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

# Plaidoyer pour l'optimisation non-lisse 

illustré par l'aide à la décision robuste

## Jérôme MALICK



Journées des Lauréats SMI 2023


ACADÉMIE

## 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)
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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

H. Attouch


## 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 $\quad F(x)=f(x)+g(x)$

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


## Nonsmooth composition $\quad F(x)=g \circ c(x)$

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

Probability functions

$$
F(x)=\mathbb{P}(h(x, \xi) \leqslant 0)
$$

- 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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My point: nonsmoothness is relevant !

## Example: $\ell_{1}$-regularized least-squares $(1 / 2)$

$$
\begin{equation*}
\min _{x \in \mathbb{R}^{d}} \frac{1}{2}\|A x-y\|^{2}+\lambda\|x\|_{1} \tag{LASSO}
\end{equation*}
$$

Illustration (on an instance with $d=2$ )


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## Example: $\ell_{1}$-regularized least-squares (2/2)

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

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\end{equation*}
$$



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

$$
\text { nuclear 63\% renewables } 14 \% \quad \text { oil/gaz/coal } 12 \%
$$


hydro $17 \%$


Question: finding "optimal" daily production schedules
Day-to-day optimization of production ("unit-commitment" )

$$
\binom{\text { simplified }}{\text { model }}\left\{\begin{array}{c}
\min \sum_{i} c_{i}^{\top} x_{i} \quad \text { (production costs) } \\
\sum_{i} x_{i}=d \quad \text { (demand constraints) } \\
\left(x_{1}, \ldots, x_{N}\right) \in X_{1} \times \cdots \times X_{N} \quad \text { (operational constraints) }
\end{array}\right.
$$

Hard optimization problem: large-scale, heterogeneous, complex ( $\geqslant 10^{6}$ variables, $\geqslant 10^{6}$ constraints)
Out of reach for (mixed-integer linear) solvers... But where is the nonsmoothness ?

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## Lagrangian decomposition

- Dual function (concave)

$$
\theta(u)=\left\{\begin{array}{c}
\min \sum_{i=1}^{N} c_{i}^{\top} x_{i}+\sum_{t=1}^{T} u^{t}\left(d^{t}-\sum_{i=1}^{N} x_{i}^{t}\right) \\
\left(x_{1}, \ldots, x_{N}\right) \in X_{1} \times \cdots \times x_{N}
\end{array}\right.
$$

- Dualizing the coupling constraint makes it decomposable by units
Nonsmooth optimization algorithm

$$
\begin{aligned}
\theta(u) & =d^{\top} u+\sum_{i=1}^{N} \theta_{i}(u) \\
\theta_{i}(u) & =\left\{\begin{array}{c}
\min \left(c_{i}-u\right)^{\top} x_{i} \\
x_{i} \in X_{i}
\end{array}\right.
\end{aligned}
$$

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

- Research in the 1990's
- In action in early 2000's
- Save money and CO2 !
S. Charousset
A. Renaud


## 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 $\odot$




## 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"

## Example 2.1: Don't forget how fragile deep learning can be!

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


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


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## Example 2.2: ML may perform poorly for some people

Example: Global model is trained on average distribution


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Example: Global model is deployed on individual clients


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Example: Global model is deployed on individual clients


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

Fairness issues, e.g.


Machine Bias


The Wastiugton just
THE ACCENT GAP

## Example 2.2: ML may perform poorly for some people

Example: Global model is deployed on individual clients


## Optimization set-up

- Training data: $\xi_{1}, \ldots, \xi_{N}$
e.g. in supervised learning: labeled data $\xi_{i}=\left(a_{i}, y_{i}\right)$ feature, label
- Train model: $f(x, \cdot)$ the loss function with $x$ the parameter/decision $(\omega, \beta, \theta, \ldots)$ e.g. least-square regression: $f(x,(a, y))=\left(x^{\top} a-y\right)^{2}$
- Compute $x$ via empirical risk minimization (a.k.a SAA)

$$
\min _{x} \frac{1}{N} \sum_{i=1}^{N} f\left(x, \xi_{i}\right)=\mathbb{E}_{\widehat{\mathbb{P}}_{N}}[f(x, \xi)] \quad \text { with } \widehat{\mathbb{P}}_{N}=\frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_{i}}
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$$

