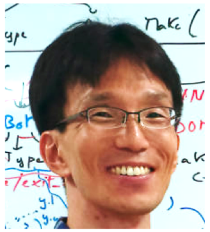
On Correctness of Automatic Differentiation for Non-Differentiable Functions

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NeurIPS 2020 (Spotlight)

Autodiff

Problem For $F : \mathbb{R}^N \to \mathbb{R}$ given by $F(x) = (F_L \circ \cdots \circ F_1)(x)$,

how to compute $\nabla F(x)$ 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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$\uparrow$

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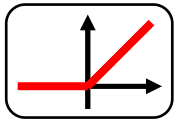
e.g., $\mathrm{ReLU}(x) = \max\{x, 0\} =$ 

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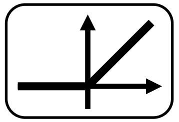
e.g., $\mathrm{ReLU}(x) = \max\{x, 0\} =$ 

non-differentiable on a measure-zero set

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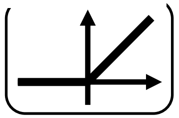
e.g., $\mathrm{ReLU}(x) = \max\{x, 0\} =$ 

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

No, measure-zero non-differentiabilities matter!

Chain Rule For $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^l$ differentiable $\overbrace{\text{everywhere}}^{\text{almost-}}$,
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Subtleties in Chain Rule (1)

Claim 1 For any $f, g : \mathbb{R} \to \mathbb{R}$,

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

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

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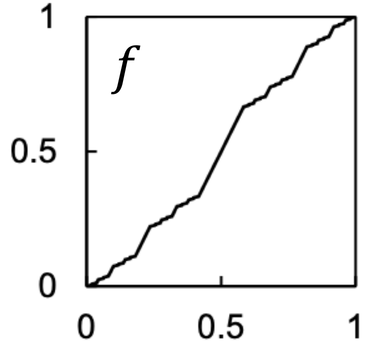
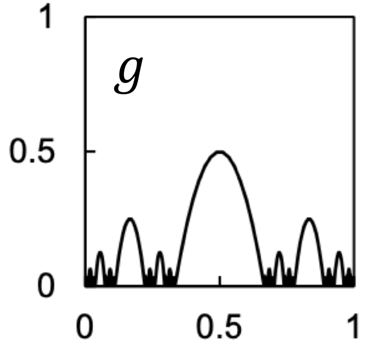
<u>Counterexample</u> Involves the Cantor function.





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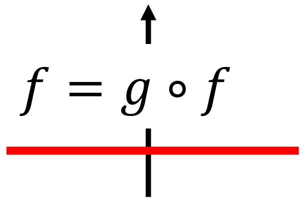
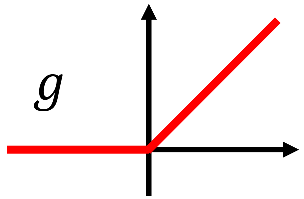
Counterexample $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

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





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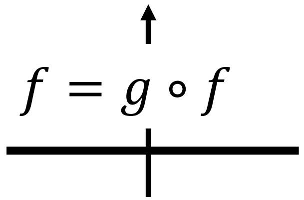

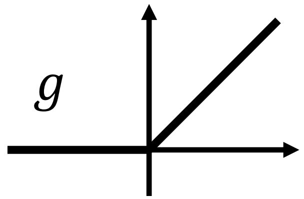

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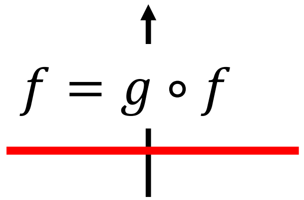

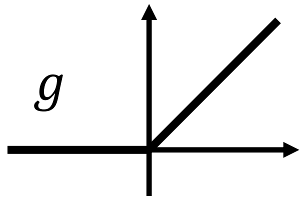

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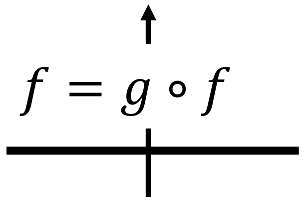
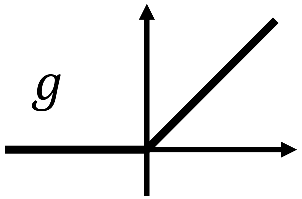
<u>Counterexample</u> $f(x) = 0$ and $g(y) = \mathrm{ReLU}(y)$.

$$\Longrightarrow \quad \underbrace{(g \circ f)'(x)}_{= 0} \qquad {\color{red} dg}\big(f(x)\big) \qquad \underbrace{f'(x)}_{= 0}$$

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





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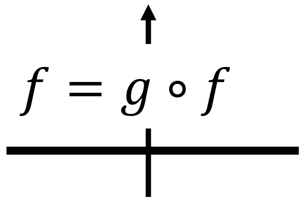

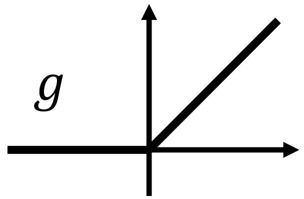

Subtleties in Chain Rule (3)

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

$\underbrace{f, g}_{}$ and $g \circ f$: a.e.-differentiable and continuous

$\boxed{\Longrightarrow}$?

