Nonsmooth differential calculus and optimization, the conservative gradient approach

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joint work with Jérôme Bolte

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Journées MOA, Nice, (Octobre, 2022)

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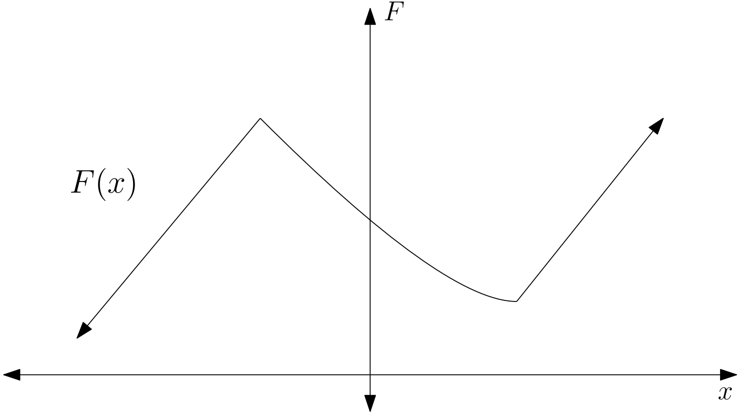
- $\boxed{\textbf{Nonsmoothness is needed:}}$ $g_i = \mathrm{relu}$, sort, maxpool, implicit layers



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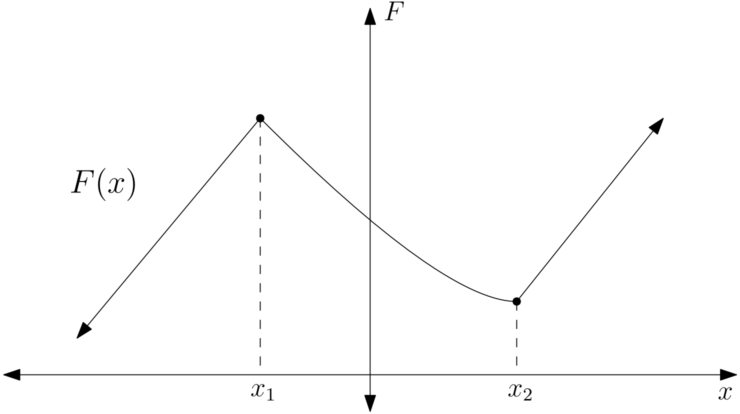

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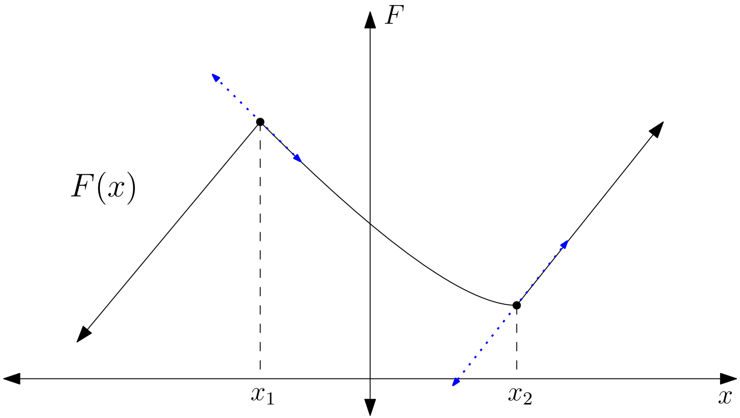

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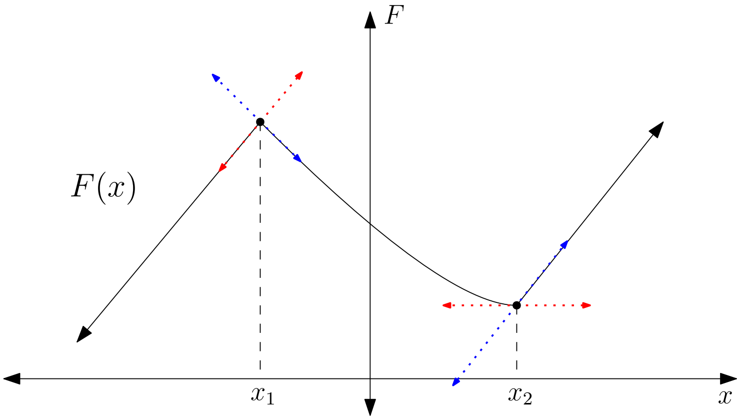

