The Era of "Non"-Optimization Problems

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presented at

OneWorld Optimization Seminar Series

3:30–4:30 PM CEST Monday September 14 2020

Based on joint work with Dr. Ying Cui at the University of Minnesota and many collaborators.

Contents of presentation

- Some general thoughts of the state of the field

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- A readiness test (a light-hearted humor)

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- A gentle touch of mathematics
- **The monograph**

Some General Thoughts

addressing the negative impact of the field of machine learning

on the optimization field,

and raising an alarm

- **Convexity and/or differentiability** have been the safe haven for optimization and its applications for decades, particularly popular in the machine learning in recent years

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to the extent that

• modellers are routinely sacrificing realism for convenience,

• algorithm designers will do whatever to stay in this comfort zone, even at the expense of potentially wrong approach,

• practitioners are content with the resulting models, algorithms, and "solutions",

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to the extent that

• modellers are routinely sacrificing realism for convenience,

• algorithm designers will do whatever to stay in this comfort zone, even at the expense of potentially wrong approach,

• practitioners are content with the resulting models, algorithms, and "solutions",

resulting in

• tools being abused,

• advances in science being stalled, and

• future being built on soft ground.

This talk

Benefits, yes or No?

Ready for the “non”-era, yes or no?

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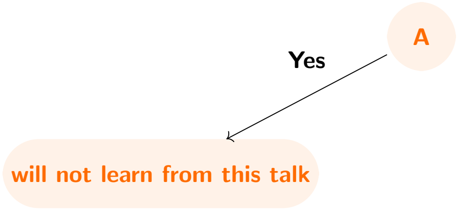
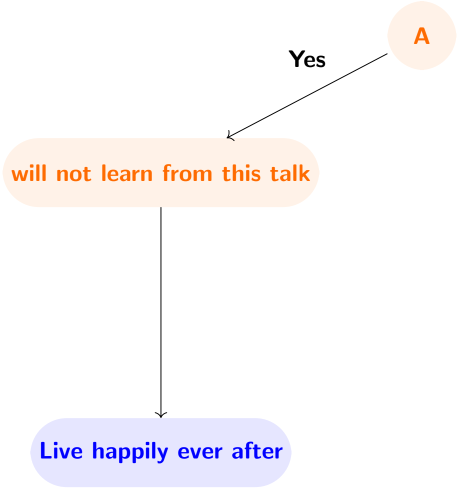
Ready for the “non”-era, yes or no?

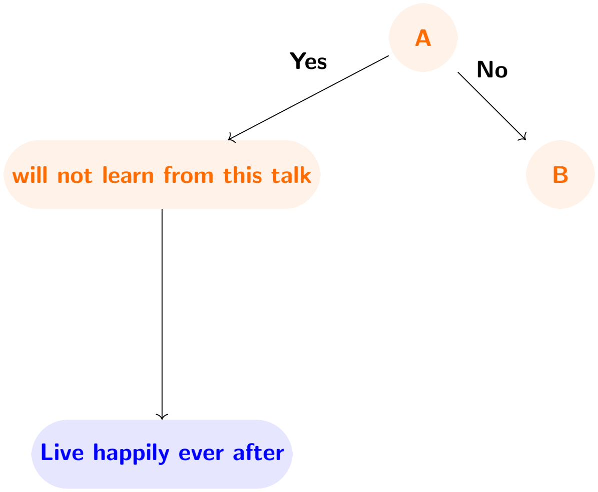
A little humor before the storm

A

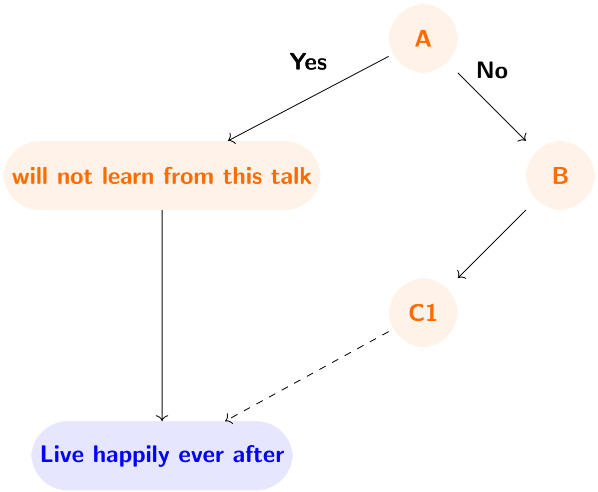
A: Are you satisfied with the comfort zone of convexity and differentiability?


