Nonsmooth implicit differentiation for optimization

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joint work with

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OWOS seminar (September 2021)

Observations:

- The classical implicit function theorem has two parts (existence and calculus)
- Nonsmooth generalizations essentially focused on existence.

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Contributions: nonsmooth generalization of the calculus part.

- Direct generalization of calculus fails.
- Our solution: use conservative Jacobians.
- Applications in compositional modeling (ML, DEQ), bilevel optimization, . . .

Plan

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Classical implicit function theorem (Dini 1877)

Let $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ be continuously differentiable with Jacobian $\mathrm{Jac}_F(x, y) = [A_x \ B_y] \in \mathbb{R}^{m\times(n+m)}$ and $(\bar{x}, \bar{y}) \in \mathbb{R}^n \times \mathbb{R}^m$ such that

$$F(\bar{x}, \bar{y}) = 0.$$

If $B_{\bar{y}}$ is invertible, then there exists $U \subset \mathbb{R}^n$ a neighborhood of $\bar{x}$ and a differentiable function $G(x)$ so that

$$\forall x \in U \qquad F(x, G(x)) = 0,$$

and $y = G(x)$ is the unique such solution in a neighborhood of $\bar{y}$.

$$\mathrm{Jac}_G(x) = -B^{-1}A, \qquad [A \ B] = \mathrm{Jac}_F(x, G(x)).$$

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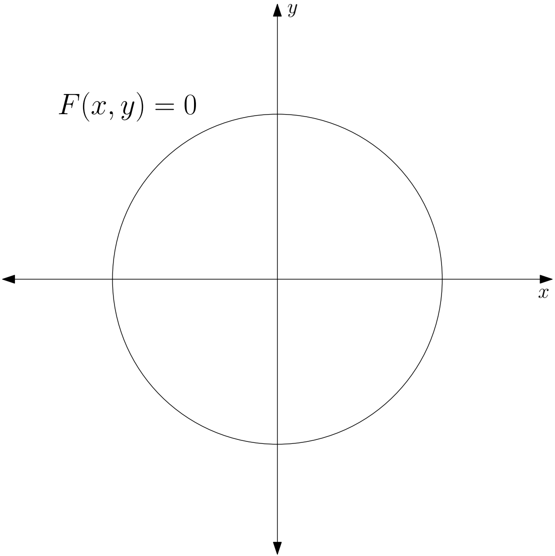
- **Existence:** Equation $F(x, y) = 0$ defines a functional relation $y = G(x)$ around $\bar{x}$.
- **Implicit differentiation:** Calculus rule for the derivative of G.

$F(x, y) = x^2 + y^2 - 1.$



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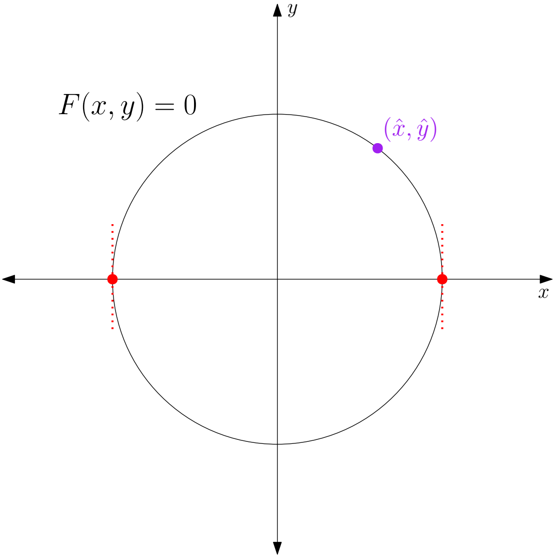

