Differentiating Nonsmooth Solutions to Parametric Monotone Inclusion Problems

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ISMP 2024 Montréal

Plan

- **Motivation**
- Conservative Gradients
- Results
- Applications
- Numerical Examples

A Motivating Example

Recall the LASSO problem:

$$\hat{x} \in \operatorname*{argmin}_{x \in \mathbb{R}^p} \frac{1}{2} \|Ax - b\|_2^2 + e^{\theta} \|x\|_1 .$$

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Given some measure of task performance $C(\hat{x}(\theta))$, how to pick the "best" value of θ?

The problem of choosing θ becomes a bilevel optimization problem:

$$\min_{\theta \in \mathbb{R}} C(\hat{x}(\theta)) \quad \text{such that} \quad \hat{x} \in \operatorname*{argmin}_{x \in \mathbb{R}^p} \frac{1}{2} \|Ax - b\|_2^2 + e^{\theta} \|x\|_1 .$$

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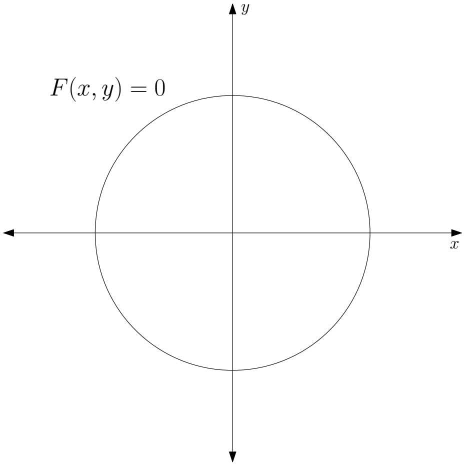
However, $\hat{x}(\cdot)$ might not be smooth (often the case in machine learning settings). We need a method to derive functions like $\hat{x}$ which are implicitly defined.

Consider the smooth function

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

and the equation

$$F(x, y) = 0.$$



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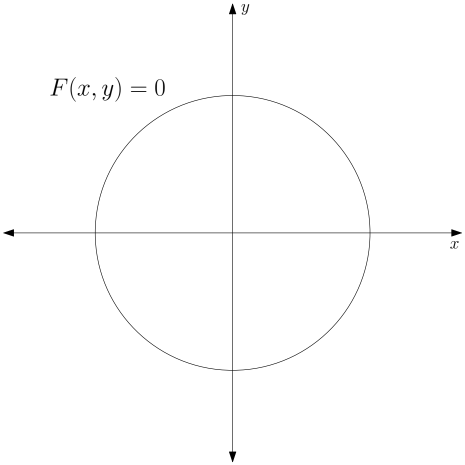

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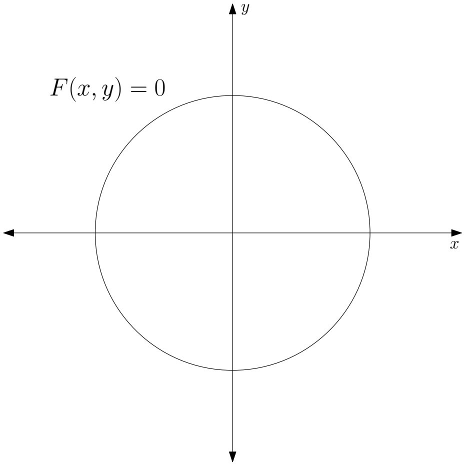

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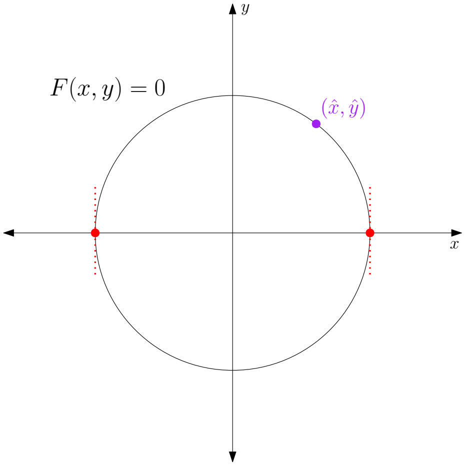

