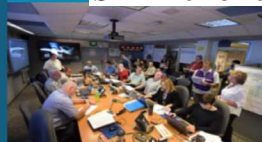


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Smoothing Techniques for Risk-Averse PDE-Constrained Optimization



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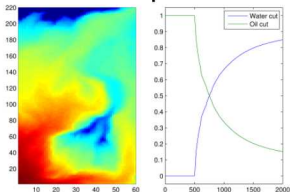
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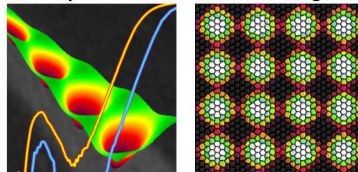
2 Motivating Applications



Reservoir Optimization



Superconductor Vortex Pinning



Courtesy Argonne National Laboratory

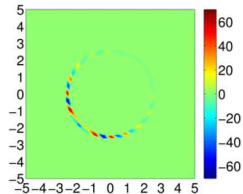
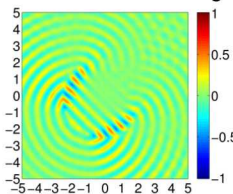
$$v = -\mathbf{K}\lambda(s)\nabla p, \quad \nabla \cdot v = q$$

$$\phi \partial_t s + \nabla \cdot (f(s)v) = \hat{q}$$

$$\gamma(\partial_t + i\mu)\psi = \epsilon\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi$$

$$\mathbf{J} = \text{Im}(\bar{\psi}(\nabla - i\mathbf{A})\psi) - (\partial_t\mathbf{A} + \nabla\mu), \quad \nabla \cdot \mathbf{J} = 0$$

Direct Field Acoustic Testing



$$-\Delta u - \kappa^2(1 + \sigma\epsilon)^2 u = z$$

3 Topology Optimization and Additive Manufacturing



Given $V_0 \in (0, 1)$ compute a density that solves:

$$\min_{0 \leq z \leq 1} \mathcal{R} \left(\int_D \mathbf{F} \cdot \mathbf{S}(z) dx + \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{S}(z) dx \right)$$

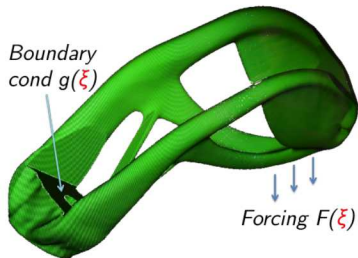
subject to $\int_D z(x) dx \leq V_0 |D|$, where $\mathbf{S}(z) = \mathbf{u}$ solves the **linear elasticity equations**

$$-\nabla \cdot (\mathbf{E}(z) : \epsilon \mathbf{u}) = \mathbf{F}, \quad \text{in } D, \text{ a.s.}$$

$$\epsilon \mathbf{u} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^\top), \quad \text{in } D, \text{ a.s.}$$

$$\epsilon \mathbf{u} \mathbf{n} = \mathbf{t}, \quad \text{on } \Gamma_t, \text{ a.s.}$$

$$\mathbf{u} = \mathbf{g}, \quad \text{on } \Gamma_d, \text{ a.s.}$$



- Uncertain external forces (loads) and boundary conditions.
- Uncertain internal forces, e.g., residual stresses due to AM.
- Uncertain material properties (porosity, etc.) due to AM.
- Compute light-weight designs that minimize the probability of structural failure.



Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a **probability space**, Z be a **reflexive Banach space**, and $\mathcal{X} := L^p(\Omega, \mathcal{F}, \mathbb{P})$ with $1 \leq p < \infty$. We consider the optimization problem

$$\min_{z \in Z_{\text{ad}}} \{ \mathcal{R}(F(z)) + \wp(z) \}$$

where $\mathcal{R} : \mathcal{X} \rightarrow (-\infty, \infty]$ is a **measure of risk**,

$F : Z \rightarrow \mathcal{X}$ is the **uncertain objective function**,

$\wp : Z \rightarrow \mathbb{R}$ is a **deterministic objective function**, and

$Z_{\text{ad}} \subseteq Z$ is a **closed, convex** set of **decision variables**.



What is risk? *Possibility of loss or injury* (Merriam Webster)

... In our optimization problem, $F(z)$ is a **risk**!