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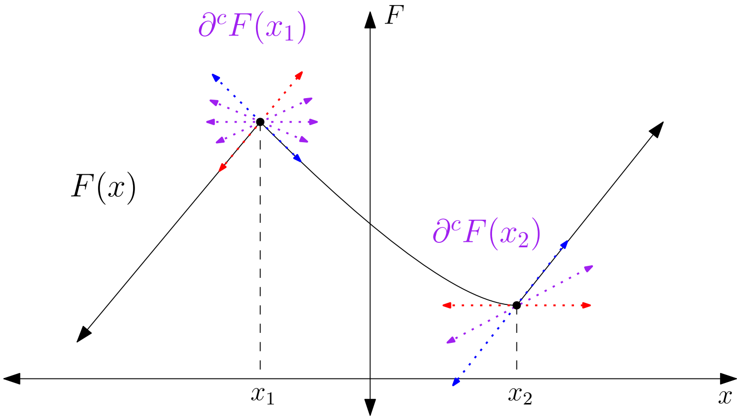

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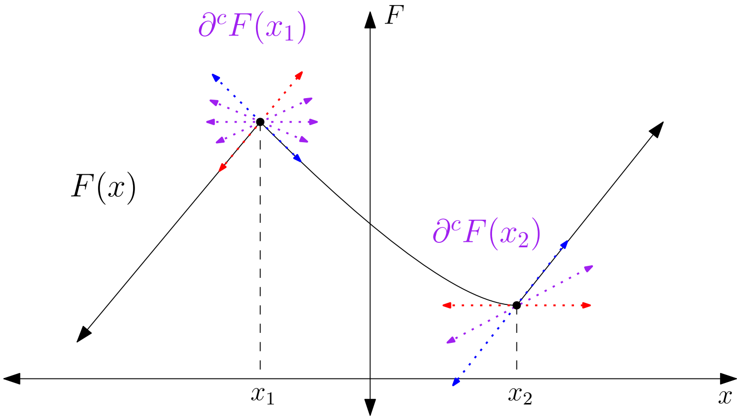

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Set valued $\mathrm{Jac}^{\,c} F \colon \mathbb{R}^p \rightrightarrows \mathbb{R}^{q\times p}$

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$\boxed{\text{But what does backprop output? What sort of gradient could it be?}}$

Plan

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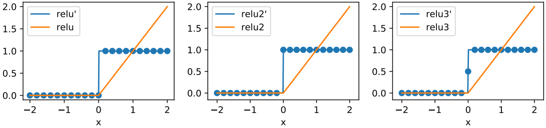

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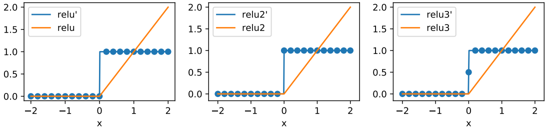

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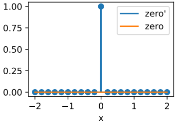

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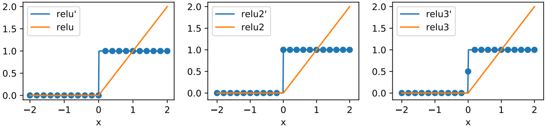

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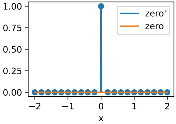

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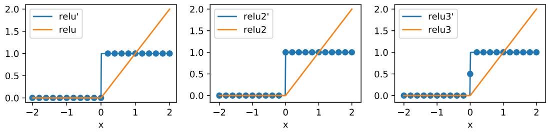

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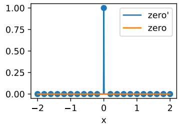

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- Spurious critical point: $\mathrm{identity}(x) := x - \mathrm{zero}(x) = x$ but $\mathrm{backprop}\,\mathrm{identity}(0) = 0$

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- **Stochastic approximation:** $\partial^c \left(\frac{1}{n} \sum_{i=1}^n \ell_i \right) \subset \frac{1}{n} \sum_{i=1}^n \partial^c \ell_i$.