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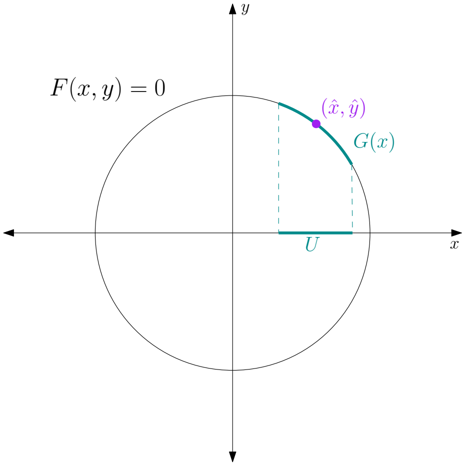

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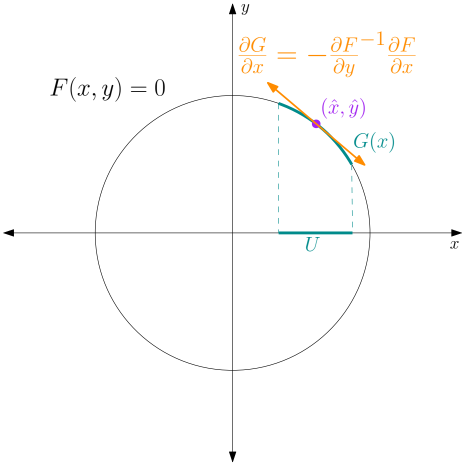

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In practice one hopes for an algorithm of the form

$$x^+ = x - \gamma d(x)$$

where $d(x)$ is some descent direction or surrogate "gradient".

Nonsmooth Implicit Function Theorem with Clarke Subdifferential

Theorem (Clarke 1976, Hiriart-Urruty 1979)

Let $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ be locally Lipschitz and $(\hat{x}, \hat{y}) \in \mathbb{R}^n \times \mathbb{R}^m$ such that

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

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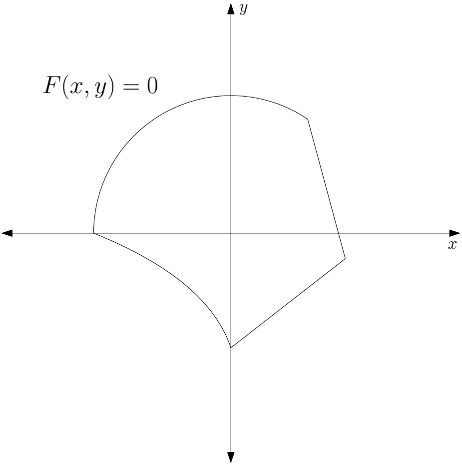

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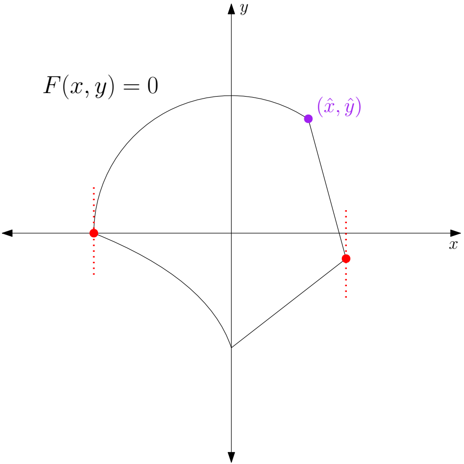

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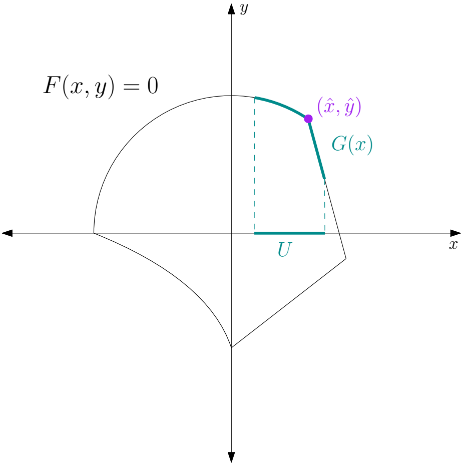