A
Yes
will not learn from this talk

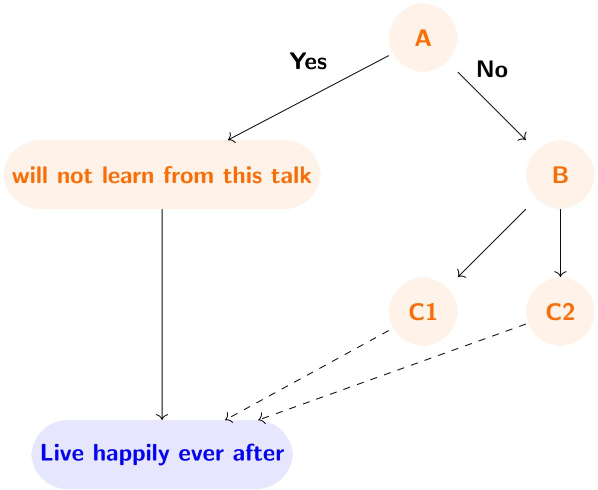

A
Yes
will not learn from this talk
Live happily ever after



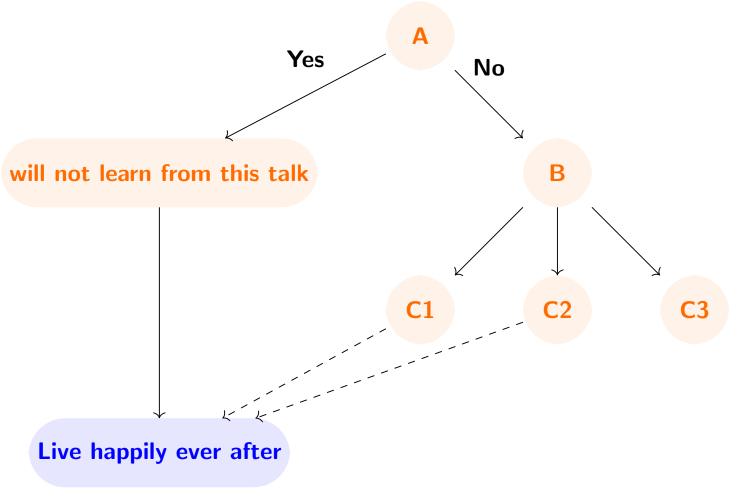
B: How to deal with non-convexity/non-smoothness?



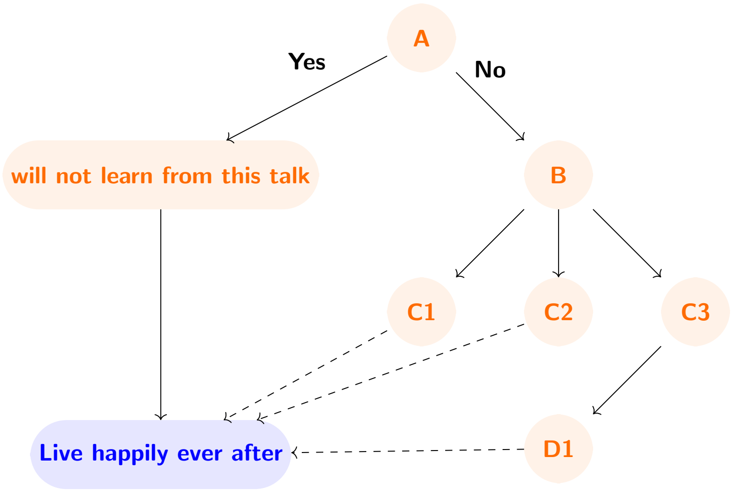
C1: Ignore these properties or give them minimal or even wrong treatment