Plan

- Objects akin to Clarke's subgradient / Jacobian (for locally Lipschitz functions).
- Lipschitz $F\colon \mathbb{R}^n \to \mathbb{R}^m$ has none or multiple conservative Jacobians $J_F\colon \mathbb{R}^n \rightrightarrows \mathbb{R}^{m\times n}$. Notation D_F if $m = 1$ for conservative gradients.
- If conservative Jacobians exist, F is called **path-differentiable**.
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Hypothesis: Fix any Lipschitz curve $\gamma \colon [0,1] \mapsto \mathbb{R}^p$

$$\frac{d}{dt} f(\gamma(t)) = \langle v, \dot{\gamma}(t) \rangle \qquad \forall v \in \partial^c f(\gamma(t)), \qquad \text{a.e.} \quad t \in [0,1]$$

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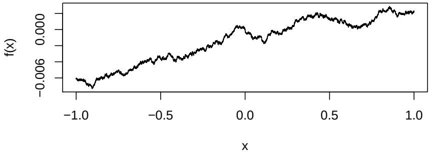

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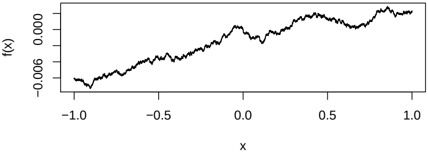

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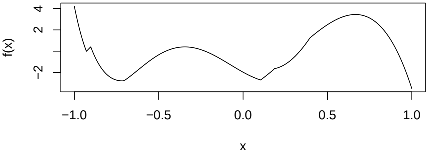

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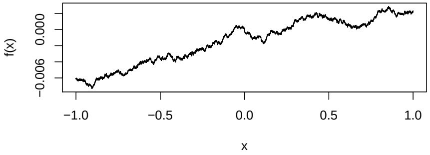

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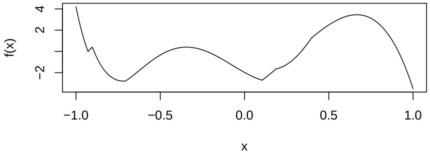

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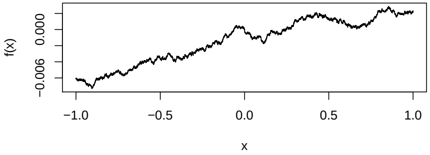

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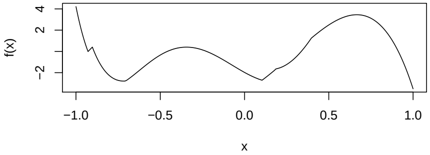

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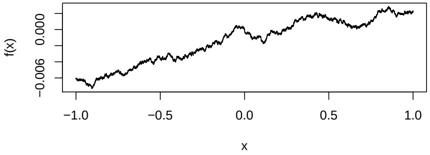

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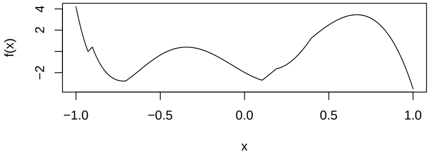

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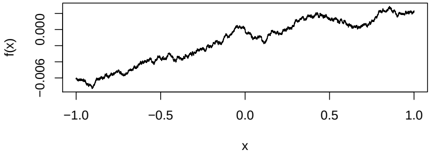

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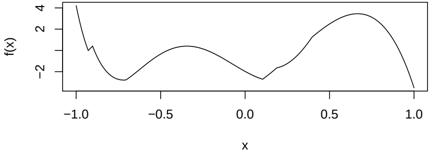
Davis et .al. 2019, **Bolte et. al. 2007:** Subgradient projection formula implies chain rule along Lipschitz curves.



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Conservative calculus example: finite sums

Conservative (outer) sum rule (Bolte-Pauwels 2019):
$f_i \colon \mathbb{R}^p \to \mathbb{R}$ path differentiable (locally Lipschitz), for $i = 1, \ldots, n$. Then $D = \sum_i \partial^c f_i$ is conservative for $f = \sum_i f_i$.

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$f_i \colon \mathbb{R}^p \to \mathbb{R}$ path differentiable (locally Lipschitz), for $i = 1, \ldots, n$. Then $D = \sum_i \partial^c f_i$ is conservative for $f = \sum_i f_i$.