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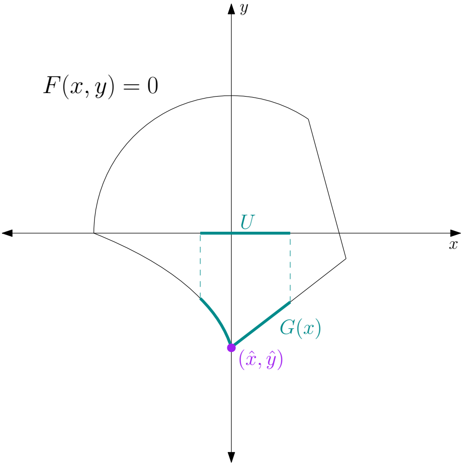

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Lack of Calculus

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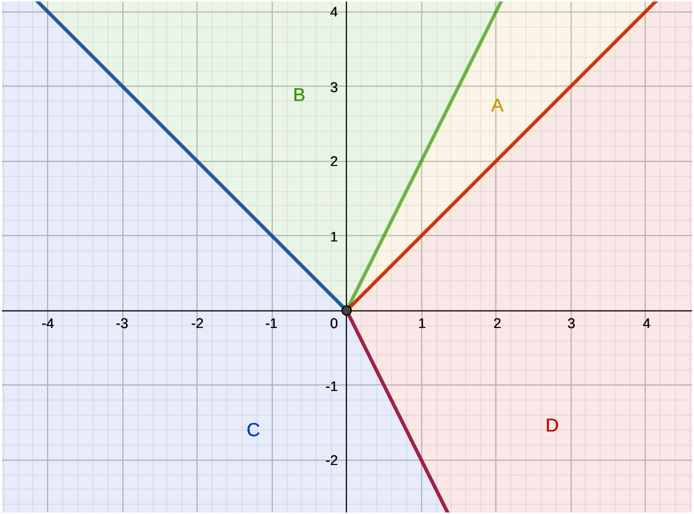
$\exists$ piecewise linear $F : \mathbb{R}^2 \to \mathbb{R}^2$ for which Clarke's inverse mapping theorem fails:

$$\exists M \in J^c_F(0,0) \quad \text{such that} \quad M^{-1} \notin J^c_{F^{-1}}(0,0)$$

Counterexample

$$F(x, y) = (|x| + y, 2x + |y|)$$



F^{-1} is linear on each region $A, B, C, \& D$.

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A set valued mapping $D_F \colon \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ is a conservative field (or conservative Jacobian) for $F : \mathbb{R}^n \to \mathbb{R}$ locally Lipschitz if:

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Take home message: conservative fields/Jacobians faithfully model what is computed by backpropagation in practice.

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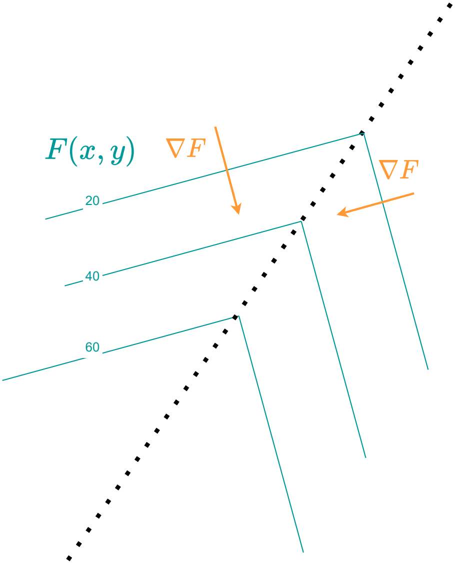