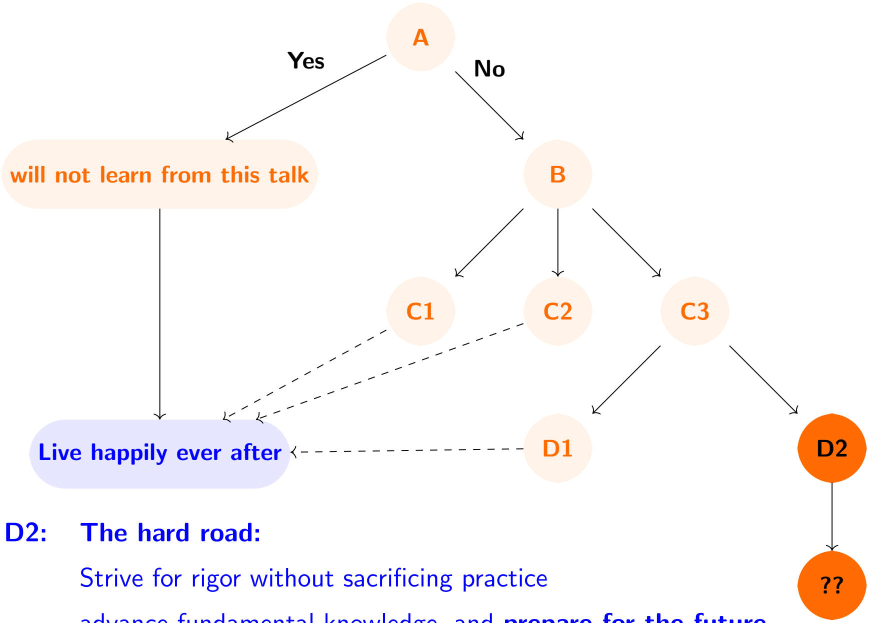
C2: Focus on stylized problems (and there are many interesting ones) and stop at them



C3: Faithfully treat these **non-properties**



D1: Employ heuristics, and potentially, leading to heuristics on heuristics when complex models are being formulated

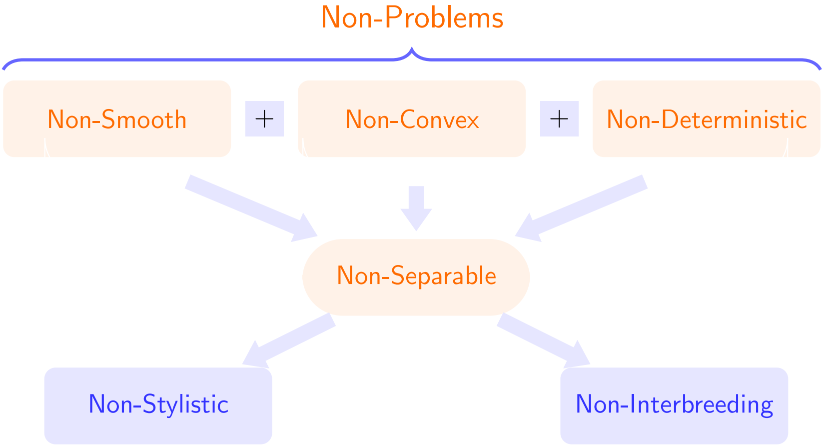


D2: The hard road:

Strive for rigor without sacrificing practice

advance fundamental knowledge, and **prepare for the future**

Features



and many more non-topics $\cdots$

Examples of Non-Problems

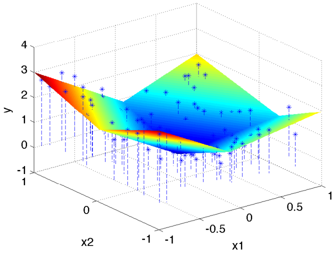
I. Structured Learning

Piecewise Affine Regression

extending classical affine regression

$$\underset{a,\alpha,b,\beta}{\textbf{minimize}} \; \frac{1}{N}\sum_{s=1}^{N}\left(y_s - \left[\underbrace{\max_{1\le i\le k_1}\left\{ (a^i)^\top x^s + \alpha_i \right\} - \max_{1\le i\le k_2}\left\{ (b^i)^\top x^s + \beta_i \right\}}_{\text{capturing all piecewise affine functions}} \right] \right)^2$$

illustrating coupled non-convexity and non-differentiability.