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Conservative calculus example: finite sums

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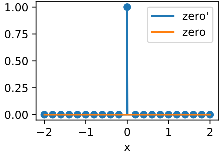

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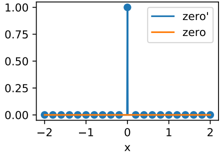

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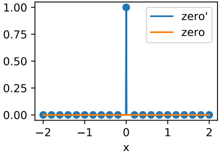

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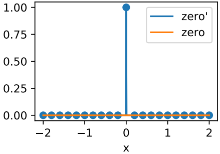

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More calculus on calculus and chain rule

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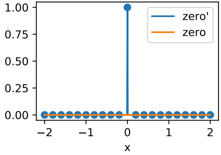

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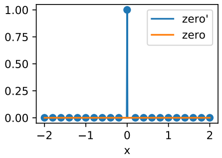

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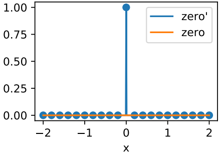

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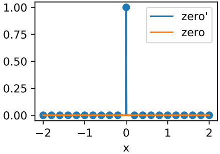

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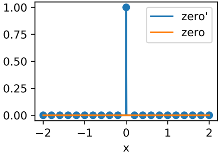

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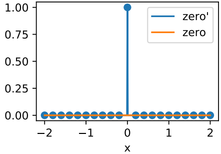

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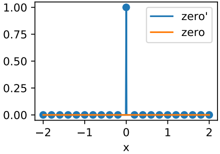

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- Widespread "conservative gradients oracles":

TensorFlow PyTorch JAX

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Theorem (Bolte-Pauwels 2019-2020):

- **Step size condition:** $\sum_{k=1}^{+\infty} \alpha_k = +\infty$ and $\alpha_k \to 0$.
- Accumulation points satisfy $0 \in \mathrm{conv}\left(\mathrm{Jac}\,^c g_L \circ \ldots \circ \mathrm{Jac}\,^c g_1\right)(\theta)$
- For "most" such sequences, accumulation points are Clarke critical $0 \in \partial^c \ell(\theta)$.
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- g_i is locally Lipschitz tame (piecewise polynomial, semi-algebraic, definable).

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$$\min_{\theta \in \mathbb{R}^p} \ell(\theta) := \frac{1}{n} \sum_{i=1}^{n} g_{i,L} \circ \ldots \circ g_{i,1}(\theta)$$

Qualitatively similar results under appropriate assumptions.

- **Subsampling:** at step k sample $i_k \subset \{1, \ldots, n\}$ uniformly at random.

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Despite differential calculus artifacts, optimization works with nonsmooth autodiff:

TensorFlow PyTorch

Plan

$f : \mathbb{R}^p \times \mathbb{R}^m \to \mathbb{R}$
μ measure on $\mathbb{R}^m$, $f(x, \cdot)$ μ-integrable for all x.
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Inversion integral / derivative:

$x \mapsto f(x,s)$, **smooth**, for all s,

$$\forall (x,s),\ \|\nabla_x f(x,s)\| \leq \kappa(s)$$

for $\kappa : \mathbb{R}^m \to \mathbb{R}_+$, μ integrable.

Gradient of F

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Abstract integrals (with Bolte, Le, 2021)

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Applications: Stochastic optimization, chain rule for parametric integrals (assumption).

Ordinary differential equations (with Marx, 2022)

$F\colon \mathbb{R}^m \to \mathbb{R}^m$ Lipschitz

$$\frac{d}{dt}X(t,\theta) = F(X(t,\theta))$$
$$X(0) = \theta \in \mathbb{R}^m.$$

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Sensitivity equation:

F, **smooth**.

$$\frac{d}{dt}M(t,\theta) = \mathrm{Jac}\, F(X(t,\theta))M(t,\theta)$$
$$M(0) = I \in \mathbb{R}^{m\times m}. \qquad (1)$$

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Applications: Neural ODE, adjoint method, optimization under ODE constraints.