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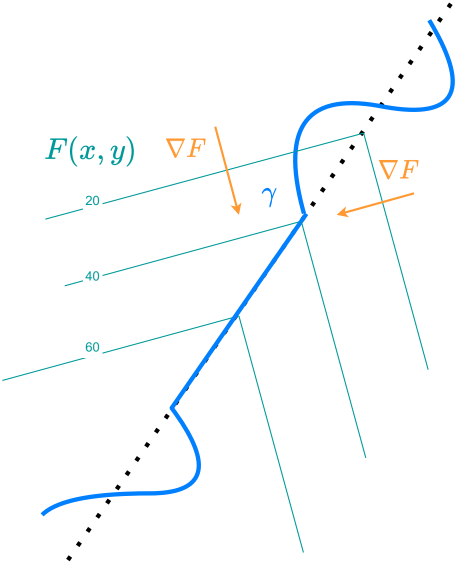

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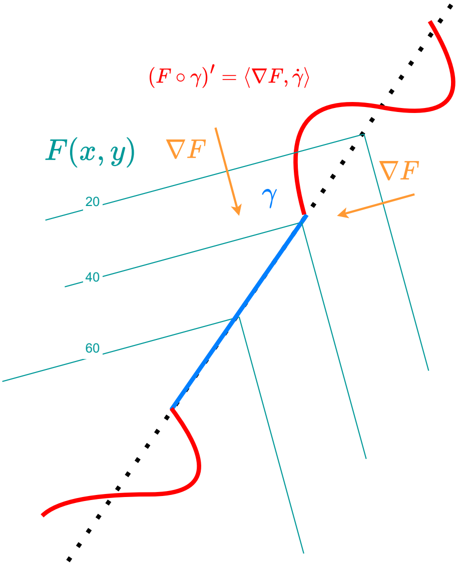

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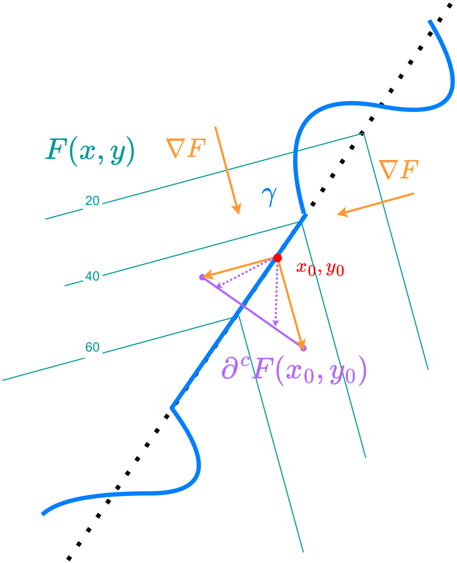

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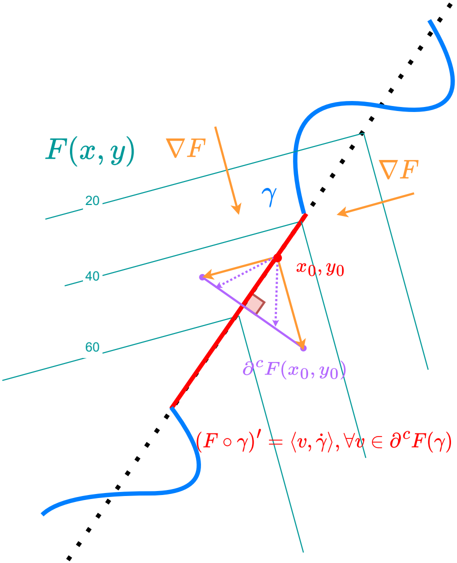

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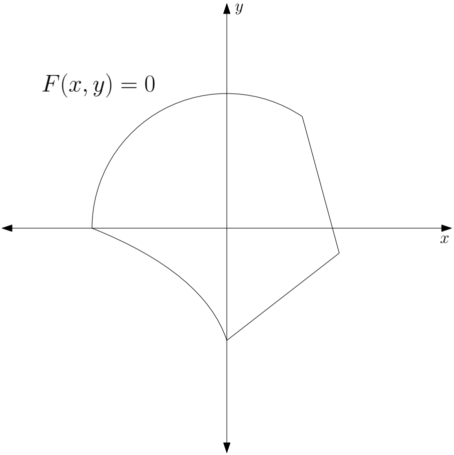