Estimate Change Points/Hyperplanes
in Linear Regression

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• It has finitely many stationary values.

• A directional stationary solution can be computed by an iterative convex-programming based algorithm.

• Leads to several classes of nonconvex nonsmooth functions; most general is a difference-of-convex function composed with a difference-of-convex function, an example of which is

$$\varphi_1\left(\max_{1\leq i\leq k_{11}}\psi^1_{1i}(x)-\max_{1\leq i\leq k_{12}}\psi^1_{2i}(x)\right)-\varphi_2\left(\max_{1\leq i\leq k_{21}}\psi^2_{1i}(x)-\max_{1\leq i\leq k_2}\psi^2_{2i}(x)\right)$$

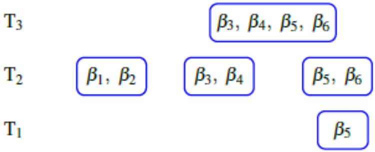
where all functions are convex.

Logical Sparsity Learning

$$\begin{aligned} \underset{\beta \in \mathbb{R}^d}{\textbf{minimize}} \quad & f(\beta) \\ \text{subject to} \quad & \sum_{j=1}^{d} a_{ij} \, | \, \beta_j \, |_0 \, \leq \, b_i, \quad i \, = \, 1, \cdots, m, \end{aligned}$$

where $| \, t \, |_0 \triangleq \begin{cases} 1 & \text{if } t \neq 0 \\ 0 & \text{otherwise.} \end{cases}$

- strong/weak hierarchy: e.g. $| \, \beta_j \, |_0 \leq | \, \beta_k \, |_0$
- cost-based variable selection: coefficients ≥ 0 but not all equal
- hierarchical/group variable selection



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• Soft formulation of ASCs is possible, leading to an objective of the kind:

$$\underset{\beta \in \mathbb{R}^d}{\textbf{minimize}}\; f(\beta) + \gamma \sum_{i=1}^{m} \left[b_i - \sum_{j=1}^{d} a_{ij} \,|\, \beta_j \,|_0 \right]_+, \quad \text{for a given } \gamma > 0.$$

• When the matrix A has negative entries, the resulting ASC set may not closed; its optimization formulation may not have a lower semi-continuous objective.

• When $|\bullet|_0$ is approximated by a folded concave function, obtain some nondifferentiable, difference-of-convex constraints.

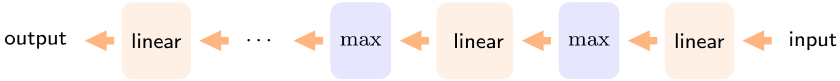
Deep Neural Network with Feed-Forward Structure

leading to multi-composite, nonconvex, nonsmooth optimization problems

$$\underset{\theta=\left\{\left(W^\ell,w^\ell\right)_{\ell=1}^L\right\}}{\textbf{minimize}} \quad \frac{1}{S}\sum_{s=1}^{S}\left[\, y_s - f_\theta(x^s)\,\right]^2$$

where f_θ is the L-fold composite function with the non-smooth max ReLU activation:

$$f_\theta(x) = \underbrace{\left(W^L \bullet + w^L\right)}_{\text{Output Layer}} \circ \cdots \circ \underbrace{\max\left(0, W^2 \bullet + w^2\right)}_{\text{Second Layer}} \circ \underbrace{\max\left(0, W^1 x + w^1\right)}_{\text{Input Layer}}$$