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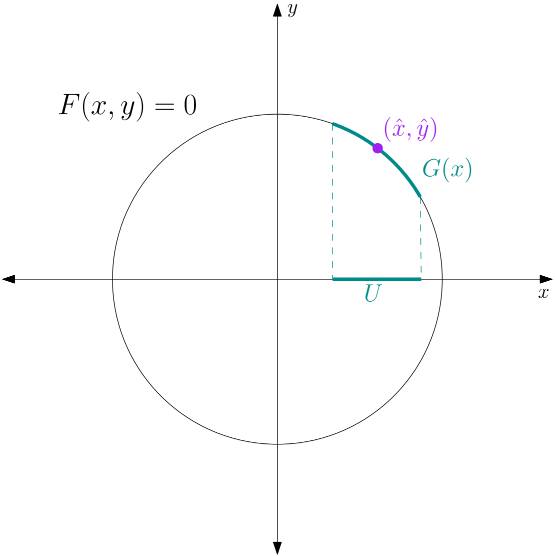

Classical inverse mapping theorem

Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable with Jacobian $\mathrm{Jac}_F : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ and $\bar{x} \in \mathbb{R}^n$ such that $\mathrm{Jac}_F(\bar{x})$ is nonsingular. Then there exists $U \subset \mathbb{R}^n$ a neighborhood of $\bar{x}$ such that F_U is a diffeomorphism. For all $x \in U$,

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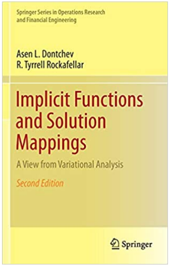

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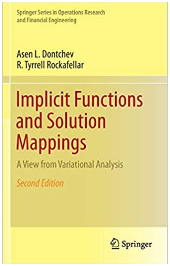

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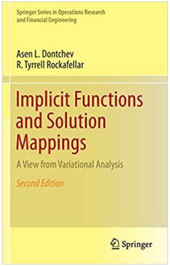

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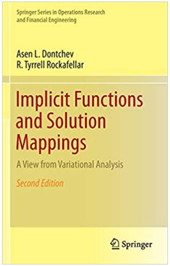

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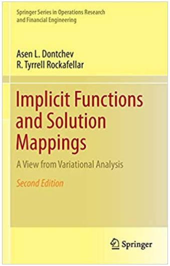

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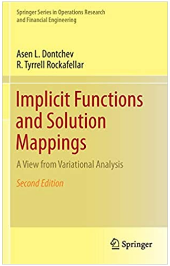

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    - Robinson (1991) directional derivatives with calculus (restricted subclass).
    - Sun (2001), semismoothness.
    - Fukui, Kurdyka, Paunescu (2007), subanalytic / tame.

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Motivation and applications:

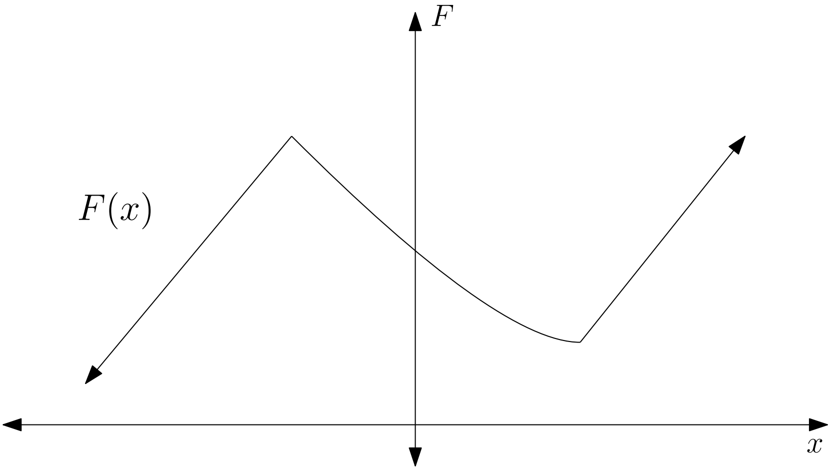
- Generalizations focused on the existence / regularity part.
- Applications:
  - Bilevel optimization: differentiate solutions of optimization problems.
  - Implicit compositional modeling: equilibrium models, declarative networks . . .

Plan

Clarke's generalized derivatives: Given a locally Lipschitz function $F : \mathbb{R}^n \to \mathbb{R}^m$, the Clarke Jacobian at a point $x \in \mathbb{R}^n$ is

$$J_F^c(x) = \mathrm{conv}\left(\left\{\lim_{k\to\infty} \mathrm{Jac}\,_F(x_k) : x_k \in \mathrm{diff}_F \text{ and } x_k \to x\right\}\right),$$

where diff_F is the set of differentiability point of F (Rademacher: full measure).