- 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 $\odot$


## (Wasserstein) Distributionally Robust Optimization

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

solve instead
$\min _{x} \max _{\mathbb{Q} \in \mathcal{U}} \mathbb{E}_{\mathbb{Q}}[f(x, \xi)]$
with $\mathcal{U}$ a neighborhood of $\widehat{\mathbb{P}}_{N}$
Wasserstein balls as ambiguity sets

$$
\begin{aligned}
& \mathcal{U}=\left\{\mathbb{Q}: W\left(\widehat{\mathbb{P}}_{N}, \mathbb{Q}\right) \leqslant \rho\right\} \\
& W\left(\widehat{\mathbb{P}}_{N}, \mathbb{Q}\right)=\min _{\pi}\left\{\mathbb{E}_{\boldsymbol{\pi}}\left[c\left(\xi, \xi^{\prime}\right)\right]:[\pi]_{1}=\widehat{\mathbb{P}}_{N},[\pi]_{2}=\mathbb{Q}\right\}
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WDRO objective function for given $x, \widehat{\mathbb{P}}_{N}, \rho$

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\left\{\begin{array} { c } 
{ \operatorname { m a x } _ { \mathbb { Q } } \mathbb { E } _ { \mathbb { Q } } [ f ( x , \xi ) ] } \\
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\end{array}\right.\right. \\
& \Leftrightarrow \min _{\lambda \geqslant 0} \lambda \rho+\mathbb{E}_{\mathbb{\mathbb { P }}_{N}}\left[\max _{\xi^{\prime}}\left\{f\left(x, \xi^{\prime}\right)-\lambda c\left(\xi, \xi^{\prime}\right)\right\}\right]
\end{aligned}
$$

...(finite dimension) nonsmooth... computable in some (specific) cases [Kuhn et al. '18]

## 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 skWDRO [Vincent, Azizian, lutzeler, Malick '24]


Try it out!
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...


## Conclusion

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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
"There is no clear cut between functions that are smooth and functions that are not. In-between there is a rather fuzzy boundary of stiff functions"

Jean-Baptiste Hiriart-Urruty Claude Lemaréchal

Convex Analysis and Minimization Algorithms II

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) $\gg$ smooth methods (gradient, conj. grad., q-Newton)
- 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 $\tau$, we have the observed load $\xi_{1}, \ldots, \xi_{\tau}$ and the current best forecast $\xi_{\tau+1}, \ldots, \xi_{T}$

W. van Ackooij
- We propose a stochastic 2-stage problem:

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

- 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, 27 k binary variables, 815 k constraints
- stochastic version (50 scenarios) : 1,200k continuous var., 700k binary var., 20,000k constraints
- Our method allows to solve it $\odot$ (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


$$
\left\{\begin{array}{l}
\min _{x \in X} c^{\top} x+\max _{\xi \in \equiv} \sum_{t=1}^{T} \psi\left(\sum_{i} x_{i}^{t}-\xi^{t}\right) \\
x,
\end{array}\right.
$$

Complex model of uncertainty set $\equiv$ (vs $\equiv$ finite or $\left.\equiv=\left[d_{\text {min }}, d_{\text {max }}\right]^{T}\right)$


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])

$$
R_{\rho}(f)=\min _{\lambda \geqslant 0} \lambda \rho+\mathbb{E}_{\mathbb{P}}\left[\max _{\xi^{\prime}}\left\{f\left(\xi^{\prime}\right)-\lambda\left\|\xi-\xi^{\prime}\right\|^{2}\right\}\right]
$$

What about smoothing ? Smoothed counterpart

$$
R_{\rho}^{\varepsilon}(f)=\min _{\lambda \geqslant 0} \lambda \rho+\varepsilon \mathbb{E}_{\mathbb{P}} \log \left(\mathbb{E}_{\xi^{\prime} \sim \pi_{0}(\cdot \mid \xi)} e^{f\left(\xi^{\prime}\right)-\lambda\left\|\xi-\xi^{\prime}\right\|^{2}}\right)
$$

(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 $\equiv \subset \mathbb{R}^{d}$, then

$$
0 \leqslant R_{\rho}(f)-R_{\rho}^{\varepsilon}(f) \leqslant\left(C \varepsilon \log \frac{1}{\varepsilon}\right) d
$$

