Optimisation: des maths pour des décisions plus robustes, résilientes, responsables

# Plaidoyer pour l'optimisation non-lisse

### illustré par l'aide à la décision robuste

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ACADÉMIE DES SCIENCES

# Mathematical Optimization ?

• branch of applied maths

(theory, algorithms, software, modeling)

applications everywhere

(industry, decision-making, sciences,...)

• being revolutionized by its interactions with data

(computational statistics, machine learning, IA)



optim. is at the core of IA, playing a fundamental role, behind the scenes

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nonsmooth optim. is at the core of IA, playing a fundamental role, behind the scenes

(French) pioneers on optimization...

worked on nonsmooth aspects



J.-J. Moreau

C. Lemaréchal H. Attouch

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## Nonsmooth objective functions are everywhere...

Max functions 
$$F(x) = \sup_{u \in U} h(u, x)$$

- robust optimization, stochastic optimization, decomposition methods
- Relaxations of combinatorial problems

### **Nonsmooth regularization** F(x) = f(x) + g(x)

- image/signal processing, inverse problems
- sparsity-inducing regularizers in machine learning

### Nonsmooth composition

$$F(x) = \mathbf{g} \circ \mathbf{c}(x)$$

- risk-averse optimization, eigenvalue optimization
- deep learning: nonsmooth activation, implicit layers

**Probability functions**  $F(x) = \mathbb{P}(h(x,\xi) \leq 0)$ 

• optimization under uncertainty, energy optimization

# So what ?...

Is nonsmoothness really important ? useful ?

### Why not just ignoring it ?

• Ex: nonsmooth deep learning

(with RELU, max-pooling or implicit layers)

- Just apply SGD with back-prog
- Or just apply quasi-Newton with (sub)gradients

### Why not smoothing it ?

- Smoothing by (inf-)convolution (e.g. Moreau regularization)
- Smoothings by overparameterization, ad hoc, or...



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# Example: $\ell_1$ -regularized least-squares (1/2)

$$\min_{x \in \mathbb{R}^{d}} \quad \frac{1}{2} \|Ax - y\|^{2} + \lambda \|x\|_{1} \qquad (\text{LASSO})$$

Illustration (on an instance with d = 2)



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$$\min_{x \in \mathbb{R}^d} \quad \frac{1}{2} \|Ax - y\|^2 + \lambda \|x\|_1 \qquad (LASSO)$$







$$\operatorname{prox}_{\gamma g}(y) = \operatorname*{argmin}_{z} \left\{ g(z) + \frac{1}{2\gamma} \|z - y\|^2 \right\}$$

(proximal-gradient) algorithms produce iterates...

...that eventually have the same support as the optimal solution

Nonsmoothness attracts (proximal) algorithms

# Today's message



Nonsmoothness is sometimes useful and always nice-looking

### Modest goals of this talk:

- Spotlights on 2 applications:
  - in industry : electricity generation
  - in learning : towards robustness and fairness
- High level: underline ideas, duality, models...

No theorems ! No algorithms ! (Almost) No references !

• For more, feel free to contact me :

jerome.malick@cnrs.fr

# Spotlight #1: Optimization of electricity production

In France: EDF produces electricity by N production units









hydro 17%



Question : finding "optimal" daily production schedules

Day-to-day optimization of production ("unit-commitment" )

Hard optimization problem: large-scale, heterogeneous, complex ( $\ge 10^6$  variables,  $\ge 10^6$  constraints)

Out of reach for (mixed-integer linear) solvers... But where is the nonsmoothness ?

# Spotlight #1: Optimization of electricity production

In France: EDF produces electricity by N production units





oil/gaz/coal 12%



hydro 17%



Question : finding "optimal" daily production schedules

Day-to-day optimization of production ("unit-commitment" )

 $\begin{pmatrix} \text{simplified} \\ \text{model} \end{pmatrix} \begin{cases} \min \sum_{i} c_i^\top x_i & (\text{production costs}) \\ \sum_{i} x_i = d & \twoheadleftarrow u \in \mathbb{R}^T & (\text{demand constraints}) \\ (x_1, \dots, x_N) \in X_1 \times \dots \times X_N & (\text{operational constraints}) \end{cases}$ 

Hard optimization problem: large-scale, heterogeneous, complex ( $\ge 10^6$  variables,  $\ge 10^6$  constraints)

Out of reach for  $(\ensuremath{\mathsf{mixed-integer}}\xspace$  linear) solvers... But where is the nonsmoothness ?