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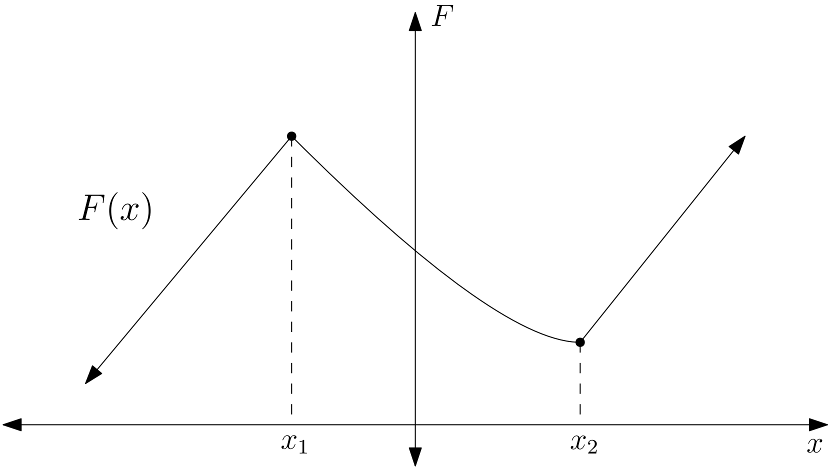
Generalized derivative



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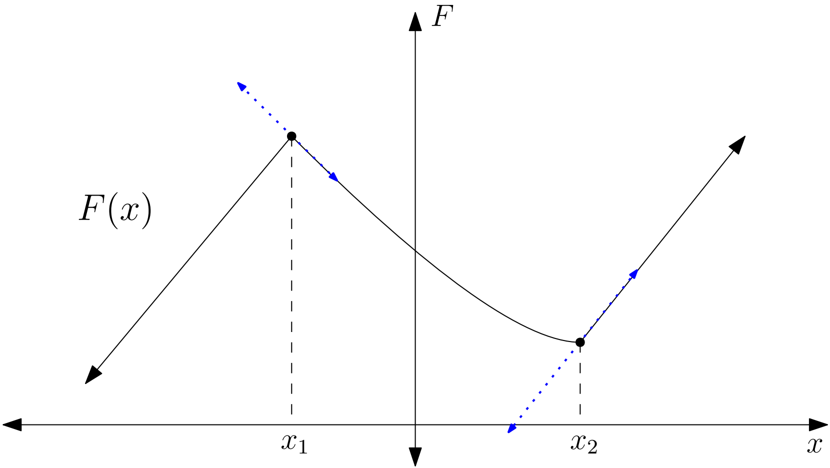

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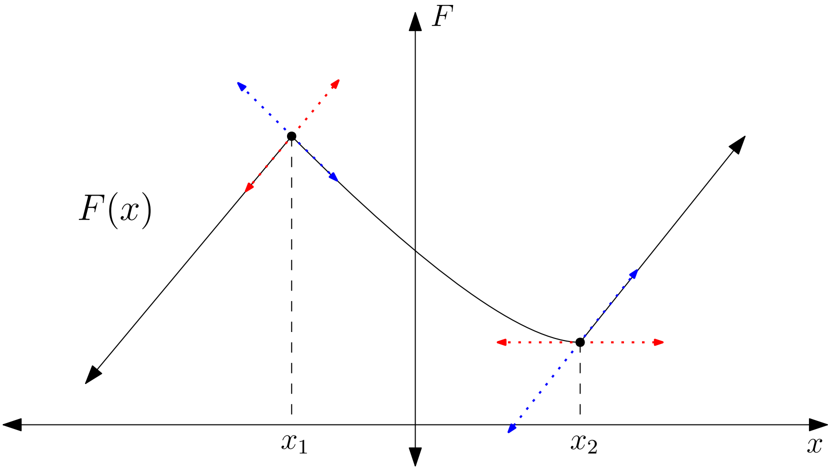

