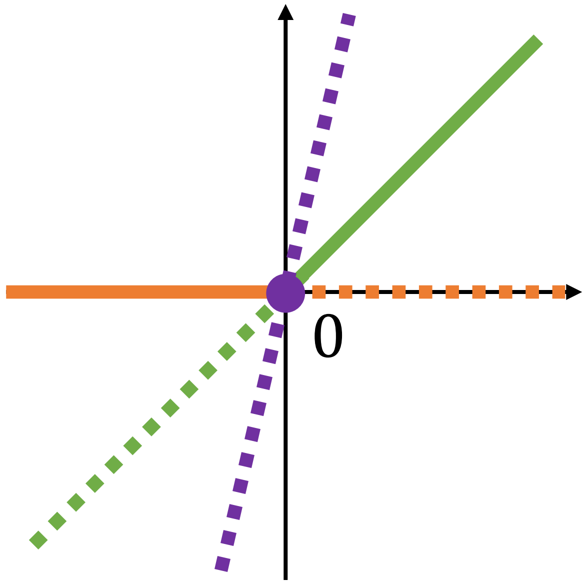

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can be a subset of $\mathbb{R}^n$

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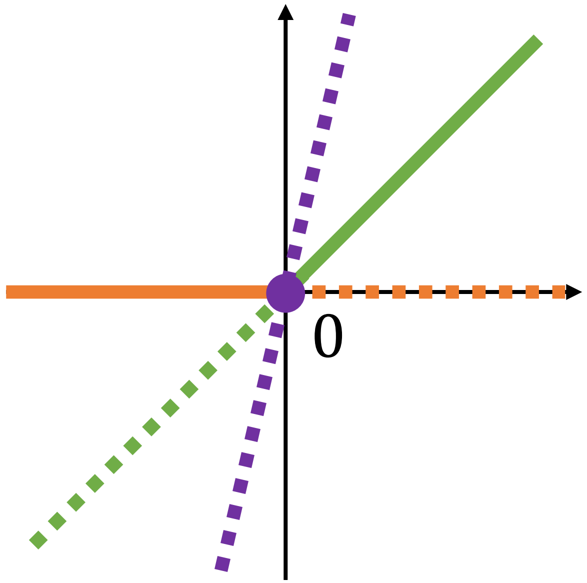

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Observation PAP functions include all functions used in practice.

Proposition PAP functions are a.e.-differentiable.

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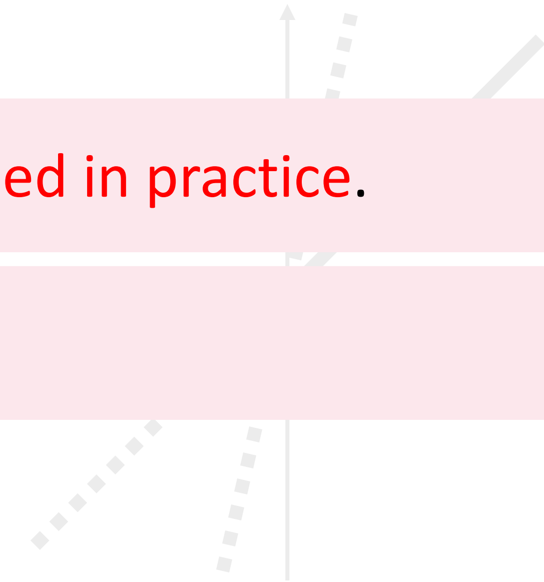

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For any non-constant, analytic function $g : \mathbb{R}^n \to \mathbb{R}$,
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PAP Functions

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Intensional Derivatives

analytic functions

<u>Example</u> $f(x) = \text{ReLU}(x)$.

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intensional derivative of f

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Intensional Derivatives

Proposition Intensional derivative is a **total function**.

Proposition Intensional derivatives **always** satisfy the **chain rule**.

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<u>Proposition</u> Intensional derivative is a total function.