# Lagrangian decomposition

• Dual function (concave)

$$\theta(u) = \begin{cases} \min \sum_{i=1}^{N} c_i^{\top} x_i + \sum_{t=1}^{T} u^t \left( d^t - \sum_{i=1}^{N} x_i^t \right) \\ (x_1, \dots, x_N) \in X_1 \times \dots \times X_N \end{cases}$$

• Dualizing the coupling constraint makes it decomposable by units

$$\theta(u) = d^{\top}u + \sum_{i=1}^{N} \theta_i(u)$$
  
$$\theta_i(u) = \begin{cases} \min (c_i - u)^{\top} x_i \\ x_i \in X_i \end{cases}$$

• Nonsmooth algorithm: inexact prox. bundle [Lemaréchal '75... '95]







A. Renaud



- Research in the 1990's
- In action in early 2000's
- Save money and CO2 !

### On the shoulders of giants

### My contributions on this topic

- Acceleration of the bundle method (using coarse linearizations) [Malick, Oliveira, Zaourar '15]
- (Level) asynchronous bundle algorithm [lutzeler, Malick, Oliveira '18]
- Denoising dual solutions (by TV-regularization) [Zaourar, Malick '13]
- Introducing weather uncertainty in the model
  - robust version of the problem + bundle method [van Ackooij, Lebbe, Malick '16]
  - 2-stage stochastic version + double decomposition algorithm [van Ackooij, Malick '15]

...handling uncertainty adds extra nonsmoothness 🙂





## Spotlight #2: towards robust, resilient, responsible decisions

Spectacular success of deep learning, in many fields/applications... E.g. in generation **Ex:** picture generated with https://stablediffusionweb.com in oct. 2023.



input: "towards robust, resilient, responsible decisions"

Flying pigs (notebooks of NeurIPS 2018, tutorial on robustness)



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"ML is a wonderful technology: it makes pigs fly" [Kolter, Madry '18]

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Attacks against self-driving cars [@ CVPR '18]



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Train-test mismatch! Low Count Error High Error Error

Server 2 100

**Example:** Global model is deployed on *individual* clients



#### Amazon : l'intelligence artificielle qui n'aimait pas les femmes



Fairness issues, e.g.



l'idée semblait prometteuse à Amazon. Mais elle s'est mise à sous-noter les femmes candidates à des postes tech.







Error

#### Amazon : l'intelligence artificielle qui n'aimait pas les femmes



Accélérer le recrutement en faisant analyser les CV par une IA : l'idée semblait prometteuse à Amazon. Mais elle s'est mise à sous-noter les femmes candidates à des postes tech.



Tost



### Fairness issues, e.g.

### **Optimization set-up**

• Training data:  $\xi_1, \ldots, \xi_N$ 

e.g. in supervised learning: labeled data  $\xi_i = (a_i, y_i)$  feature, label

- Train model: f(x, ·) the loss function with x the parameter/decision (ω, β, θ, ...)
   e.g. least-square regression: f(x, (a, y)) = (x<sup>T</sup>a y)<sup>2</sup>
- Compute x via empirical risk minimization (a.k.a SAA)

$$\min_{\mathbf{x}} \frac{1}{N} \sum_{i=1}^{N} f(\mathbf{x}, \xi_i) = \mathbb{E}_{\widehat{\mathbb{P}}_N}[f(\mathbf{x}, \xi)] \quad \text{with } \widehat{\mathbb{P}}_N = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i}$$

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- Prediction with x for different data  $\xi$ 
  - Adversarial attacks (e.g. flying pigs, driving cakes...)
  - Presence of bias, e.g. heterogeneous data
  - Distributional shifts:  $\mathbb{P}_{\text{train}} \neq \mathbb{P}_{\text{test}}$
- Solution: take possible variations into account during training