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$$\boxed{\underset{z \in \mathcal{Z};\, u}{\textbf{minimize}}\ \zeta_\rho(z;u) \triangleq \frac{1}{S}\sum_{s=1}^{S}\left[\varphi_s(u^{s;L}) + \rho\,\underbrace{\sum_{\ell=1}^{L}\sum_{j=1}^{N_\ell}\left|\,u_j^{s;\ell} - \psi_j^\ell(z^\ell, u^{s;\ell-1})\,\right|}_{\text{penalizing the components}}\right]}$$

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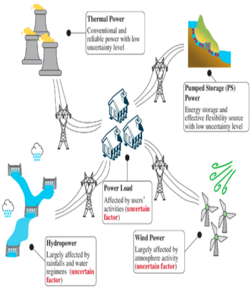
• Framework allows the treatment of data perturbation.

• Leads to an advanced study of exact penalization and error bounds of nondifferentiable optimization problems.

Examples of Non-Problems

II. Smart Planning

Power Systems Planning



ω_1: uncertain renewable energy generation
ω_2: uncertain demand of electricity

x: production from traditional thermal plants

y: production from backup fast-ramping generators

$$\underset{x \in X}{\textbf{minimize}} \quad \varphi(x) + \mathbb{E}_{\omega_1, \omega_2}\left[\psi(x, \omega_1, \omega_2)\right]$$

where the recourse function is

$$\psi(x, \omega_1, \omega_2) \triangleq \underset{y}{\textbf{minimum}}\, y^\top c\left([\omega_2 - x - \omega_1]_+\right)$$
$$\textbf{subject to} \quad A(\omega)x + Dy \geq \xi(\omega)$$

Unit cost of fast-ramping generators depends on

- observed renewable production & demand of electricity
- shortfall due to the first-stage thermal power decisions

Comments

• Leads to the study of the class of two-stage linearly bi-parameterized stochastic program with quadratic recourse:

$$\operatorname*{\mathbf{minimize}}_{x} \quad \zeta(x) \triangleq \varphi(x) + \mathbf{E}_{\tilde{\xi}}\left[\psi(x,\tilde{\xi})\right] \quad \textbf{subject to} \quad x \in X \subseteq \mathbb{R}^{n_1},$$

where the recourse function $\psi(x,\xi)$ is the optimal objective value of the quadratic program (QP): with Q being symmetric positive semidefinite:

$$\begin{array}{rll}\psi(x,\xi) \triangleq & \operatorname*{minimum}_{y} & \left[\, f(\xi) + G(\xi)x \,\right]^\top y + \frac{1}{2}\, y^\top Q y \\ & \text{subject to} & y \in Y(x,\xi) \triangleq \left\{ y \in \mathbb{R}^{n_2} \mid A(\xi)x + Dy \geq b(\xi) \right\}.\end{array}$$

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• The recourse function $\psi(\bullet,\xi)$ is of the implicit convex-concave kind.

• Developed a Regularization, Convexification, sampling combined method for computing a *generalized critical point* with almost sure convergence guarantee.

(Simplified) Defender-Attacker Game with Costs

Underlying problem is: $\boxed{\textbf{minimize } c^\top x \text{ subject to } Ax = b \text{ and } x \geq 0}$

Defender's problem: Anticipating the attacker's disruption $\delta \in \Delta$, the defender undertakes the operation by solving the problem:

$$\underset{x \geq 0}{\textbf{minimize}} \quad (c + \delta c)^\top x + \underbrace{\rho \left\| \left[(A + \delta A)x - b - \delta b \right]_+ \right\|_\infty}_{\text{constraint residual}}$$

Attacker's problem: Anticipating the defender's activity x, the attacker aims to disrupt the defender's operations by solving the problem:

$$\underset{\delta \in \Delta}{\textbf{maximum}} \quad \underbrace{\lambda_1 (c + \delta c)^\top x}_{\text{disrupt objective}} + \underbrace{\lambda_2 \left\| \left[(A + \delta A)x - b - \delta b \right]_+ \right\|_\infty}_{\text{disrupt constraints}} - \underbrace{C(\delta)}_{\text{cost}}.$$