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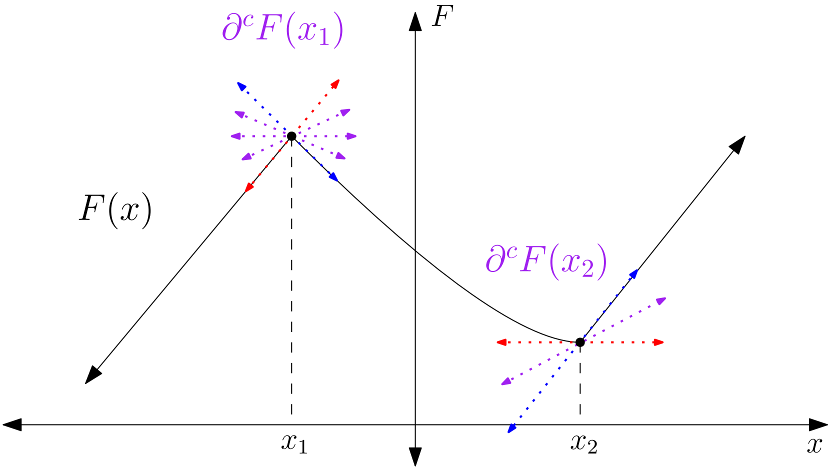

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$$F(\bar{x},\bar{y})=0.$$

If, $\forall[A\ B]\in J_F^c(\bar{x},\bar{y})$, B is invertible, then $\exists U\subset\mathbb{R}^n$ a neighborhood of $\bar{x}$ and a locally Lipschitz function $G(x)$ so that

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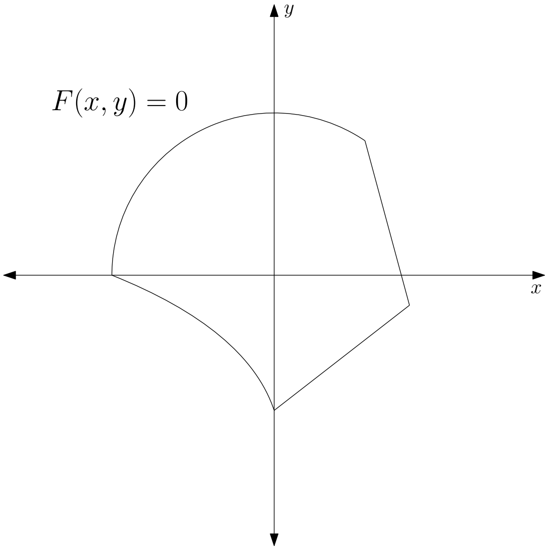

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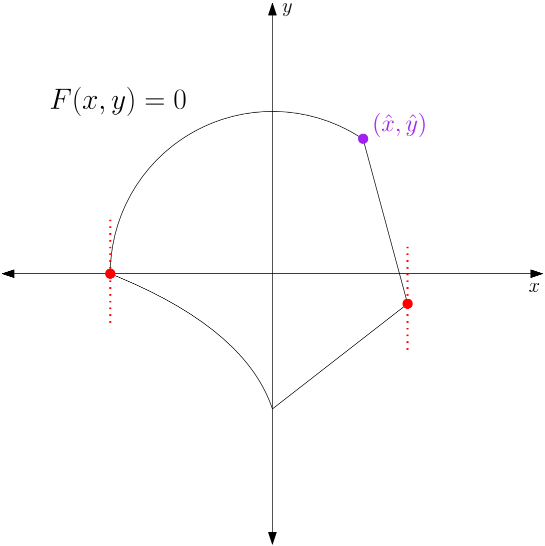