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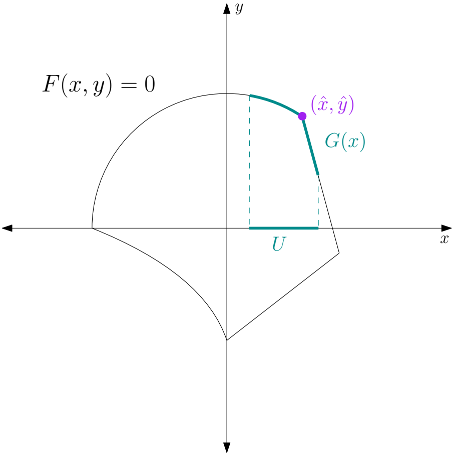

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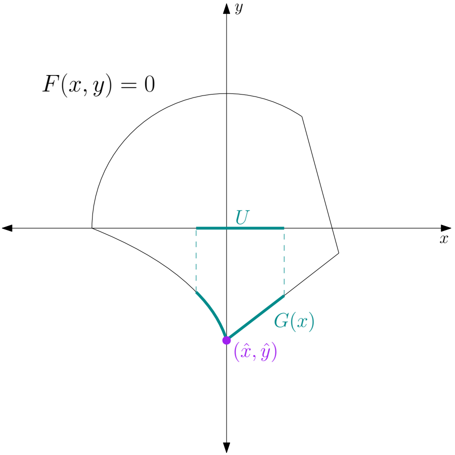

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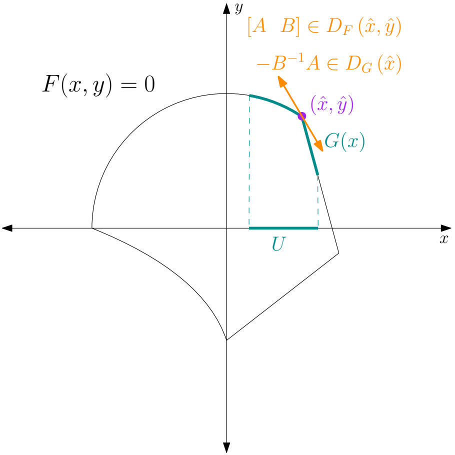

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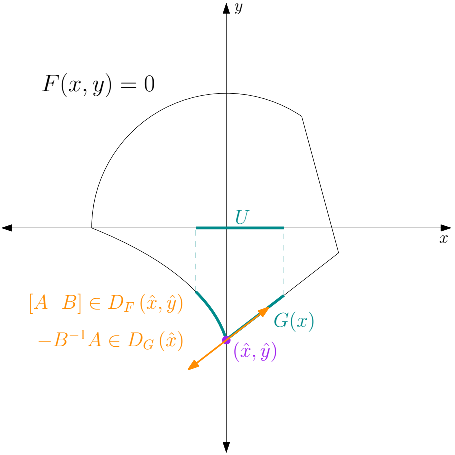

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- Conservative Gradients
- Results
- **Applications**
- Numerical Examples

With our new theorem we can answer the question:

how to differentiate the solution to a nonsmooth convex optimization problem ?

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- Set-valued implicit function theorems + semismooth localizations [Gferer, Outrata 2024].
- etc.

We recall the LASSO problem:

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A fixed point condition for optimality:

$$\underbrace{\mathrm{prox}_{e^{\theta}\|\cdot\|_1}(\hat{x} - A^T(A\hat{x} - b)) - \hat{x}}_{F(\theta, x)} = 0.$$

the proximal mapping here is simply the "soft thresholding" operator, which is path differentiable. Thus, the function F is path differentiable.