...and nonsmoothness comes into play C

Rather than

 $\min \mathbb{E}_{\widehat{\mathbb{P}}_{N}}[f(\mathbf{x},\xi)]$ 

solve instead

 $\min_{\mathsf{x}} \max_{\mathbb{Q} \in \mathcal{U}} \mathbb{E}_{\mathbb{Q}}[f(\mathsf{x},\xi)]$ 



with  ${\mathcal U}$  a neighborhood of  $\widehat{\mathbb{P}}_N$ 

Wasserstein balls as ambiguity sets

$$\mathcal{U} = \{ \mathbb{Q} : W(\widehat{\mathbb{P}}_N, \mathbb{Q}) \leq \rho \}$$
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**WDRO objective function** for given *x*,  $\widehat{\mathbb{P}}_N$ ,  $\rho$ 

$$\begin{cases} \max_{\mathbb{Q}} \mathbb{E}_{\mathbb{Q}}[f(x,\xi)] \\ W(\widehat{\mathbb{P}}_{N},\mathbb{Q}) \leqslant \rho \end{cases} \Leftrightarrow \begin{cases} \max_{\mathbb{Q},\pi} \mathbb{E}_{\mathbb{Q}}[f(x,\xi)] \\ [\pi]_{1} = \widehat{\mathbb{P}}_{N}, [\pi]_{2} = \mathbb{Q} \\ \min_{\pi} \mathbb{E}_{\pi}[c(\xi,\xi')] \leqslant \rho \end{cases}$$

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 $\Leftrightarrow \min_{\lambda \ge 0} \lambda \rho + \mathbb{E}_{\widehat{\mathbb{P}}_{N}}[\max_{\xi'} \{f(x,\xi') - \lambda c(\xi,\xi')\}]$ 

...(finite dimension) nonsmooth... computable in some (specific) cases [Kuhn *et al.* '18] ...actually many more [Vincent, Azizian, lutzeler, Malick '24]

## Illustration: (W)DRO reshapes test histograms

Classification task, federated learning context [Laguel, Pillutla, Harchaoui, Malick '23]

ConvNet with EMNIST dataset (1730 users, 179 images/users)

Histogram over users of test misclassification error: standard vs. robust (dashed lines: 10%/90%-quantiles)



## Main current topic in my group

### Our work

- Applications in federated learning [Laguel, Pillutla, Harchaoui, Malick '23]
- (abstract, entropic) regularizations of WDRO [Azizian, lutzeler, Malick '22]
- Statistical guarantees [Azizian, lutzeler, Malick '23] [Le, Malick '24]
- Numerical work for an easy-to-use toolbox skWDR0 [Vincent, Azizian, lutzeler, Malick '24]



robustify our model with skWDRO !

scikitlearn interface + pytorch wrapper

# Conclusion

### Main take-aways

- Nonsmooth optimization rocks
- Electricity managment optimization is huge Handling size (and uncertainty) leads to nonsmooth optimization
- Deep learning works very well... unless it does not Handling robustness leads to nonsmooth optimization
- More work is needed resilience, fairness...

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Merci à vous pour votre confiance et pour votre écoute aujourd'hui

## Remark: smooth but stiff problems



### J.-B. Hiriart-Urruty C. Lemaréchal

In sharp contrast with smoothing-like approaches:

 Toy example from the book (Section VIII.3.3): for a smooth problem, run usual algorithms nonsmooth methods (prox/level-bundle) >>> smooth methods (gradient, conj. grad., q-Newton)

"There is no clear cut between

functions that are smooth and

In-between there is a rather fuzzy boundary of stiff functions"

functions that are not.

- Real-life example in energy optimization :
  - problem of managment of reservoirs : smooth
  - state-of-the-art algos to solve it : nonsmooth

Nonsmoothness can help, even for (difficult) smooth problems



### Two-stage stochastic unit-commitment

- The schedule x is sent to the grid-operator (RTE) before being activated and before observing uncertainty
- In real time, a new production schedule can be sent at certain times
- At time τ, we have the observed load ξ<sub>1</sub>,...,ξ<sub>τ</sub> and the current best forecast ξ<sub>τ+1</sub>,...,ξ<sub>τ</sub>
- We propose a stochastic 2-stage problem:



W. van Ackooij

$$\begin{cases} \min c^{\top}x + \mathbb{E}[c(x,\xi)] \\ x \in X, \quad \sum_{i} x_{i} = d \end{cases} \quad \text{where } c(x,\xi) = \begin{cases} \min c^{\top}y \\ y \in X, \quad \sum_{i} y_{i} = \xi \\ y \text{ coincides with } x \text{ on } 1, \dots, \tau \end{cases}$$

- 2nd stage model: same as 1st stage but with smaller horizon
- fine operational modeling vs difficult to compute
- complexity of  $c(x,\xi)$  only allows for simple modeling of randomness

• New algo: double decomposition (by units and scenarios) using the same ingredients