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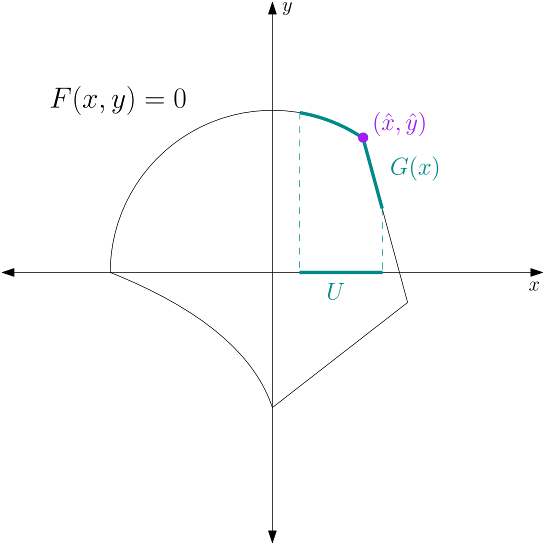

Lipschitz implicit function theorem (Hiriart Urruty 1979, Clarke 1976)

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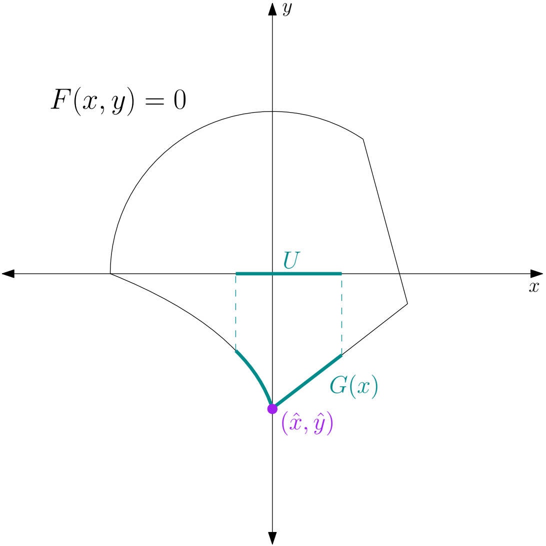

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Formal inverse differentiation? For all $x \in U$,

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From Clarke's book: consider the function $F\colon \mathbb{R}^2 \to \mathbb{R}^2$

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$$F\colon \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} |x| + y \\ 2x + |y| \end{pmatrix}$$

- $F(0) = 0$
- $J^c F(0) = \left\{ \begin{pmatrix} \alpha & 1 \\ 2 & \beta \end{pmatrix}, \alpha, \beta \in [-1, 1] \right\}$
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Explicit piecewise affine inverse.

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\begin{aligned}
F^{-1}(u,v) &= (v-u, 2u-v) && \text{for } (u,v)\in A,\\
F^{-1}(u,v) &= \frac{1}{3}(u+v, 2u-v) && \text{for } (u,v)\in B,\\
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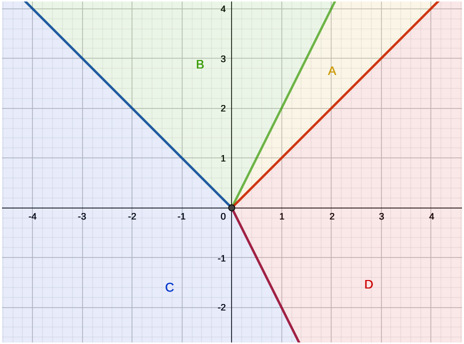

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Plan

Conservative gradients / Jacobians:

- Objects akin to Clarke's subgradient / Jacobian (for locally Lipschitz functions).
- A given function $F : \mathbb{R}^n \to \mathbb{R}^m$ has multiple conservative Jacobians $J_F : \mathbb{R}^n \rightrightarrows \mathbb{R}^{m \times n}$.
- Compatible with compositional calculus rules
  - $J_F : \mathbb{R}^n \rightrightarrows \mathbb{R}^{m \times n}$ conservative for $F : \mathbb{R}^n \to \mathbb{R}^m$.
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- **Lazy gradient oracle:** Bianchi-Hachem-Schechtman (2020).
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- **Semi-smoothness:** Davis-Drusvyatskiy (2021).

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Vanishing step sizes, almost surely all accumulation points are critical points: $0 \in \partial^c f(\bar{\theta})$.

