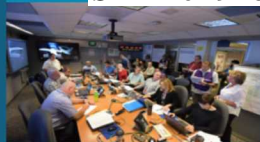


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 Laboratories

SAND2019-8675C

A Primal-Dual Algorithm for Large-Scale Risk Minimization



Drew P. Kouri, Thomas M. Surowiec
International Conference on Stochastic Programming
Trondheim, Norway

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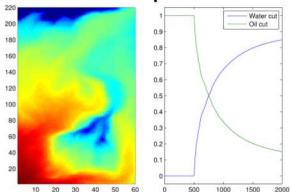
Administration under contract DE-NA0003525.

2 Motivating Applications

Simulation Constrained Optimization



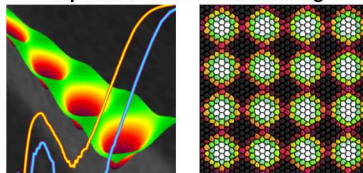
Reservoir Optimization



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

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

Superconductor Vortex Pinning



Courtesy Argonne National Laboratory

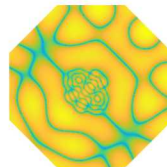
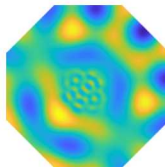
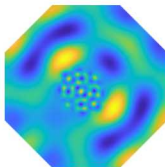
$$\gamma(\partial_t + i\mu)\psi = \epsilon\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi$$

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

Direct Field Acoustic Testing



<https://blogs.nasa.gov/orion/2016/03/07/engineers-test-new-acoustics-method-on-flown-orion/>



$$\Delta u + \kappa^2(1 + \sigma\epsilon)^2 u = 0,$$

$$\nabla u \cdot n + i\chi\kappa\gamma u = i\rho_0\omega(1 - \chi)z$$

3 Simulation Constrained Optimization

Stochastic Problem Formulation



Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a **probability space**, let U and Z be **reflexive Banach spaces** and let Y be a **Banach space**. We consider the optimization problem

$$\min_{z \in Z_{\text{ad}}} \{ \mathcal{R}(f(S(z), \xi)) + \wp(z) \} \quad \text{where} \quad u = S(z, \xi) \quad \text{solves} \quad e(u, z, \xi) = 0 \quad \text{a.s.}$$

Here $\xi : \Omega \rightarrow \Xi$ are **random parameters (i.e., boundary/initial conditions, etc.)**

$f : U \times \Xi \rightarrow \mathbb{R}$ is a **state (simulation variable) objective function**,

$\wp : Z \rightarrow \mathbb{R}$ is a **control (design, etc.) objective function**,

$e : U \times Z \times \Xi \rightarrow Y$ is the **simulation constraint**, and

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

Computational Cost to Evaluate $F(z) := f(S(z, \xi), \xi)$ **and Its Derivatives:**

Value $e(u, z, \xi) = 0$

Gradient $e(u, z, \xi) = 0$

HessVec $e(u, z, \xi) = 0$

$$e_u(u, z, \xi)s = -e_z(u, z, \xi)v$$

$$e_u(u, z, \xi)^* \lambda = -f_u(u, \xi)$$

$$e_u(u, z, \xi)^* \lambda = -f_u(u, \xi)$$

$$e_u(u, z, \xi)^* p = L_{uu}(u, z, \lambda, \xi)s - L_{uz}(u, z, \lambda, \xi)v$$



What is **risk** and how should we **quantify** it?

Risk (noun): *Possibility of loss or injury* (Merriam Webster)

Optimistic Problem Formulations

- ▶ **Risk-Neutral Approach:**
Minimize *on average*

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

- ▶ **Reliability Approach:**
Minimize *probability of loss*

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

Conservative Problem Formulations

- ▶ **Risk-Averse Approach:**
Model *risk preferences*

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

- ▶ **Buffered Approach:**
Minimize *buffered probability*

$$\mathcal{R}(F(z)) = \text{bPOE}_x(F(z)).$$



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Average Value-at-Risk and Buffered Probability



A **risk measure** is any $\mathcal{R} : \mathcal{X} \rightarrow (-\infty, \infty]$ such that $\mathcal{R}(C) = C$ for all $C \in \mathbb{R}$.