We **cannot** directly minimize $F(z) + \wp(z) \in \mathcal{X} := L^p(\Omega, \mathcal{F}, \mathbb{P})$

... How should we quantify our risk?

- ▶ **Traditional Stochastic Programming:** Minimize *on average*

$$\mathcal{R}(F(z)) = \mathbb{E}[F(z)].$$

- ▶ **Risk-Averse Stochastic Programming:** Model *risk preferences*

$$\mathcal{R}(F(z)) = \mathbb{E}[F(z)] + c\mathbb{E}[(F(z) - \mathbb{E}[F(z)])_+]^p]^{1/p}.$$

- ▶ **Probabilistic Optimization:** Minimize the *probability of loss*

$$\mathcal{R}(F(z)) = \mathbb{P}(F(z) > \tau).$$

- ▶ **Stochastic Orders:** Model risk preference with a *benchmark* Y

$$\mathbb{P}(F(z) \leq x) \leq \mathbb{P}(Y \leq x) \quad \forall x \in \mathbb{R}.$$



$\mathcal{R} : \mathcal{X} \rightarrow (-\infty, \infty]$ is a **coherent** measure of risk if it satisfies

- (R1) **Subadditivity:** $\mathcal{R}(X + X') \leq \mathcal{R}(X) + \mathcal{R}(X')$
- (R2) **Monotonicity:** $X \geq X'$ a.s. $\implies \mathcal{R}(X) \geq \mathcal{R}(X')$
- (R3) **Translation Equivariance:** $\mathcal{R}(X + t) = \mathcal{R}(X) + t, \quad \forall t \in \mathbb{R}$
- (R4) **Positive Homogeneity:** $\mathcal{R}(tX) = t\mathcal{R}(X), \quad \forall t > 0$

Note: $\{(R1) + (R4) \implies \text{convexity}\} \quad \text{and} \quad \{\text{convexity} + (R4) \implies (R1)\}$

Examples of **coherent** risk measures with $X \in \mathcal{X}$:

- ▶ Risk Neutral: $\mathcal{R}(X) = \mathbb{E}[X]$
- ▶ Mean Plus Semideviation: $\mathcal{R}(X) = \mathbb{E}[X] + c\mathbb{E}[(X - \mathbb{E}[X])_+^p]^{1/p}, \quad c \in (0, 1)$
- ▶ Conditional Value-at-Risk: $\mathcal{R}(X) = \inf \{t + (1 - \beta)^{-1}\mathbb{E}[(X - t)_+]\}, \quad \beta \in (0, 1)$

Ph. Artzner, F. Delbaen, J.-M. Eber and D. Heath, *Coherent measures of risk*. Math. Finance, 1999.

7 Coherent Measures of Risk

Some Good and *Not* So Good Properties?



Biconjugate Representation: Recall $\mathcal{R}^*(\vartheta) = \sup_X \{\mathbb{E}[\vartheta X] - \mathcal{R}(X)\}$

- If \mathcal{R} is proper, **convex** and lsc

$$\iff \mathcal{R}(X) = \sup \{ \mathbb{E}[\vartheta X] - \mathcal{R}^*(\vartheta) \mid \vartheta \in \text{dom}(\mathcal{R}^*) \}$$

- If \mathcal{R} is **translation equivariant** and **monotonic**

$$\iff \text{dom}(\mathcal{R}^*) \subseteq \{ \vartheta \in \mathcal{X}^* \mid \mathbb{E}[\vartheta] = 1, \vartheta \geq 0 \text{ a.s.} \}$$

- If \mathcal{R} is **positive homogeneous**

$$\iff \mathcal{R}(X) = \sup_{\vartheta \in \text{dom}(\mathcal{R}^*)} \mathbb{E}[\vartheta X]$$

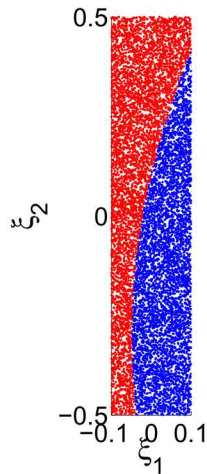
Optimal $\vartheta^* \in \text{dom}(\mathcal{R}^*)$ are called **risk identifiers**