Verification of Invertibility - Example With LASSO

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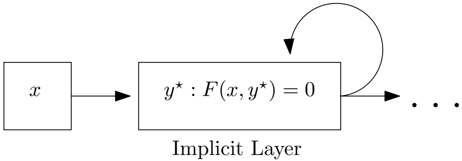
Proposition (Prop. 5 [Bolte, Le, Pauwels, S.F. 21])

Define, $\forall \theta \in \mathbb{R}$, the matrix $A_{\mathcal{E}}$ by taking the columns of A indexed by $\mathcal{E}$. If, $\forall \theta \in \mathbb{R}$, the matrix $A_{\mathcal{E}}^T A_{\mathcal{E}}$ is full rank, then $\hat{x}(\cdot)$ is a path differentiable function with a conservative Jacobian given by

$$D_{\hat{x}} : \theta \rightrightarrows \left\{ \left[-e^{\theta} (\mathrm{Id}_p - \mathrm{diag}(q)(\mathrm{Id}_p - A^T A))^{-1} \mathrm{diag}(q) \mathrm{sign}(\hat{x} - A^T (A\hat{x} - b)) \right] : q \in \mathcal{M}(\theta) \right\}$$

where $$\mathcal{M}(\theta) = \left\{ q : q_i \in \begin{cases} \{1\} & \text{if } i \in \mathcal{S} \\ [0,1] & \text{if } i \in \mathcal{E} \setminus \mathcal{S} \\ \{0\} & \text{if } i \notin \mathcal{E} \end{cases} \right\}.$$

Deep Learning with Implicit Layers



- Deep equilibrium networks [Bai, Kolter, Koltun 2019].
- Implicit networks [El Ghaoui, Gu, Travacca, Askari, Tsai 2019].
- Declarative networks [Gould, Hartley, Campbell 2019].
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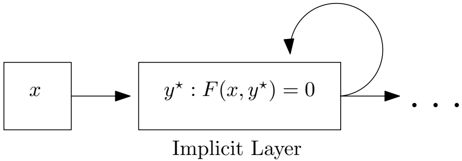

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conservative Jacobians $+$ path differentiable implicit function theorem

$\Longrightarrow$ convergence guarantees (every acc. point is a Clarke stationary point almost surely, objective values converge) for these network types.

Consider two parametric maximal monotone operators $\mathcal{A}_\theta$ and $\mathcal{B}_\theta$ and the inclusion

$$0 \in \mathcal{A}_\theta(x^\star) + \mathcal{B}_\theta(x^\star)$$

where $\mathcal{A}_\theta$ is set-valued but $\mathcal{B}_\theta$ is Lipschitz continuous. Note: We assume that $x^\star(\theta)$ is unique for each θ.

Generalizing to Monotone Inclusions/Generalized Equations

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$$\underbrace{R_{\gamma\mathcal{A}_\theta}(x - \gamma\mathcal{B}_\theta x)}_{H(\theta,x)} = x$$

We call H the Forward-Backward mapping. Formally we denote $T(\theta, x) := R_{\gamma\mathcal{A}_\theta}(x)$ and $S(\theta, x) := x - \gamma\mathcal{B}_\theta(x)$ the forward and backward maps which gives an equation we can apply the IFT to:

$$F(\theta, x) := H(\theta, x) - x = 0.$$

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We will assume that F is path differentiable jointly in (θ, x).

Choice of Conservative Jacobian

Beware: conservative Jacobians are not unique and not defined pointwise!

$$\text{Example: path differentiable } f : \mathbb{R} \to \mathbb{R}, \quad \tilde{\mathcal{J}}_f(x) = \begin{cases} \mathcal{J}_f(x) \cup \{1\} & x \in \mathbb{N} \\ \mathcal{J}_f(x) & x \notin \mathbb{N} \end{cases}$$

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We take the product of Clarke Jacobians of the forward and backward maps giving