For example, $\mathcal{R}(X) = \mathbb{E}[X]$, $\mathcal{R}(X) = \mathbb{E}[X] + \mathbb{E}[|X - \mathbb{E}[X]|^p]^{1/p}$, or $\mathcal{R}(X) = \text{AVaR}_\beta(X)$.

The **Average Value-at-Risk** is the *average of the* $(1 - \beta) \times 100\%$ *largest scenarios*:

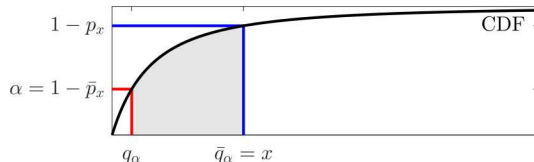
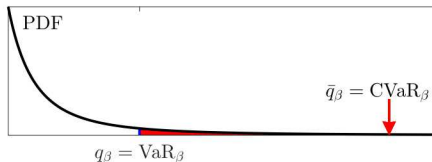
$$\text{AVaR}_\beta(X) = \frac{1}{1 - \beta} \int_\beta^1 q_\alpha(X) \, d\alpha = \min_{t \in \mathbb{R}} \left\{ t + \frac{1}{1 - \beta} \mathbb{E}[\max\{0, X - t\}] \right\}.$$

The **Buffered Probability** is the *probability that* $\text{AVaR}_\beta(X)$ *exceeds a threshold* x :

$$\text{bPOE}_x(X) = 1 - \beta \quad \text{where } \beta \text{ solves } \text{AVaR}_\beta(X) = x,$$

which can be computed by solving the convenient 1D convex optimization problem

$$\text{bPOE}_x(X) = \min_{t \geq 0} \mathbb{E}[\max\{0, t(X - x) + 1\}].$$



6 Coherent Measures of Risk

Ph. Artzner et al., Mathematical Finance, 9(3), 1999.



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

(R1) **Subadditivity:** $\mathcal{R}(X + X') \leq \mathcal{R}(X) + \mathcal{R}(X')$

(R2) **Monotonicity:** $X \geq X' \text{ a.s.} \implies \mathcal{R}(X) \geq \mathcal{R}(X')$

(R3) **Translation Equivariance:** $\mathcal{R}(X + t) = \mathcal{R}(X) + t, \quad \forall t \in \mathbb{R}$

(R4) **Positive Homogeneity:** $\mathcal{R}(tX) = t\mathcal{R}(X), \quad \forall t > 0$

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

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

Examples of risk measures that are **coherent**:

► Mean-Plus-Semideviation: $\mathcal{R}(X) = \mathbb{E}[X] + c\mathbb{E}[\max\{0, X - \mathbb{E}[X]\}^p]^{1/p}, \quad c \in (0, 1)$

► Average Value-at-Risk: $\mathcal{R}(X) = \inf_t \{t + (1 - \beta)^{-1} \mathbb{E}[\max\{X - t, 0\}]\}, \quad \beta \in (0, 1)$

Examples of risk measures that are **not coherent**:

► Mean-Deviation: $\mathcal{R}(X) = \mathbb{E}[X] + \mathbb{E}[|X - \mathbb{E}[X]|^p]^{1/p} \quad \text{Violates (R2)!}$

► Entropic Risk: $\mathcal{R}(X) = \log \mathbb{E}[\exp X] \quad \text{Violates (R4)!}$

7 Is Nondifferentiability *Really* an Issue?



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

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

Nonsmooth, nonconvex, & stochastic simulation-constrained optimization:

- Algorithms for **nonsmooth, nonconvex** problems often converge **(sub)linearly**!
- Evaluating the **cost function** requires **simulations for every sample**!
- Evaluating **(sub)gradients** requires additional **linear solves for every sample**!

A small, nonconvex, & nonsmooth example: AVaR minimization of Burger's equation:

- **Bundle Method:** Required $\mathcal{O}(10^8)$ nonlinear and $\mathcal{O}(10^8)$ linearized solves.
- **Smoothing + Newton:** Required $\mathcal{O}(10^6)$ nonlinear and $\mathcal{O}(10^7)$ linearized 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.