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

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

Subtleties in Chain Rule (3)

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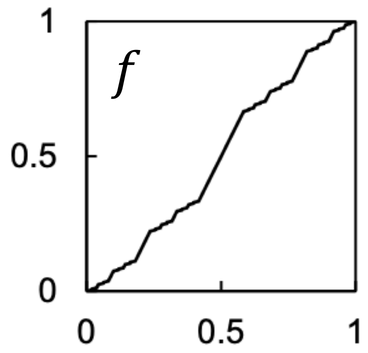
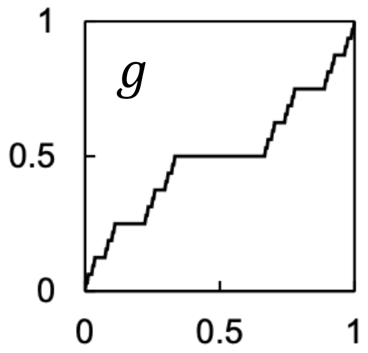
$$\cancel{\Longrightarrow} \quad \underbrace{(g \circ f)'(x) \cancel{=} dg\big(f(x)\big) \cdot df(x)}_{\exists\, df, dg \,:\, \mathbb{R} \to \mathbb{R} \text{ such that } df \overset{\text{a.e.}}{=} f',\; dg \overset{\text{a.e.}}{=} g', \text{ and}} \qquad \text{for a.e. } x \in \mathbb{R}.$$

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





Our Results

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

Our Result Disprove this and related claims.

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Question How to recover this claim?

Theorem F_l's are differentiable everywhere $\cancel{\Longrightarrow}$ autodiff correctly computes $\nabla F(x)$.

? almost-

almost-everywhere

✓

Our Result Disprove this and related claims.

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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 everywhere,

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Our Result Prove this claim for a wide class of F_l's.

Theorem F_l's are ~~differentiable everywhere~~ $\boxed{\Rightarrow}$ autodiff correctly computes $\nabla F(x)$.

~~almost-~~

so-called "PAP"

almost-everywhere

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PAP Functions

Definition $f : \mathbb{R}^n \to \mathbb{R}^m$ is PAP (= Piecewise Analytic under Analytic Partition)

roughly iff f can be "decomposed" into $f_1\big|_{A_1}, f_2\big|_{A_2}, \cdots$ such that

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

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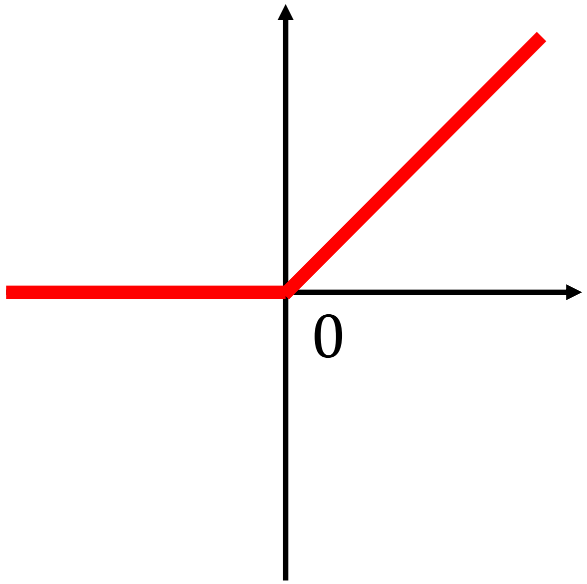
Example $f(x) = \mathrm{ReLU}(x)$.



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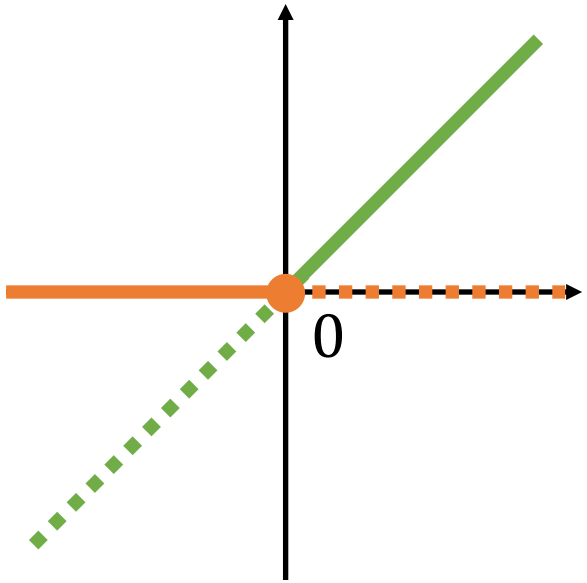
Example $f(x) = \mathrm{ReLU}(x)$.