Example (Conditional Value-at-Risk): $\mathcal{R} = \text{CVaR}_\beta$

$$\text{dom}(\mathcal{R}^*) = \left\{ \vartheta \in \mathcal{X}^* \mid \mathbb{E}[\vartheta] = 1, 0 \leq \vartheta \leq \frac{1}{1-\beta} \text{ a.s.} \right\}$$

Differentiability: If $\mathcal{R} : \mathcal{X} \rightarrow \mathbb{R}$ is **coherent**, then \mathcal{R} is **Fréchet differentiable**

$$\iff \exists \vartheta \in \mathcal{X}^* \text{ with } \vartheta \geq 0 \text{ a.s., } \mathbb{E}[\vartheta] = 1, \text{ and } \mathcal{R}(X) = \mathbb{E}[\vartheta X] \text{ for all } X \in \mathcal{X}$$



8 Is Nondifferentiability *Really* an Issue?

Example: Optimal control of Burger's equation using CVaR

- Problem size is **small**: 1D spatial domain, 4D stochastic domain
- PDE is nonlinear \implies Objective function is not convex
- CVaR risk measure quantifies *tail weight* and is **not** differentiable

Application of a *nonconvex nonsmooth* optimization algorithm:

β	0.1	0.5	0.9
# iter	9,740	10,035	10,128

Required $\mathcal{O}(10^8)$ nonlinear and $\mathcal{O}(10^8)$ linearized PDE solves!

Application of smoothed \mathcal{R} with globalized Newton's method:

Required $\mathcal{O}(10^6)$ nonlinear and $\mathcal{O}(10^7)$ linearized PDE solves!

Solving real world problems is intractable without ...

- ▶ Better **nonsmooth** optimization algorithm or **differentiable** \mathcal{R}
- ▶ **Adaptive/variable fidelity** approximation in physical and stochastic space
- ▶ In optimization, accuracy is **not** required far from a solution

9 Epi-Regularized Risk Measures

Let $\mathcal{R}, \Phi : \mathcal{X} \rightarrow (-\infty, \infty]$ satisfy:

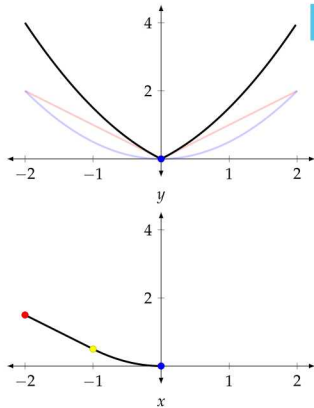
1. \mathcal{R}, Φ are proper, closed and convex
2. $\text{dom } \mathcal{R}^* \subseteq \text{dom } \Phi^*$
3. $(\text{dom } \mathcal{R}^* - \text{dom } \Phi^*)$ contains a neighborhood of 0

The **epi-regularization** of \mathcal{R} is given by

$$\mathcal{R}_\varepsilon(X) := \inf_{Y \in \mathcal{X}} \{ \mathcal{R}(X - Y) + \varepsilon \Phi(Y/\varepsilon) \}, \quad \varepsilon > 0$$

Properties of $\mathcal{R}_\varepsilon^\Phi$:

1. $(\mathcal{R}_\varepsilon^\Phi)^*(\vartheta) = \mathcal{R}^*(\vartheta) + \varepsilon \Phi^*(\vartheta)$ with $\text{dom}(\mathcal{R}_\varepsilon^\Phi)^* = \text{dom } \mathcal{R}^* \cap \text{dom } \Phi^* = \text{dom } \mathcal{R}^*$
2. $-\varepsilon \Phi(0) \leq \mathcal{R}(X) - \mathcal{R}_\varepsilon^\Phi(X) \leq \varepsilon \Phi^*(\vartheta) \quad \forall \vartheta \in \partial \mathcal{R}(X)$
3. **Coherent Risk:** $\mathcal{R}_\varepsilon^\Phi$ is convex, translation equivariant and monotonic
4. **Coherent Risk:** $\mathcal{R}_\varepsilon^\Phi$ is **not** positively homogeneous $\implies \mathcal{R}_\varepsilon^\Phi$ is **not** coherent



9 Epi-Regularized Risk Measures

Let $\mathcal{R}, \Phi : \mathcal{X} \rightarrow (-\infty, \infty]$ satisfy:

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2. $\text{dom } \mathcal{R}^* \subseteq \text{dom } \Phi^*$
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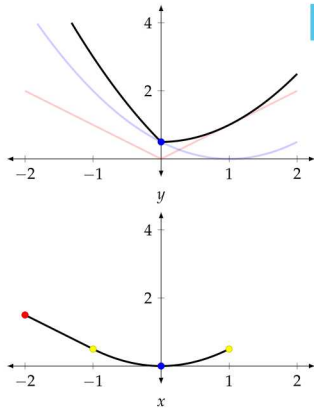
$$\mathcal{R}_\varepsilon(X) := \inf_{Y \in \mathcal{X}} \{ \mathcal{R}(X - Y) + \varepsilon \Phi(Y/\varepsilon) \}, \quad \varepsilon > 0$$

Differentiability of $\mathcal{R}_\varepsilon^\Phi$:

1. If Φ^* is *strictly convex* on $\text{dom } \mathcal{R}^*$, then $\mathcal{R}_\varepsilon^\Phi$ is *Hadamard differentiable*
2. If, in addition, Φ^* is *weak* closed* and satisfies

$$\theta_k \rightharpoonup^* \theta \quad \text{in } \mathcal{X}^* \quad \text{and} \quad \Phi^*(\theta_k) \rightarrow \Phi^*(\theta) \quad \implies \quad \theta_k \rightarrow \theta \quad \text{in } \mathcal{X}^*,$$

then $\mathcal{R}_\varepsilon^\Phi$ is *continuously Fréchet differentiable*



Example: Optimized Certainty Equivalents

Let $u(t) = -v(-t)$ is a normalized, concave utility function and define $\mathcal{R}(X) = \inf_t \{t + \mathbb{E}[v(X - t)]\}$ and $\Phi(X) = \mathbb{E}[\phi(X)]$, then

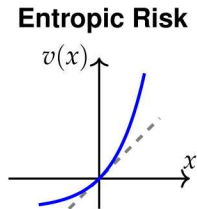
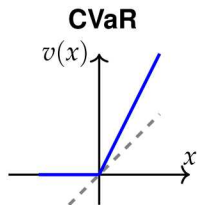
$$\begin{aligned}\mathcal{R}_\varepsilon^\Phi(X) &= \inf_{Y \in \mathcal{X}} \left\{ \inf_{t \in \mathbb{R}} \{t + \mathbb{E}[v(X - Y - t)]\} + \varepsilon \Phi(Y/\varepsilon) \right\} \\ &= \inf_{t \in \mathbb{R}} \left\{ t + \inf_{Y \in \mathcal{X}} \mathbb{E}[v(X - Y - t) + \varepsilon \phi(Y/\varepsilon)] \right\}\end{aligned}$$

Decomposability of \mathcal{X} ensures that

$$\mathcal{R}_\varepsilon^\Phi(X) = \inf_{t \in \mathbb{R}} \left\{ t + \mathbb{E} \left[\inf_{y \in \mathbb{R}} \{v(X - y - t) + \varepsilon \phi(y/\varepsilon)\} \right] \right\}$$

The inner infimum is the **infimal convolution** of $v(x)$ with $\phi(x)$

$$\Rightarrow \mathcal{R}_\varepsilon^\Phi(X) = \inf_{t \in \mathbb{R}} \{t + \mathbb{E}[v_\varepsilon^\phi(X - t)]\}!$$





Results: If $\Phi(0) < \infty$ and $\Phi(1) < \infty$, then

- ▶ $\mathcal{R}_{\varepsilon_n}$ *Mosco converges* to \mathcal{R} for $\varepsilon_n \downarrow 0$
- ▶ $\mathcal{R}_{\varepsilon_n}$ *pointwise converges* to \mathcal{R} for $\varepsilon_n \downarrow 0$
- ▶ If $\Phi(0) \leq 0$, then $\mathcal{R}_{\varepsilon}^{\Phi}$ *monotonically increases* to \mathcal{R} as $\varepsilon \downarrow 0$

Recall: $G_n : \mathcal{X} \rightarrow (-\infty, \infty]$ *Mosco converges* to $G : \mathcal{X} \rightarrow (-\infty, \infty]$ if