Generic triviality, generic rigidity

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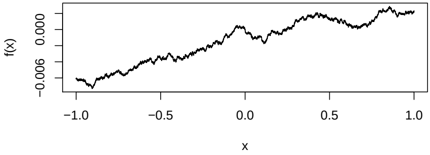

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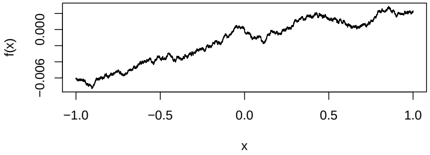

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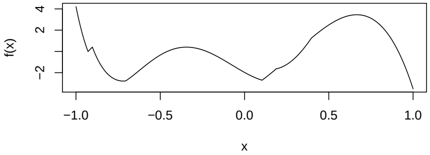

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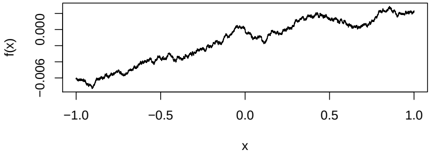

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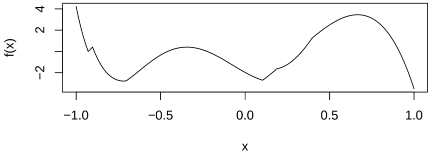

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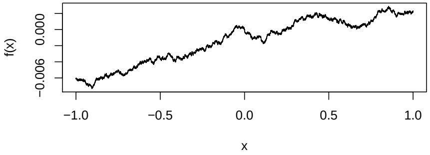

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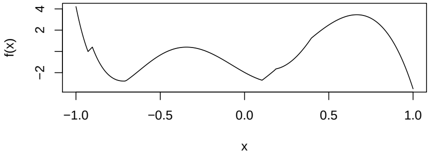

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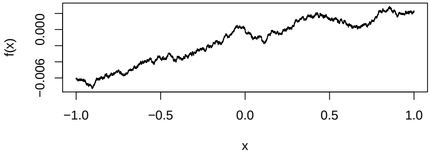

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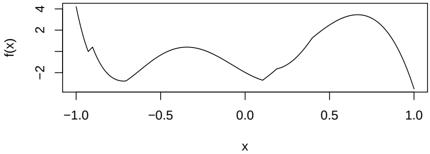

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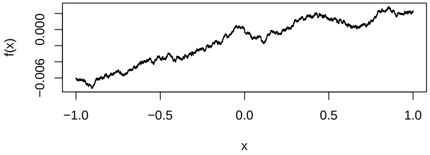

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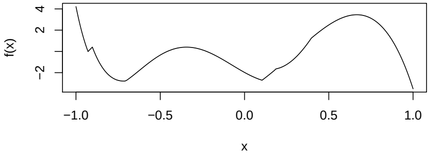
Davis et .al. 2019, **Bolte et. al. 2007:** Subgradient projection formula implies chain rule along AC curves.



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Results:

- $D(x) = \{\nabla f(x)\}$ for *almost all* $x \in \mathbb{R}^p$.
- $\partial^c f(x) \subset \mathrm{conv}(D(x))$ for all $x \in \mathbb{R}^p$.
- Sum, linear combinations, compositions of conservative Jacobians are conservative.

Conservative gradient and optimization

$$\min_{\theta \in \mathbb{R}^p} \ell(\theta) := \frac{1}{N} \sum_{i=1}^{N} \ell_i(\theta) \quad \text{with} \quad \ell_i = g_{i,L} \circ g_{i,L-1} \circ \ldots \circ g_{i,1}$$

Assumption: For $i \in \{1, \ldots, N\}$ and $j \in \{1, \ldots, L\}$,

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For $i \in \{1, \ldots, N\}$, set $D_i = \prod_{j=1}^{L} J_{i,j}$.

- D_i is a conservative gradient for ℓ_i.
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Conservative gradient and optimization

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- **Step size:** $\sum_{k=1}^{+\infty} \alpha_k = +\infty$ and $\alpha_k = o(1/\log(k))$.
- **Boundedness:** there exists $M > 0$, $\|\theta_k\| \leq M$ almost surely.
- Almost surely, $\ell(\theta_k)$ converges, accumulation points satisfy $0 \in \sum_{i=1}^{N} \mathrm{conv}(D_i(\bar{\theta}))$
- For "most" such sequences, accumulation points are Clarke critical $0 \in \partial^c \ell(\theta)$.