8 Epi-Regularized Risk Measures

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

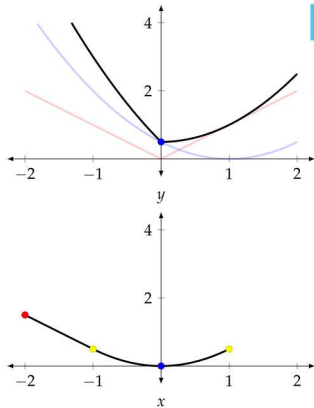
$$\mathcal{R}_\varepsilon^\Phi(X) := \inf_{Y \in \mathcal{X}} \{ \mathcal{R}(X - Y) + \varepsilon \Phi(Y/\varepsilon) \}, \quad \varepsilon > 0$$

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

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

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

1. $|\mathcal{R}(X) - \mathcal{R}_\varepsilon^\Phi(X)| = \mathcal{O}(\varepsilon)$
2. \mathcal{R} **coherent** $\implies \mathcal{R}_\varepsilon^\Phi$ is a **convex** risk measure, but is **not** coherent
3. If Φ^* is *strictly convex* on $\text{dom } \mathcal{R}^*$, then $\mathcal{R}_\varepsilon^\Phi$ is *Hadamard differentiable*
4. If, in addition, Φ is a *potential*, then $\mathcal{R}_\varepsilon^\Phi$ is *continuously differentiable*



9 Epi-Regularized Risk Measures

Application to Expected Regret Functions



Let $v : \mathbb{R} \rightarrow \mathbb{R}$ and $\phi : \mathbb{R} \rightarrow \mathbb{R}$ be convex and define

$$\mathcal{R}(X) = \mathbb{E}[v(X)] \quad \text{and} \quad \Phi(X) = \mathbb{E}[\phi(X)].$$

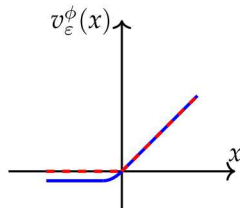
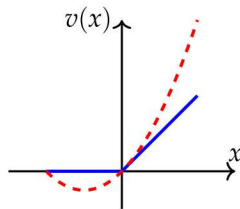
The **decomposability** of \mathcal{X} ensures that

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

where the inner infimum, v_ε^ϕ , is the **infimal convolution** of v with ϕ !

Example: If $v(x) = \max\{0, x\}$ and $\phi(x) = \frac{1}{2}x^2 + x$, then

$$v_\varepsilon^\phi(x) = \begin{cases} -\frac{\varepsilon}{2} & \text{if } x \leq -\varepsilon \\ \frac{1}{2\varepsilon}x^2 + x & \text{if } -\varepsilon < x < 0 \\ x & \text{if } x \geq 0 \end{cases} .$$





We consider the optimization problem:

$$\min_{w \in W_{\text{ad}}} \{g(w) + \Psi(G(w))\} \quad (\text{P})$$

- W_{ad} is a **closed, convex** subset of the **reflexive Banach space** W ,
- $g : W \rightarrow \mathbb{R}$ is **weakly lower semicontinuous**,
- $G : W \rightarrow \mathcal{X} := L^2(\Omega, \mathcal{F}, \mathbb{P})$ is **weak-to-strong continuous**,
- $\Psi : \mathcal{X} \rightarrow \mathbb{R}$ is **convex, monotonic** and **positively homogeneous**,
- $\exists \gamma \in \mathbb{R}$ such that $\{w \in W_{\text{ad}} \mid g(w) + \Psi(G(w)) \leq \gamma\}$ is **nonempty** and **bounded**.

Consequences: Problem (P) **has a solution** and Ψ is **continuous, subdifferentiable** and

$$\Psi(X) = \sup_{\theta \in \mathfrak{A}} \mathbb{E}[\theta X] \quad \forall X \in \mathcal{X} \quad \text{where} \quad \mathfrak{A} := \partial\Psi(0) \subseteq \{\theta \in \mathcal{X} \mid \theta \geq 0 \text{ a.s.}\}$$

$$\implies \min_{w \in W_{\text{ad}}} \{g(w) + \Psi(G(w))\} = \min_{w \in W_{\text{ad}}} \sup_{\theta \in \mathfrak{A}} \{\ell(w, \theta) := g(w) + \mathbb{E}[\theta G(w)]\}.$$

Notation: Let $K := \sup_{\theta \in \mathfrak{A}} \|\theta\|_{\mathcal{X}}$ denote the Lipschitz modulus of Ψ at $X = 0$.