- Many variations are possible.
- Offer alternative approaches to the convexity-based robust formulations.
- **Adversarial Programming**

Robustification of nonconvex problems

A general nonlinear program:

$$\begin{array}{ll} \underset{x \in S}{\textbf{minimize}} & \theta(x) + f(x) \\ \textbf{subject to} & H(x) = 0, \quad \text{where} \end{array}$$

• S is a closed convex set in $\mathbb{R}^n$ not subject to alterations,
• θ and f are real-valued functions defined on an open convex set $\mathcal{O}$ in $\mathbb{R}^n$ containing S,
• $H : \mathcal{O} \to \mathbb{R}^m$ is a vector-valued (nonsmooth) function that can be used to model both inequality constraints $g(x) \leq 0$ and equality constraints $h(x) = 0$.

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Robust counterpart: with separate perturbations

$$\left.\begin{array}{ll} \underset{x \in S}{\textbf{minimize}} & \theta(x) + \underset{\widehat{\delta} \in \widehat{\Delta}}{\textbf{maximum}}\, f(x, \widehat{\delta}) \\ \textbf{subject to} & \underbrace{H(x, \widetilde{\delta}) = 0, \quad \forall\, \widetilde{\delta} \in \widetilde{\Delta}}_{\text{easily infeasible}} \end{array}\right\} \quad \begin{array}{l} \text{in current way} \\ \text{of modeling} \end{array}$$

New formulation

via a pessimistic value-function minimization: given $\gamma > 0$,

$$\boxed{\underset{x \in S}{\textbf{minimize}} \quad \theta(x) + v_\gamma(x)}$$

where $v_\gamma(x)$ models constraint violation with cost of model attacks:

$$v_\gamma(x) \quad \triangleq \quad \textbf{maximum} \text{ over } \boldsymbol{\delta} \in \boldsymbol{\Delta} \text{ of}$$

$$\phi_\gamma(x, \boldsymbol{\delta}) \quad \triangleq \quad f(x, \boldsymbol{\delta}) + \gamma \left[\underbrace{\| H(x, \boldsymbol{\delta}) \|_\infty}_{\text{constraint residual}} - \underbrace{C(\boldsymbol{\delta})}_{\text{attack cost}} \right]$$

with the novel features:

- combined perturbation $\boldsymbol{\delta}$ in joint uncertainty set $\boldsymbol{\Delta} \subseteq \mathbb{R}^L$;
- robustify constraint satisfaction via penalization

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- Showed that the value function admits an explicit form under piecewise structures of $f(\bullet, \boldsymbol{\delta})$ and $H(\bullet, \boldsymbol{\delta})$, a linear structure of $C(\boldsymbol{\delta})$ with a set-up component, and special simplex-type uncertainty set $\boldsymbol{\Delta}$.

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• Introduced a Majorization-Minimization (MM) algorithm for solving a unified formulation:

$$\underset{x \in S}{\textbf{minimize}}\ \varphi(x) \triangleq \theta(x) + v(x) \quad \text{with}$$

$$v(x) \triangleq \max_{1 \leq j \leq J} \underset{\boldsymbol{\delta} \in \boldsymbol{\Delta} \cap \mathbb{R}^L_+}{\textbf{maximum}} \left[g_j(x, \boldsymbol{\delta}) - h^j(x)^\top \boldsymbol{\delta} \right],$$

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• Implemented algorithm and reported computation results to demonstrate the viability of the robust paradigm in the "non"-framework.

Examples of Non-Problems

III. Operations Research meets Statistics

Composite CVaR and bPOE minimization

for risk-based statistical estimation to control left and right-tail distributions simultaneously

Interval Conditional Value-at-Risk of a random variable Z, at levels $0 \leq \alpha < \beta \leq 1$, treating two-sided estimation errors,

$$\begin{aligned}\text{In-CVaR}_\alpha^\beta(Z) &\triangleq \frac{1}{\beta - \alpha} \int_{\mathrm{VaR}_\beta(Z) > z \geq \mathrm{VaR}_\alpha(Z)} z \, dF_Z(z) \\ &= \frac{1}{\beta - \alpha} \left[(1-\alpha)\mathrm{CVaR}_\alpha(Z) - (1-\beta)\mathrm{CVaR}_\beta(Z) \right]\end{aligned}$$