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Conservative gradients / Jacobians:

- Objects akin to Clarke's subgradient / Jacobian.
- Compatible with compositional calculus rules
- Have a minimizing behavior similar to subgradients in optimization.

Plan

Clarke's inverse mapping theorem:

- $F : \mathbb{R}^n \to \mathbb{R}^n$ locally Lipschitz
- Clarke Jacobian $J_F^c : \mathbb{R}^n \rightrightarrows \mathbb{R}^{n \times n}$
- $\bar{x} \in \mathbb{R}^n$ such that $J_F^c(\bar{x}) \subset \mathbb{R}^{n \times n}$ only contains nonsingular matrices.

Then there exists $U \subset \mathbb{R}^n$ a neighborhood of $\bar{x}$ such that F_U is a bi-Lipschitz homeomorphism.

Failure of formal differentiation

$$J_{F^{-1}}^c(y) \neq J_F^c(F^{-1}(y))^{-1} := \left\{ M^{-1},\ M \in J_F^c(F^{-1}(y)) \right\}$$

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- $\forall [A\ B] \in J_F^c(\bar{x}, \bar{y})$, B is invertible

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and $y = G(x)$ is the unique such solution in a neighborhood of $\bar{y}$.

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- Preserved by inversion / implicit definition.

$\Rightarrow$ convergence of small step first order methods.

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Plan

Assumption: ℓ and f locally Lipschitz. For any θ,

- the inner argmin is a singleton

$$\begin{aligned} \min_{\theta \in \mathbb{R}^p} \quad & \ell(x(\theta)) \\ \text{s.t.} \quad & x(\theta) \in \operatorname*{argmin}_{x \in \mathbb{R}^m} f(x, \theta) \end{aligned}$$

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Example: Lasso hyperparameter optimization (Bertrand *et. al.* 2020).

$$x(\theta) \in \operatorname*{argmin}_{x \in \mathbb{R}^m} \frac{1}{2}\|Ax - b\|_2^2 + \theta\|x\|_1, \qquad \theta > 0$$

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$\Rightarrow$ recover LARS algorithm + convergence of small step first order methods.

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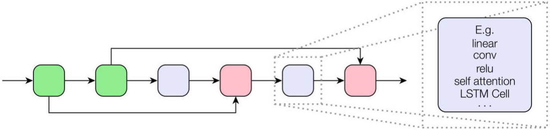
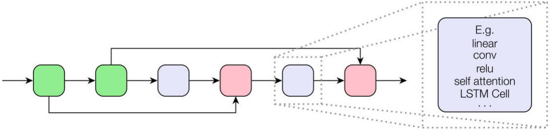


Image courtesy: `implicit-layers-tutorial.org`

Neural networks:
Compositional models, elementary blocks called *layers* (parametric functions).



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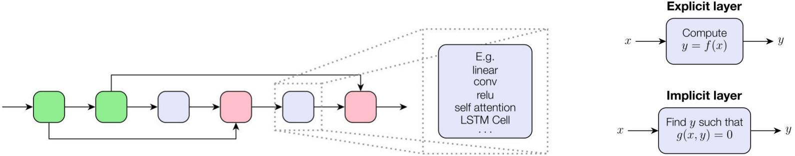

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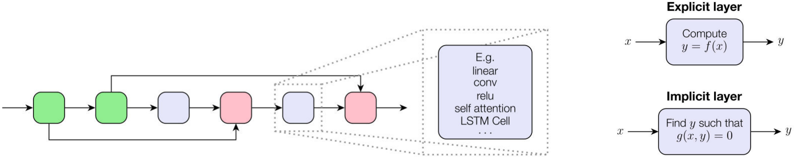

Image courtesy: `implicit-layers-tutorial.org`

Examples: Equilibrium networks (Bai *et. al.* 2019), implicit networks (El Ghaoui *et. al.* 2019) declarative networks (Gould *et. al.* 2019), optimization layers (Agrawal *et. al.* 2019)