Motivated by the method of multipliers, we define the *generalized augmented Lagrangian*

$$L(w, \lambda, r) := \max_{\theta \in \mathfrak{A}} \left\{ g(w) + \mathbb{E}[\theta G(w)] - \frac{1}{2r} \mathbb{E}[(\lambda - \theta)^2] \right\}, \quad r > 0.$$

Relation to Epi-Regularization: As a consequence of convex duality,

$$L(w, \lambda, r) = g(w) + \min_{Y \in \mathcal{X}} \left\{ \Psi(G(w) - Y) + \mathbb{E}[\lambda Y] + \frac{r}{2} \mathbb{E}[Y^2] \right\} = g(w) + \Psi_{1/r}^\Phi(G(w))$$

where $\Phi(Y) = \mathbb{E}[\lambda Y] + \frac{1}{2} \mathbb{E}[Y^2] \implies 0 \leq \Psi(X) - \Psi_{1/r}^\Phi(X) \leq K^2/r$ for all $X \in \mathcal{X}$.

Consequences: $L(\cdot, \lambda, r)$ is *continuously differentiable* with derivative given by

$$\nabla_w L(w, \lambda, r) = \mathbf{P}_{\mathfrak{A}}(rG(w) + \lambda).$$

$L(w, \cdot, r)$ is also *continuously differentiable* with derivative given by

$$\nabla_\lambda L(w, \lambda, r) = (\mathbf{P}_{\mathfrak{A}}(rG(w) + \lambda) - \lambda)/r.$$



We can rewrite the *generalized augmented Lagrangian* in the more revealing form

$$L(w, \lambda, r) = g(w) + \mathbb{E}[\lambda G(w)] + \frac{r}{2} \mathbb{E}[G(w)^2] - \frac{1}{2r} \mathbb{E}[\{(\text{Id} - \mathbf{P}_{\mathfrak{A}})(rG(w) + \lambda)\}^2].$$

Equality Constraints ($G(w) = 0$): Let Ψ be the *indicator function* of $\{0\}$, then $\mathfrak{A} = \mathcal{X}$ and

$$L(w, \lambda, r) = g(w) + \mathbb{E}[\lambda G(w)] + \frac{r}{2} \mathbb{E}[G(w)^2].$$

Inequality Constraints ($G(w) \leq 0$): Let Ψ be the *indicator function* of $\{X \in \mathcal{X} \mid X \leq 0 \text{ a.s.}\}$, then $\mathfrak{A} = \{\theta \in \mathcal{X} \mid \theta \geq 0 \text{ a.s.}\}$ and

$$L(w, \lambda, r) = g(w) + \frac{1}{2r} \mathbb{E}[\max\{0, rG(w) + \lambda\}^2] - \frac{1}{2r} \mathbb{E}[\lambda^2].$$



Initialize: Given $\lambda_0 \in \mathfrak{A}$ and $r_0 > 0$.

While(“Not Converged”)

1. Find $w_{k+1} \in W_{\text{ad}}$ that *approximately* minimizes $L(\cdot, \lambda_k, r_k)$.
2. Set $\lambda_{k+1} = \mathbf{P}_{\mathfrak{A}}(r_k G(w_{k+1}) + \lambda_k)$.
3. Update r_{k+1} .

EndWhile

Practical Implementation: If W is a **Hilbert space**, then “**Converged**” could mean

$$\|w_{k+1} - \mathbf{P}_{W_{\text{ad}}}(w_{k+1} - \nabla_w L(w_{k+1}, \lambda_k, r_k))\|_W \leq \tau_w \quad \text{and} \quad \|\lambda_k - \lambda_{k+1}\|_{\mathcal{X}} \leq \tau_{\lambda}.$$

Moreover, we can update $r_{k+1} = \rho_r r_k$ for some $\rho_r > 0$ if $\|\lambda_k - \lambda_{k+1}\|_{\mathcal{X}} > \tau_{\lambda,k}$ with $\tau_{\lambda,k} > 0$.



Example: Suppose $\Psi(X) = \mathbb{E}[\max\{0, X\}]$, then $\mathfrak{A} = \{\theta \in \mathcal{X} \mid 0 \leq \theta \leq 1 \text{ a.s.}\}$.