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<u>Proposition</u> Intensional derivative $\overset{\text{a.e.}}{=}$ standard derivative.

$\{x \in \mathbb{R}^n \mid df(x) \neq Df(x)\}$ is contained in
a countable union of the zero-sets of (non-const) analytic func's.

Correctness of Autodiff

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Theorem For any $h = h_L \circ \cdots \circ h_1$ with PAP h_l,
autodiff computes an intensional derivative of h,
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if autodiff uses an intensional derivative of h_l for "D"h_l,

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First-order → higher-order.

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Difference from Clarke-subdifferentials.

- Intentional derivative: $\partial^i f \in \mathcal{P}([\mathbb{R}^n \to \mathbb{R}^{m\times n}])$.
- Clarke-subdifferential: $\partial^c f \in [\mathbb{R}^n \to \mathcal{P}(\mathbb{R}^{m\times n})]$.

  → Difficult to extend to higher-order derivatives.

High-Level Messages

We often have discrepancy between theory and practice of ML algorithms.

But our theoretical understanding on such discrepancy is still limited.

ML Algorithm	Theory	Practice
Autodiff	differentiable func's	a.e.-differentiable func's

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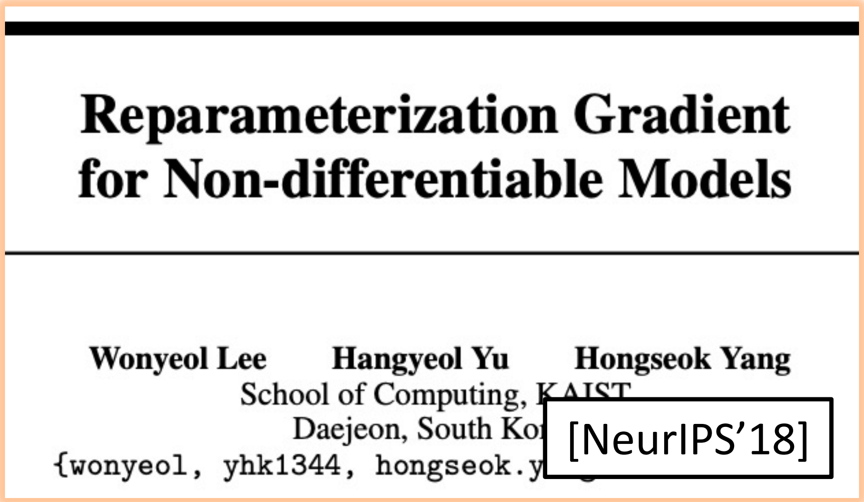
Algorithm for estimating
$\nabla_\theta \int f_\theta(z)dz$



Reparameterization Gradient for Non-differentiable Models

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School of Computing, KAIST
Daejeon, South Ko
{wonyeol, yhk1344, hongseok.y

[NeurIPS'18]

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Autodiff and many more	differentiable func's	a.e.-differentiable func's
Variational inference, …	func's with finite integrals (and other nice properties)	func's with infinite integrals (or some bad properties)

Towards Verified Stochastic Variational Inference for Probabilistic Programs

WONYEOL LEE, School of Computing, KAIST, South Korea
HANGYEOL YU, School of Computing, KAIST, South Korea
XAVIER RIVAL, INRIA Paris, Département d'Informatique of ENS, and CNRS/PSL U
HONGSEOK YANG, School of Computing, KAIST, South Korea

[POPL'20]

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Most algorithms	func's on reals	func's on floating-points

Verifying Bit-Manipulations of Floating-Point

Wonyeol Lee Rahul Sharma Alex Aiken
Stanford University, USA
{wonyeol, sharmar, aiken}@cs.stanford.edu

[PLDI'16]

On Automatically Proving the Correctness of `math.h` Implementations

WONYEOL LEE*, Stanford University, USA
RAHUL SHARMA, Microsoft Research, India
ALEX AIKEN, Stanford University, USA

[POPL'18]

Comments? Questions?