## Entropic regularization: OT vs. WDRO

KL (Kullback-Leiber) divergence: $\mathrm{KL}(\mu \mid \nu)= \begin{cases}\int \log \frac{\mathrm{d} \mu}{\mathrm{d} \nu} \mathrm{d} \mu & \mu \ll \nu \\ +\infty & \text { otherwise }\end{cases}$
OT: Sinkhorn distance, very popular from [Cuturi '13]

$$
\min _{\pi}\left\{\mathbb{E}_{\pi}\left[\left\|\xi-\xi^{\prime}\right\|^{2}\right]+\varepsilon \operatorname{KL}\left(\pi \mid \pi_{0}\right): \pi \text { with marginals }[\pi]_{1}=\mathbb{P} \text { and }[\pi]_{2}=\mathbb{Q}\right\}
$$

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

$$
\left\{\begin{array}{c}
\max _{\boldsymbol{\pi}} \quad \mathbb{E}_{[\pi]_{2}}[f(\xi)]-\varepsilon \operatorname{KL}\left(\pi \mid \pi_{0}\right) \\
{[\pi]_{1}=\mathbb{P}} \\
\mathbb{E}_{\boldsymbol{\pi}}\left[\left\|\xi-\xi^{\prime}\right\|^{2}\right]+\delta \operatorname{KL}\left(\pi \mid \pi_{0}\right) \leqslant \rho
\end{array}\right.
$$

Subtility:
in OT, take $\pi_{0}=\mathbb{P} \otimes \mathbb{Q}$

$$
[\pi]_{1}=\mathbb{P},[\pi]_{2}=\mathbb{Q} \Rightarrow \boldsymbol{\pi} \ll \pi_{0}
$$

but in WDRO, $\left[\pi_{0}\right]_{2}$ not fixed !
vs $\pi_{0}\left(\mathrm{~d} \xi, \mathrm{~d} \xi^{\prime}\right) \propto \mathbb{P}(\mathrm{d} \xi) \mathbb{I}_{\xi^{\prime} \in \equiv} e^{-\frac{\left\|\xi-\xi^{\prime}\right\|^{2}}{\sigma}} \mathrm{~d} \xi^{\prime}$

## DRO/superquantile in action in federated learning

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

Step 3 of 3: Aggregate updates contributed by all clients

Step 3 of 3: Aggregate updates contributed by tail clients only




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 $F_{i}$ are G-Lipschitz and with gradients L-Lipshitz

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

with $t$ : nb comm. rounds, $\tau$ : nb local updates, and $\Delta$ : initial error
where $\Phi_{\theta}^{\mu}(x)=\inf _{y}\left\{\bar{R}_{\theta}(y)+\frac{\mu}{2}\|y-x\|^{2}\right\} \quad$ (Moreau@ 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 $\xi_{1}, \ldots, \xi_{N} \sim \mathbb{P}_{\text {train }} \quad$ (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 : $\quad R_{\rho}(x)=\max _{W\left(\mathbb{P}_{N}, Q\right) \leqslant \rho} \mathbb{E}_{\mathbb{Q}}[f(x, \xi)]$
- Obviously, if $\rho, N$ large enough such that $W\left(\mathbb{P}_{\text {train }}, \widehat{\mathbb{P}}_{N}\right) \leqslant \rho$, then

- It requires $\rho \propto 1 / \sqrt[s]{N}$ [Fournier and Guillin '15] (issue)
- Not optimal: $\rho \propto 1 / \sqrt{N}$ 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 $\delta \in(0,1), \quad$ if $\rho \geqslant O\left(\sqrt{\frac{\log 1 / \delta}{N}}\right)=\rho_{n}$ then w.p. $1-\delta$,

Generalization guarantee: $\quad R_{\rho}(x) \geqslant \mathbb{E}_{\mathbb{P}_{\text {train }}}[f(x, \xi)]$
Distribution shifts:

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

Asymptotic tightness:

$$
W(\mathbb{P}, \mathbb{Q})^{2} \leqslant \rho\left(\rho+\rho_{n}\right) \quad \text { it holds } \quad R_{\rho}(x) \leqslant \max _{\mathbb{Q}} \mathbb{E}_{\mathbb{Q}}[f(x, \xi)]
$$

- 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]