$$\begin{aligned}
\mathcal{J}_{H_\theta}(\theta, x) &= \mathrm{Jac}^c_{\mathcal{T}}(S(\theta, x)) \times \mathrm{Jac}^c_{S}(\theta, x) \\
&= \Big\{ \begin{bmatrix} A & B \end{bmatrix} \times \begin{bmatrix} \mathrm{Id}_p & 0 \\ -C & \mathrm{Id}_n - \gamma D \end{bmatrix} : [A \ B] \in \mathrm{Jac}^c_{\mathcal{T}}(\theta, x - \gamma \mathcal{B}_\theta(x)), \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad [C \ D] \in \mathrm{Jac}^c_{\mathcal{B}}(\theta, x) \Big\} \\
&= \Big\{ \begin{bmatrix} A - BC & B(\mathrm{Id}_n - \gamma D) \end{bmatrix} : [A \ B] \in \mathrm{Jac}^c_{\mathcal{T}}(\theta, x - \gamma \mathcal{B}_\theta(x)), [C \ D] \in \mathrm{Jac}^c_{\mathcal{B}}(\theta, x) \Big\}
\end{aligned}$$

which is a conservative Jacobian for H.

Strong Monotonicity is All You Need™

Theorem (Bolte, Pauwels, S.F. 2024)

Assume that $\mathcal{B}_\theta$ is β-Lipschitz continuous and that either $\mathcal{A}_\theta$ or $\mathcal{B}_\theta$ is α-strongly monotone, for some $\alpha, \beta > 0$, uniformly in θ. For $\gamma \in (0, \frac{2\alpha}{(\alpha+\beta)^2})$, the invertibility condition holds and $x^\star$ is path differentiable with a conservative Jacobian whose formula is computable from $\mathcal{J}_H(x^\star(\theta))$.

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Proof.

If $\mathcal{A}_\theta$ or $\mathcal{B}_\theta$ is α-strongly monotone, then either T or S is a strict contraction, and we can choose γ to ensure that the composition H is a strict contraction. Then, the product of Clarke Jacobians will have norm < 1. □

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Corollary

The solution to the optimization problem

$$\min_{x \in \mathbb{R}^p} f_\theta(x) + g_\theta(x),$$

where f_θ is β-Lipschitz smooth and g_θ is nonsmooth, is path differentiable if either f_θ or g_θ is α-strongly convex.

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Piecewise quadratic objective function posed as a bilevel problem:

$$\min_{x,y,s} \quad (x - s_1)^2 + 4\,(y - s_2)^2 \qquad \text{such that}$$

$$s \in \arg\max \left\{ \, (a + b)\,(-2x + y + 2) : a \in [0, 3], b \in [0, 5] \, \right\}$$

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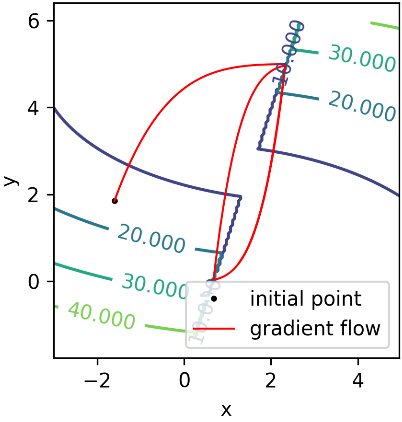

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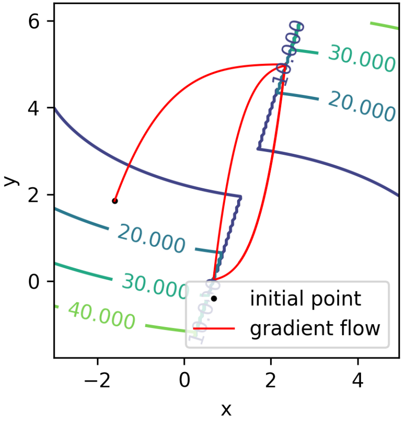