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Classical implicit differentiation:

F **smooth,** assume

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Solutions to $F(\theta, x) = 0$ locally parametrized by $G : U \to \mathbb{R}^n$, **smooth:**

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Applications: Differentiate $G(x)$ uniquely defined as $F(x, G(x)) = 0$.
parametric optimization, bilevel optimization, implicit modeling, hyperparameter tuning.

Algorithmic unrolling (with Bolte, Vaiter, 2022)

$F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$, algorithmic recursion, $x_0(\theta) \in \mathbb{R}^n$

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$$\mathrm{Jac}\, x_{k+1}(\theta) = B \mathrm{Jac}\, x_k(\theta) + A$$
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Limiting **jacobian.**

$$\mathrm{Jac}\, x_k(\theta) \underset{k\to\infty}{\to} \mathrm{Jac}\, \bar{x}(\theta)$$
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$$\begin{aligned} \mathrm{Jac}\, x_{k+1}(\theta) &= B \mathrm{Jac}\, x_k(\theta) + A \\ [A, B] &= \mathrm{Jac}\, F(\theta, x_k(\theta)) \end{aligned}$$

Limiting **jacobian.**

$$\mathrm{Jac}\, x_k(\theta) \underset{k \to \infty}{\to} \mathrm{Jac}\, \bar{x}(\theta)$$
$$= (I - B)^{-1} A,\ [A, B] = \mathrm{Jac}\, F(\theta, \bar{x}(\theta))$$

Nonsmooth unrolling :

F **path-differentiable**.

Conservative jacobian propagation:

$$D_{k+1}(\theta) = \big\{ B D_k(\theta) + A \quad [A, B] \in \mathrm{Jac}^{\,c} F(\theta, x_k(\theta)) \big\}$$

Limiting **conservative jacobian:**

$$D_k(\theta) \underset{k \to \infty}{\to} \bar{D}(\theta)$$
$$\supset \left\{ (I - B)^{-1} A, \quad [A, B] \in \mathrm{Jac}^{\,c} F(\theta, \bar{x}(\theta)) \right\}$$

$F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$, algorithmic recursion, $x_0(\theta) \in \mathbb{R}^n$

$$x_{k+1}(\theta) = F(\theta, x_k(\theta)).$$

For all θ, $x \to F(x, \theta)$ is ρ Lipschitz, $\rho < 1$: $\quad x_k(\theta) \underset{k\to\infty}{\to} \bar{x}(\theta)$.

Classical asymptotics (Gilbert 92):

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Applications: Differentiation of forward-backward, Douglas-Rachford, ADMM).

Plan

Initial motivation an results:

- study nonsmooth automatic differentiation.
- compositional calculus rules: sum, product, composition.
- require chain rule along Lipschitz curves: ubiquitous in applications.
- optimization: qualitative convergence of first order methods.

Extensions:

- Optimization algorithm variations.
- Extensions of conservative calculus.

Not presented

- Proof details.
- Parametric optimality for max structured functions.
- Complexity considerations (with Bolte, Boustany, Pesquet-Popescu)

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Thanks.

Ongoing work on "conservative calculus"

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Thanks.

$$\min_{\theta \in \mathbb{R}^p} \ell(\theta) := g_L \circ \ldots \circ g_1(\theta)$$

Assumption:

- g_i is locally Lipschitz tame (piecewise polynomial, semi-algebraic, definable).

First order algorithm: fix $\theta_0 \in \mathbb{R}^p$, $(\alpha_k)_{k\in\mathbb{N}}$ positive sequence

$$\theta_{k+1} \in \theta_k - \alpha_k \left(\mathrm{Jac}^{\,c} g_L \circ \ldots \circ \mathrm{Jac}^{\,c} g_1\right)(\theta_k).$$

Theorem (Bolte-Pauwels 2020):

- **Step size condition:** $\sum_{k=1}^{+\infty} \alpha_k = +\infty$ and $\alpha_k \to 0$.
- Accumulation points satisfy $0 \in \mathrm{conv}\left(\mathrm{Jac}^{\,c} g_L \circ \ldots \circ \mathrm{Jac}^{\,c} g_1\right)(\theta)$
- There is a meagre Lebesgue null set X_0 and finite set $\Lambda \in \mathbb{R}_+$ such that if $\theta_0 \notin X_0$ and $\alpha_k \notin \Lambda$, $k \in \mathbb{N}$, accumulation points are Clarke critical $0 \in \partial^c \ell(\theta)$.