### Numerical illustration for stochastic unit-commitment

- On a 2013 EDF instance (medium-size)
  - deterministic problem : 50k continuous variables, 27k binary variables, 815k constraints
  - stochastic version (50 scenarios) : 1,200k continuous var., 700k binary var., 20,000k constraints
- Our method allows to solve it  $\bigcirc$  (in reasonable time)
- Observation: generation transferred from cheap/inflexible to expensive/flexible
- Example: production schedules for 2 units: determinist vs stochastic



### **Robust unit-commitment**

A simple robust approach (VanAckooij Lebbe Malick '15)

- get rid of bound constraint
- penalize instead the worst gap



$$\begin{cases} \min c^{\top} x + \max_{\xi \in \Xi} \sum_{t=1}^{T} \psi \left( \sum_{i} x_{i}^{t} - \xi^{t} \right) \\ x \in X \end{cases}$$

Complex model of uncertainty set  $\Xi$  (vs  $\Xi$  finite or  $\Xi = [d_{\min}, d_{\max}]^T$ )



The model of Minoux 2012

- is finite but of high cardinality
- expresses temporal dependencies
- preserves a fast computability

### WDRO objective to be minimized

Dual WDRO is nonsmooth (which complicates resolution [Kuhn et al. '18])

$$R_{\rho}(f) = \min_{\lambda \ge 0} \lambda \rho + \mathbb{E}_{\mathbb{P}}[\max_{\xi'} \{f(\xi') - \lambda \|\xi - \xi'\|^2\}]$$

What about smoothing ? Smoothed counterpart

$$R^{\varepsilon}_{\rho}(f) = \min_{\lambda \geqslant 0} \ \lambda \rho + \varepsilon \operatorname{\mathbb{E}_{\mathbb{P}}} \log \left( \operatorname{\mathbb{E}_{\xi' \sim \pi_0(\cdot \mid \xi)} e^{\frac{f(\xi') - \lambda \|\xi - \xi'\|^2}{\varepsilon}} \right)$$

(Nice interpretation as entropy-regularized WDRO)

### Theorem (approximation bounds for WDRO [Azizian, lutzeler, M. '21])

Under mild assumptions (non-degeneracy, lipschitz), if the support of  $\mathbb{P}$  is contained in a compact convex set  $\Xi \subset \mathbb{R}^d$ , then

$$0 \leqslant R_{
ho}(f) - R_{
ho}^{arepsilon}(f) \leqslant \left(C \varepsilon \log rac{1}{arepsilon}
ight) d$$

### Entropic regularization: OT vs. WDRO

KL (Kullback-Leiber) divergence: 
$$KL(\mu|\nu) = \begin{cases} \int \log \frac{d\mu}{d\nu} d\mu & \mu \ll \nu \\ +\infty & \text{otherwise} \end{cases}$$

OT: Sinkhorn distance, very popular from [Cuturi '13]

in **OT**, take  $\pi_0 = \mathbb{P} \otimes \mathbb{Q}$  $[\pi]_1 = \mathbb{P}, [\pi]_2 = \mathbb{Q} \Rightarrow \pi \ll \pi_0$ 

 $\min_{\boldsymbol{\pi}} \left\{ \mathbb{E}_{\boldsymbol{\pi}}[\|\boldsymbol{\xi} - \boldsymbol{\xi}'\|^2] + \varepsilon \operatorname{\mathsf{KL}}(\boldsymbol{\pi}|\boldsymbol{\pi}_0) : \boldsymbol{\pi} \text{ with marginals } [\boldsymbol{\pi}]_1 = \mathbb{P} \text{ and } [\boldsymbol{\pi}]_2 = \mathbb{Q} \right\}$ 

WDRO: entropic regularization, seemingly new [Azizian, lutzeler, M. '21]

$$\begin{cases} \max_{\boldsymbol{\pi}} \quad \mathbb{E}_{[\boldsymbol{\pi}]_2}[f(\xi)] - \varepsilon \operatorname{\mathsf{KL}}(\boldsymbol{\pi}|\pi_0) \\ [\boldsymbol{\pi}]_1 = \mathbb{P} \\ \mathbb{E}_{\boldsymbol{\pi}}[\|\xi - \xi'\|^2] + \delta \operatorname{\mathsf{KL}}(\boldsymbol{\pi}|\pi_0) \leqslant \rho \end{cases}$$

Subtility:

vs but in WDRO, 
$$[\pi_0]_2$$
 not fixed !  
 $\pi_0(d\xi, d\xi') \propto \mathbb{P}(d\xi) \mathbb{I}_{\xi' \in \Xi} e^{-\frac{\|\xi - \xi'\|^2}{\sigma}} d\xi'$ 

# DRO/superquantile in action in federated learning

Only step 3 differs between Standard ERM approach and our DRO approach



DRO approach is fully compatible with secure aggregation and differential privacy [Pillutla, Laguel, M., Harchaoui '22]

### **Convergence** analysis

Analysis when  $F_i$  are smooth (and nonconvex)

Challenges: non-smoothness of  $R_{\theta}$ , biais due to local participation,...