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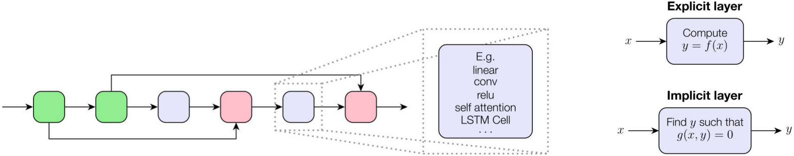

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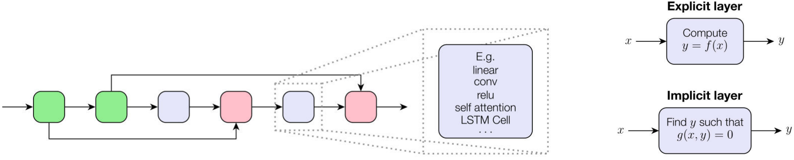

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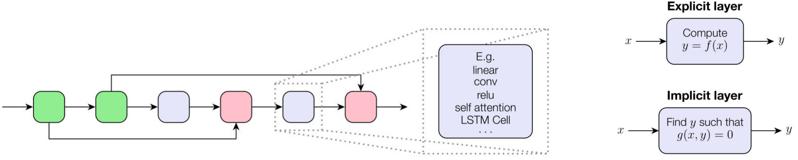

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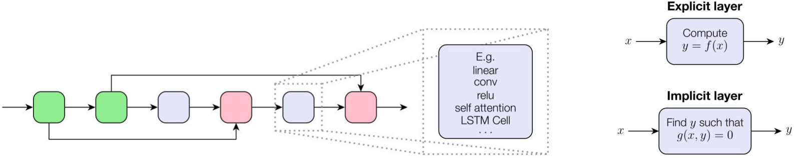

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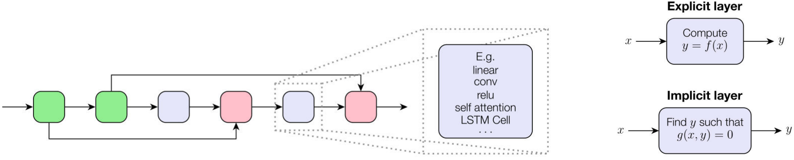

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$\Rightarrow$ invertibility condition for nonsmooth implicit differentiation
$\Rightarrow$ convergence of small steps training algorithms.

Plan

Implicit differentiation applied to:

$$\begin{aligned} \min_{x,y,s} \quad & \ell(x, y, s) := (x - s_1)^2 + 4(y - s_2)^2 \\ \text{s.t.} \quad & s \in \arg\max\{(a + b)(-2x + y + 2) : a \in [0, 3], b \in [0, 5]\}. \end{aligned}$$

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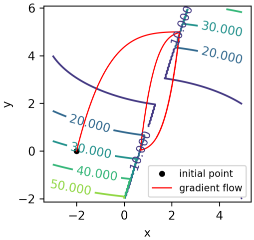

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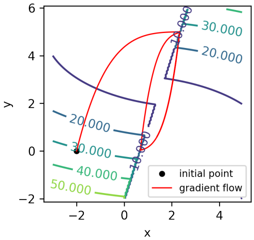

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Pathological Examples - Cyclic "*gradient*" orbits

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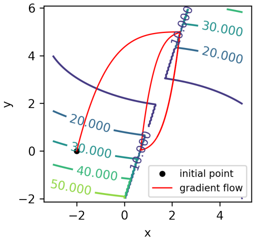

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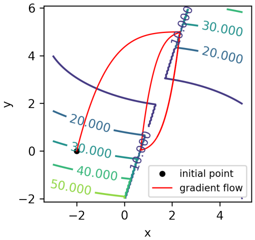

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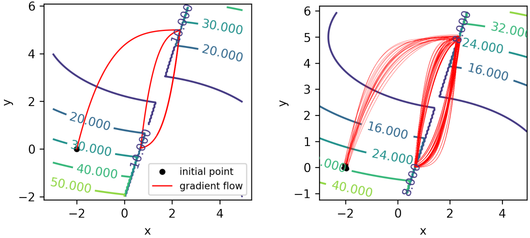

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Thanks.