1. For all $X_n \rightharpoonup X$ in \mathcal{X} , we have

$$\liminf_{n \rightarrow \infty} G_n(X_n) \geq G(X)$$

2. For all $X \in \mathcal{X}$, there exists $X_n \rightarrow X$ in \mathcal{X} such that

$$\limsup_{n \rightarrow \infty} G_n(X_n) \leq G(X)$$

\implies Minimizers of G_n converge to minimizers of G (cf. Γ -convergence)



$$\min_{z \in Z_{\text{ad}}} \{J(z) := \mathcal{R}(F(z)) + \wp(z)\} \rightsquigarrow \min_{z \in Z_{\text{ad}}} \{J_{\varepsilon}(z) := \mathcal{R}_{\varepsilon}^{\Phi}(F(z)) + \wp(z)\}$$

► **Consistency of Minimizers:**

Let $z_n \in Z_{\text{ad}}$ denote a minimizer of J_{ε_n} with $\varepsilon_n \downarrow 0$.

If F is *completely continuous*

$$z \rightharpoonup z^* \text{ in } Z \implies F(z) \rightarrow F(z^*) \text{ in } \mathcal{X}.$$

Then any *weak limit point* of $\{z_n\}$ minimizes F over Z_{ad} .

► **Consistency of First-Order Stationary Points:**

Let $z_n \in Z_{\text{ad}}$ denote a 1st-order stationary point of J_{ε_n} with $\varepsilon_n \downarrow 0$, i.e.,

$$0 \in \partial_C J_{\varepsilon_n}(z_n) + \mathcal{N}_{Z_{\text{ad}}}(z_n).$$

If ∇F is *completely continuous*

$$z \rightharpoonup z^* \text{ in } Z \implies \nabla F(z) \rightarrow \nabla F(z^*) \text{ in } L^p(\Omega, \mathcal{F}, \mathbb{P}; Z^*).$$

Then any *weak limit point*, z , of $\{z_n\}$ satisfies $0 \in \partial_C J(z) + \mathcal{N}_{Z_{\text{ad}}}(z)$.



Let the following conditions hold:

- ▶ $z \in Z_{\text{ad}}$ is a minimizer of J and $z_\varepsilon \in Z_{\text{ad}}$ is a minimizer of J_ε
- ▶ F and \wp are continuously Fréchet differentiable
- ▶ Either $(h_\varepsilon := z_\varepsilon - z)$
 1. F is twice continuously Fréchet differentiable and $\exists K \in \mathcal{X}$ s.t. $K \in (0, \infty)$ a.s. and

$$K \|z_\varepsilon - z\|_Z^2 \leq \int_0^1 \int_0^1 \nabla^2 F(z + \tau th_\varepsilon)(h_\varepsilon, h_\varepsilon) d\tau dt \text{ a.s.}$$

2. \wp is twice continuously Fréchet differentiable and $\exists L > 0$ such that

$$L \|z_\varepsilon - z\|_Z^2 \leq \int_0^1 \int_0^1 \nabla^2 \wp(z + \tau th_\varepsilon)(h_\varepsilon, h_\varepsilon) d\tau dt$$

Then, $\exists \vartheta \in \partial \mathcal{R}(F(z))$ and $c > 0$ such that

$$c \|z_\varepsilon - z\|_Z^2 \leq \varepsilon (\Phi(0) + \Phi^*(\vartheta))$$

Epi-Regularized CVaR with $\Phi(X) = \frac{1}{2} \mathbb{E}[X^2] + \mathbb{E}[X] \implies \Phi(0) = 0$ **and** $\Phi^*(\vartheta) \leq \frac{\beta^2}{2(1-\beta)}$

Nonconvex Stochastic Programming in \mathbb{R}^n



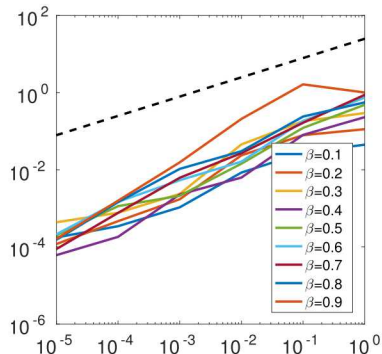
Let $\gamma > 0$ and $\bar{z} \in [-1, 1]^n$ be fixed. Consider the optimization problem

$$\min_{z \in \mathbb{R}^n} \left\{ \mathcal{R} \left(\frac{1}{2} (1 - \tanh(\eta \xi^\top z)) \right) + \frac{\gamma}{2} z^\top z \right\}$$

where ξ is uniformly distributed on $[0, 1]^n$ and $\eta = \text{sgn}(\xi^\top \bar{z})$.