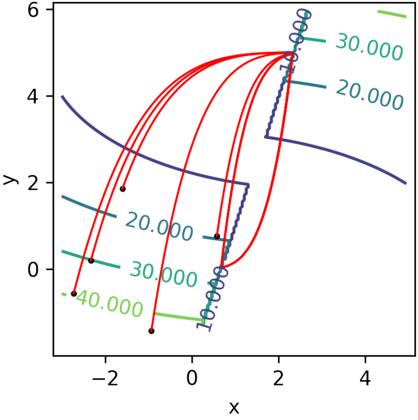

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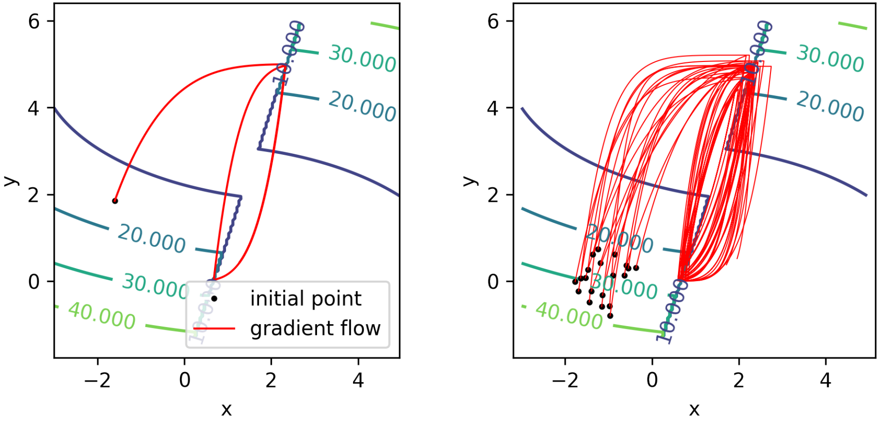

Pathological Examples - Optimizing a Quadratic Two Ways

$$\text{Let } L(u) = L(x, y, z) = \left(10(y-x), x(28-z)-y, xy-\tfrac{8}{3}z\right)$$

Explicit formulation

$$\max_{u \in \mathbb{R}^3} \quad u^T L(u)$$

$$\iff$$

Implicit formulation

$$\max_{u \in \mathbb{R}^3} \quad u^T z \quad \text{such that}$$

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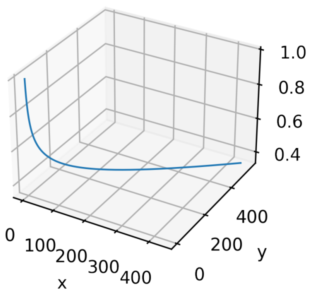

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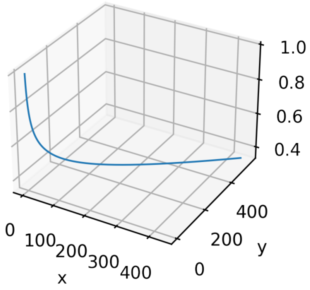
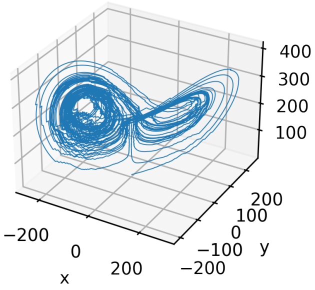


$\not\Leftrightarrow$



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Practical implications:

- Method to compute the gradient of solutions to convex optimization problems.
- Applications in machine learning (bilevel hyperparameter tuning, implicit neural networks, . . .).

Nonsmooth Implicit Differentiation for Machine Learning (NeurIPS, 2021)

Jérôme Bolte, Tâm Lê, Edouard Pauwels, Antonio Silveti-Falls

https://arxiv.org/abs/2106.04350

Differentiating Nonsmooth Solutions to Parametric Monotone Inclusion Problems (SIAM Optimization, 2024)

Jérôme Bolte, Edouard Pauwels, Antonio Silveti-Falls

https://arxiv.org/abs/2212.07844

N data points, L layers:

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

Each layer $g_{i,j}$ is semialgebraic (or definable) and path differentiable - can be explicit or implicit.
$N = 1, L = 2$ recovers bilevel optimization problem setting.
Define

$$w_{k+1} = w_k - s\alpha_k v_k \qquad v_k \in J_{I_k}(w_k)$$

for $(\alpha_k)_{k \in \mathbb{N}} \in \ell^1 \setminus \ell^2$
For almost all w_0, for almost all $s \in (s_{\min}, s_{\max})$, $\ell(w_k)$ converges and all acc. points of $(w_k)_{k \in \mathbb{N}}$ are clarke critical.