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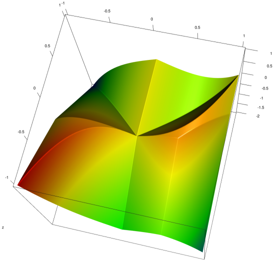
Semi-algebraic?

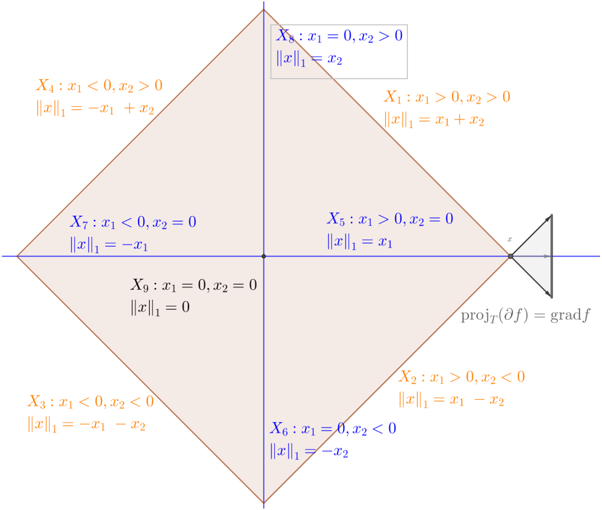
Basic set: Solution set of finitely many polynomial inequalities.
Set: Finite union of Basic semi-algebraic sets.
Function, set valued map: Semi-algebraic graph.
Examples: polynomials, square root, quotients, norm, relu, rank ...



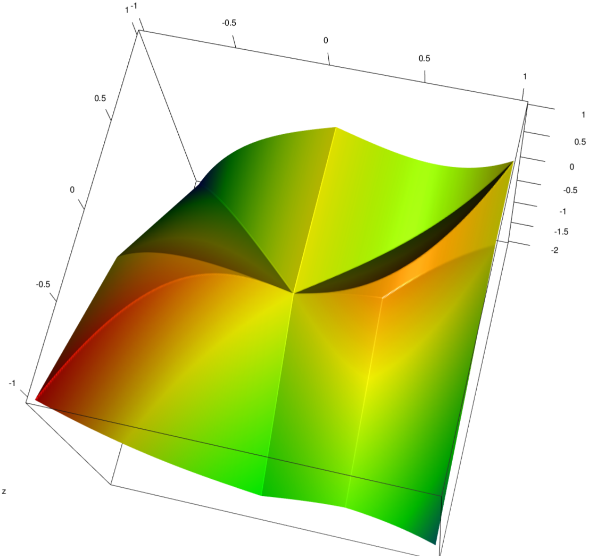
Tarski Seidenberg: first order formula involving semi-algebraic sets $\rightarrow$ semi-algebraic.

- gradient / subgradient of semi-algebraic function, partial minima, composition ....

Variational stratification: [Bolte-Daniilidis-Lewis (2007)]
Example: Projection formula .



Variational stratification: [Bolte-Daniilidis-Lewis (2007)]
Example: Projection formula $f(x_1, x_2) = |x_1| + |x_2|$.



Let $D \colon \mathbb{R}^p \rightrightarrows \mathbb{R}^p$ be a semi-algebraic (or definable), graph closed, locally bounded and $f \colon \mathbb{R}^p \to \mathbb{R}$, $r \in \mathbb{N}^*$. Then the following are equivalent

- D is a conservative field for f.
- (f, D) has a C^r variational stratification: there exists a stratification $\{M_i\}_{i \in I}$ of $\mathbb{R}^p$ such that
  - The restriction f_{M_i} of f to M_i is C^r for all $i \in I$.
  - For all $x \in \mathbb{R}^p$, set M_x the active stratum, T_x its tangent space at x.

$$P_{T_x} D(x) = \{\mathrm{grad}\ f_{M_x}(x)\}.$$

Whitney stratification: finite partition of $\mathbb{R}^p$ into C^r embedded manifolds (+ technical condition).

Applies to backprop:

- Morse-Sard condition.
- artefacts are "negligible" in a geometric sense.