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Buffered probability of exceedance/deceedance at level $\tau > 0$

$$\text{bPOE}(Z;\tau) \triangleq 1 - \min \left\{ \alpha \in [0,1] \,:\, \text{CVaR}_{\alpha}(Z) \geq \tau \right\}$$

$$\text{bPOD}(Z;u) \triangleq \min \left\{ \beta \in [0,1] \,:\, \text{In-CVaR}_{0}^{\beta}(Z) \geq u \right\}.$$

Buffered probability of interval $(\tau, u]$

We have the following bound for an interval probability:

$$\mathbb{P}(u \geq Z > \tau) \, \leq \, \mathsf{bPOE}(Z;\tau) + \mathsf{bPOD}(Z;u) - 1 \triangleq \mathsf{bPOI}_{\tau}^{u}(Z).$$

Two risk minimization problems of a composite random functional:

$$\underbrace{\underset{\theta\in\Theta}{\textbf{minimize}} \;\; \text{In-CVaR}_{\alpha}^{\beta}(\mathcal{Z}(\theta))}_{\substack{\text{a difference of two convex} \\ \text{SP value functions}}} \quad \text{and} \quad \underbrace{\underset{\theta\in\Theta}{\textbf{minimize}} \;\; \mathsf{bPOI}_{\tau}^{u}(\mathcal{Z}(\theta))}_{\substack{\text{a stochastic program with} \\ \text{a difference-of-convex objective}}},$$

where

$$\mathcal{Z}(\theta) \triangleq c \circ \left[\underbrace{g(\theta;Z) - h(\theta;Z)}_{g(\bullet;z) - h(\bullet;z) \text{ is difference of convex}} \right],$$

with $c : \mathbb{R} \to \mathbb{R}$ being a univariate piecewise affine function, Z is a m-dimensional random vector, and for each z, $g(\bullet;z)$ and $h(\bullet;z)$ are both convex functions.

Comments

- The In-CVaR minimization leads to the following stochastic program:

$$\textbf{minimize over } \theta \in \Theta \text{ of}$$

$$\underbrace{\underset{\eta_1 \in \Upsilon_1}{\textbf{minimum}} \, \mathbf{E}_{\widetilde{\omega}} \left[\, \varphi_1(\theta, \eta_1; \widetilde{\omega}) \, \right]}_{\text{denoted } v_1(\theta)} - \underbrace{\underset{\eta_2 \in \Upsilon_2}{\textbf{minimum}} \, \mathbf{E}_{\widetilde{\omega}} \left[\, \varphi_2(\theta, \eta_2; \widetilde{\omega}) \, \right]}_{\text{denoted } v_2(\theta)}$$

Both functions v_1 and v_2 are (convex) value functions of a univariate expectation minimization; thus overall objective is a difference-of-convex objective.

Comments

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Both functions v_1 and v_2 are (convex) value functions of a univariate expectation minimization; thus overall objective is a difference-of-convex objective.

- Developed a convex programming based sampling method for computing a critical point of the objective

Comments

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$$\boxed{\begin{array}{l} \textbf{minimize} \text{ over } \theta \in \Theta \text{ of} \\[1em] \underbrace{\underset{\eta_1 \in \Upsilon_1}{\textbf{minimum}} \, \mathbf{E}_{\widetilde{\omega}} \left[\varphi_1(\theta, \eta_1; \widetilde{\omega}) \right]}_{\text{denoted } v_1(\theta)} - \underbrace{\underset{\eta_2 \in \Upsilon_2}{\textbf{minimum}} \, \mathbf{E}_{\widetilde{\omega}} \left[\varphi_2(\theta, \eta_2; \widetilde{\omega}) \right]}_{\text{denoted } v_2(\theta)} \end{array}}$$

Both functions v_1 and v_2 are (convex) value functions of a univariate expectation minimization; thus overall objective is a difference-of-convex objective.