- $(f_1(x) = 0, A_1 = \{x \in \mathbb{R} : x \le 0\})$,
  $(f_2(x) = x, A_2 = \{x \in \mathbb{R} : x > 0\})$.



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

Example $f(x) = \mathrm{ReLU}(x)$.

- $(f_1(x) = 0, A_1 = \{x \in \mathbb{R} : x \leq 0\})$,
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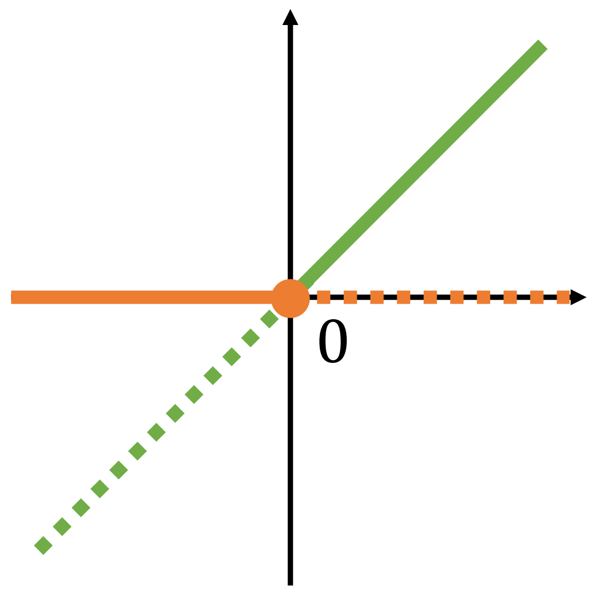
analytic functions



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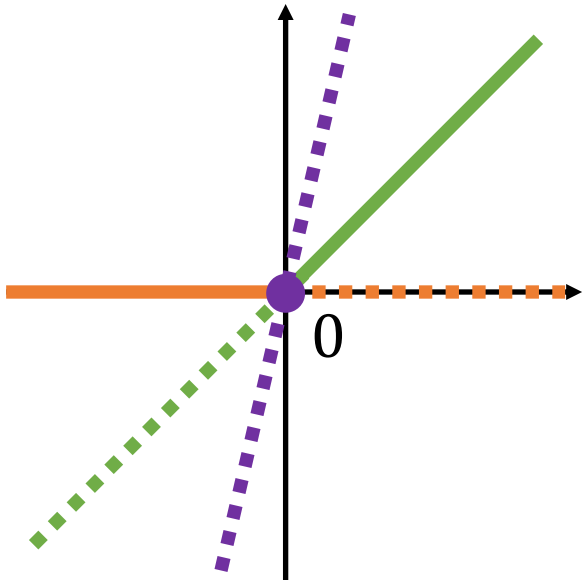

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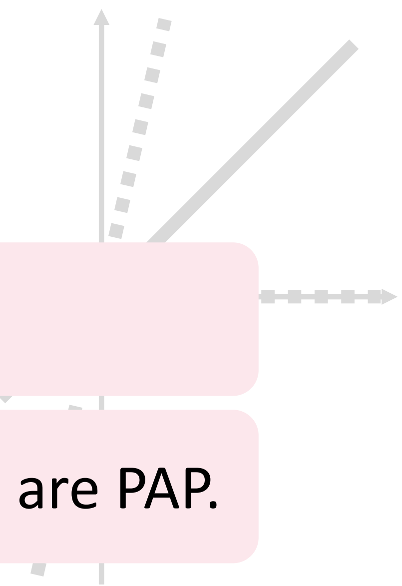

Proposition PAP implies a.e.-differentiability.

Observation Virtually all functions used in practice are PAP.

Intensional Derivatives

analytic functions

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analytic functions

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$$\boxed{df(x)} = \begin{cases} 0 & \text{for } x \leq 0 \\ 1 & \text{for } x > 0 \end{cases}$$

intensional derivative of f

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Intensional Derivatives

<u>Proposition</u> Intensional derivatives satisfy the chain rule.

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

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<u>Theorem</u> For PAP functions,

what autodiff computes is an intensional derivative,

and thus autodiff correctly computes gradients a.e.

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or $x < 0$
or $x > 0$
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High-Level Messages

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- PAP functions and intensional derivatives would play an important role, when we try to deal with such subtleties (e.g., arising from other ML algorithms).