Epi-regularization Error in Optimal Solutions:

- ▶ $\mathcal{R}(X) = \text{CVaR}_\beta[X]$ with $\beta \in \{0.1, 0.2, \dots, 0.9\}$
- ▶ $\Phi(X) = \frac{1}{2} \mathbb{E}[X^2] + \mathbb{E}[X]$ with $\varepsilon \in \{10^{-5}, 10^{-4}, \dots, 10^0\}$





Let $D_0 \subseteq D \subset \mathbb{R}^2$ and $\alpha > 0$. We consider the optimization problem

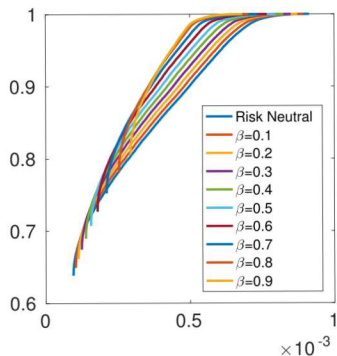
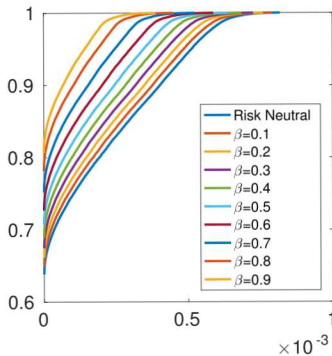
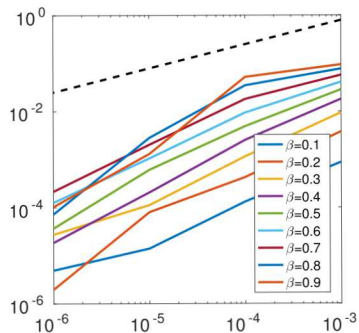
$$\min_{z \in Z_{\text{ad}}} \frac{1}{2} \text{CVaR}_\beta \left(\int_{D_0} (1 - S(z; x, \xi))_+^2 \, dx \right) + \frac{\alpha}{2} \int_D z(x)^2 \, dx$$

where $S(z) = u \in L^q(\Omega, \mathcal{F}, \mathbb{P}; H^1(D))$ solves the weak form of

$$\begin{aligned} -\kappa(\xi) \Delta u(\xi) + c(\xi) u(\xi) &= B(\xi) z + f && \text{in } D, \text{ a.s.} \\ \kappa(\xi) \nabla u(\xi) \cdot n &= 0 && \text{on } \partial D, \text{ a.s.} \end{aligned}$$

Coefficients: $\kappa(\xi) = 2.5 \times 10^{\xi_1}$, $c(\xi) = 1.45 \times 10^{\xi_2}$, $r(\xi) = 10^{\xi_3}$, and $\zeta(\xi) = B(\xi) z \in L^2(\Omega, \mathcal{F}, \mathbb{P}; H^1(D))$ solves the weak form of

$$\begin{aligned} -r(\xi) \Delta \zeta(\xi) + \zeta(\xi) &= z && \text{in } D, \text{ a.s.} \\ r(\xi) \nabla \zeta(\xi) \cdot n &= 0 && \text{on } \partial D, \text{ a.s.} \end{aligned}$$

**Left:** CDF of full objective.**Center:** CDF of random objective.**Right:** Control errors.

Conclusions:

- ▶ **Numerical solution** of risk-averse PDE-optimization is **expensive**
- ▶ Most **coherent risk measures** are **not** Fréchet differentiable
- ▶ Use **infimal convolution** to **smooth** risk measures
- ▶ Appropriate assumptions ensure smoothed risk **is** Fréchet differentiable
- ▶ Proved **consistency** of minimizers and first-order stationary points

Open Problems:

- ▶ Path-following methods for smoothed risk measures
- ▶ Algorithms for **nonsmooth**, **nonconvex** risk-averse PDE-optimization
- ▶ Analysis and algorithms for **probabilistic** PDE-optimization
- ▶ Analysis and algorithms for **dominance-constrained** PDE-optimization