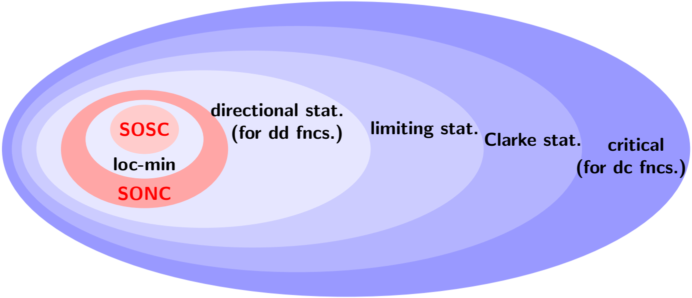
- Developed a convex programming based sampling method for computing a critical point of the objective

- Numerical results demonstrated superior performance in the handling of outliers in regression and classification problems.

A touch of mathematics

bridging computations with theory

First of All, What Can be Computed?



Relationship between the stationary points.

- Stationarity:
  - <u>smooth case:</u> $\nabla V(x) = 0$
  - <u>nonsmooth case:</u> $0 \in \partial V(x)$ [subdifferential: many calculus rules fail]

  e.g. $\partial V_1(x) + \partial V_2(x) \neq \partial(V_1 + V_2)(x)$
  unless one of them is continuously differentiable
- directional stationarity: $V'(x; d) \geq 0$ for all the directions d.

• The sharper the concept, the harder to compute.

Computational Tools

- **Built on a theory of surrogation, supplemented by exact penalization of stationary solutions**
- **A fusion of first-order and second-order algorithms**
  - Dealing with non-convexity: majorization-minimization algorithm
  - Dealing with non-smoothness: nonsmooth Newton algorithm
  - Dealing with pathological constraints: (exact) penalty method
- **An integration of sampling and deterministic methods**
  - Dealing with population optimization: in statistics
  - Dealing with stochastic programming: in operations research
  - Dealing with risk minimization: in financial management and tail control

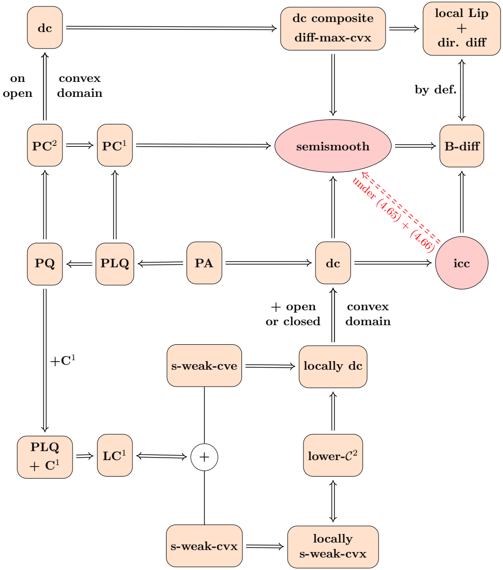
Classes of Nonsmooth Functions

Pervasive in applications

Progressively broader:

- Piecewise smooth*: e.g. piecewise linear-quadratic
- Difference-of convex: facilitates algorithmic design via convex majorization
- Semismooth: enables fast algorithms of the Newton-type
- Bouligand differentiable: locally Lipschitz + directionally differentiable
- Sub-analytic and semi-analytic

$*$ and many more.


dc
dc composite
diff-max-cvx
local Lip
+
dir. diff
on
open
convex
domain
by def.
PC^2
PC^1
semismooth
B-diff
under (4.65) + (4.66)
PQ
PLQ
PA
dc
icc
+ open
or closed
convex
domain
+C^1
s-weak-cve
locally dc
PLQ
+ C^1
LC^1
+
lower-$\mathcal{C}^2$
s-weak-cvx
locally
s-weak-cvx

Completed Monograph:

Modern Nonconvex Nondifferentiable Optimization

Ying Cui and Jong-Shi Pang

submitted to publisher (Friday September 11, 2020)

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