**Theorem ([Pillutla, Laguel, M., Harchaoui '23])** Suppose F<sub>i</sub> are G-Lipschitz and with gradients L-Lipshitz

$$\mathbb{E} \|\nabla \Phi^{2L}_{\theta}(x_t)\|^2 \leqslant \sqrt{\frac{\Delta L G^2}{t}} + (1-\tau)^{1/3} \left(\frac{\Delta L G}{t}\right)^{2/3} + \frac{\Delta L}{t}$$

with t: nb comm. rounds,  $\tau$ : nb local updates, and  $\Delta$ : initial error

where  $\Phi^{\mu}_{\theta}(x) = \inf_{y} \left\{ \bar{R}_{\theta}(y) + \frac{\mu}{2} \|y - x\|^2 \right\}$  (Moreau  $\heartsuit$  enveloppe) [Davis Drus. '21]  $\bar{R}_{\theta}$  an approximation of  $R_{\theta}$  with unbiased gradient [Levy *et al* '21]

+ result of linear convergence when  $F_i$  are convex (add smoothing and regularization)

## Quantile by secure aggregation



## Existing statistical guarantees of WDRO

- Suppose  $\xi_1, \ldots, \xi_N \sim \mathbb{P}_{\text{train}}$  (where  $\xi \in \mathbb{R}^d$ )
- Computations with  $\widehat{\mathbb{P}}_{N} = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_{i}}$  and guarantees with  $\mathbb{P}_{\text{train}}$  ?
- We manipulate the WDRO risk :  $R_{\rho}(x) = \max_{W(\widehat{\mathbb{P}}_{N}, \mathbb{Q}) \leqslant \rho} \mathbb{E}_{\mathbb{Q}}[f(x, \xi)]$
- Obviously, if  $\rho, N$  large enough such that  $W(\mathbb{P}_{train}, \widehat{\mathbb{P}}_N) \leq \rho$ , then



- It requires  $ho \propto 1/\sqrt[d]{N}$  [Fournier and Guillin '15] (issue)
- Not optimal:  $ho \propto 1/\sqrt{N}$  suffices
  - asymptotically [Blanchet et al '22]
  - in particular cases [Shafieez-Adehabadeh et al '19]
  - or with error terms [Gao '22]

### Extended exact generalization guarantees of WDRO

Our approach: a direct "optim." approach (work to get a concentration on the dual function)

### Theorem ([Azizian, lutzeler, M. '23], [Le, M. '24])

Assumptions: parametric family  $f(\theta, \cdot)$  + compactness on  $\theta$  + compactness on  $\xi$  + non-degeneracy

For 
$$\delta \in (0,1)$$
, if  $\rho \geqslant O\left(\sqrt{\frac{\log 1/\delta}{N}}\right) = \rho_n$  then w.p.  $1 - \delta$ ,

Generalization guarantee:  $R_{
ho}(x) \geqslant \mathbb{E}_{\mathbb{P}_{train}}[f(x,\xi)]$ 

Distribution shifts:

$$W(\mathbb{P},\mathbb{Q})^2 \leqslant 
ho(
ho-
ho_n)$$
 it holds  $R_
ho(x) \geqslant \mathbb{E}_\mathbb{Q}\left[f(x,\xi)\right]$ 

Asymptotic tightness:

$$W(\mathbb{P},\mathbb{Q})^2 \leqslant 
ho(
ho+
ho_n)$$
 it holds  $R_
ho(x) \leqslant \max_{\mathbb{Q}} \mathbb{E}_{\mathbb{Q}}\left[f(x,\xi)\right]$ 

- Universal result: deep learning, kernels, family of invertible mappings (e.g. normalizing flows)
- Retrieve existing results in linear/logistic regressions [Shafieez-Adehabadeh et al '19]