While(“Not Converged”)

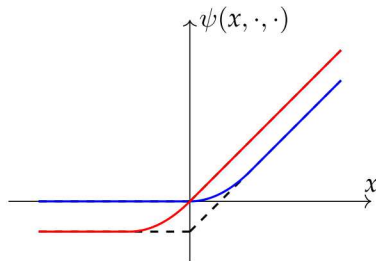
1. Find $w_{k+1} \in W_{\text{ad}}$ that *approximately* solves

$$\min_{w \in W_{\text{ad}}} \{g(w) + \mathbb{E}[\psi(G(w), \lambda_k, r_k)]\}.$$

2. Set $\lambda_{k+1} = \max\{0, \min\{1, r_k G(w_{k+1}) + \lambda_k\}\}$.

3. Update r_{k+1} .

EndWhile



$$\psi(x, t, r) = \begin{cases} -\frac{1}{2r}t^2 & \text{if } rx + t < 0 \\ \frac{r}{2}x^2 + tx & \text{if } 0 \leq rx + t \leq 1 \\ \frac{1}{r}\{(rx + t) - \frac{1}{2}(t^2 + 1)\} & \text{if } 1 < rx + t \end{cases}$$

Note: Equivalent to the **method of multipliers** applied to the smooth reformulation

$$\min_{w \in W_{\text{ad}}, s, \eta \in \mathcal{X}} \{g(w) + \mathbb{E}[\eta]\} \quad \text{subject to} \quad G(w) - \eta + s = 0, \quad \eta \geq 0, \quad s \geq 0 \text{ a.s.}$$



1. **Primal Variables:** Let $\epsilon_k \rightarrow \epsilon^* \geq 0$ and $r_k \rightarrow r^* \leq \infty$. If the iterates $\{w_k\} \subset W_{\text{ad}}$ are ϵ_k -minimizers, then **any weak accumulation point of $\{w_k\}$ is a $(\epsilon^* + \frac{K^2}{r^*})$ -minimizer of the original problem.**
2. **Dual Variables:** If, in addition, $\{\epsilon_k\}$ satisfies

$$\epsilon_k = \frac{\gamma_k^2}{2r_k}, \quad \sum_{k=0}^{\infty} \gamma_k < \infty, \quad \text{and} \quad \gamma_k \geq 0,$$

then **the dual variables $\{\lambda_k\}$ converge weakly to a maximizer of the dual problem.**

3. **Primal Variables:** Let $\epsilon_k \rightarrow 0$ and $r_k \rightarrow \infty$, and suppose g and G are continuously differentiable. If the iterates $\{w_k\} \subset W_{\text{ad}}$ are ϵ_k -stationary points then **any weak accumulation point of $\{w_k\}$ is a stationary point of the original problem.**



Elliptic 1d: $D = (-1, 1)$, $\alpha = 10$, $Z = Z_{\text{ad}} = L^2(D)$

$$\min_{z \in Z_{\text{ad}}} \mathcal{R} \left(\frac{1}{2} \int_D (S(z) - 1)^2 \, dx \right) + \frac{\alpha}{2} \int_D z^2 \, dx$$

where $u = S(z)$ solves

$$\begin{aligned} -\partial_x(\epsilon(\xi) \partial_x u(\xi)) &= f(\xi) + z && \text{in } D \text{ a.s.} \\ [u(\xi)](-1) = 0, \quad [u(\xi)](1) &= 0 && \text{a.s.} \end{aligned}$$

Elliptic 2d: $D = (0, 1)^2$, $\alpha = 10^{-5}$, $Z = \mathbb{R}^9$, $Z_{\text{ad}} = \{z \in Z \mid 0 \leq z \leq 1\}$

$$\min_{z \in Z_{\text{ad}}} \mathcal{R} \left(\frac{1}{2} \int_D S(z)^2 \, dx \right) + \alpha \|z\|_1$$

where $u = S(z)$ solves

$$\begin{aligned} -\nabla(\epsilon(\xi) \nabla u(\xi)) + \mathbb{V}(\xi) \cdot \nabla u(\xi) &= f(\xi) - Bz && \text{in } D \text{ a.s.} \\ u(\xi) &= 0 && \text{on } \Gamma_d = \{0\} \times (0, 1) \text{ a.s.} \\ \epsilon(\xi) \nabla u(\xi) \cdot n &= 0 && \text{on } \partial D \setminus \Gamma_d \text{ a.s.} \end{aligned}$$



Burgers: $D = (0, 1)$, $\alpha = 10^{-3}$, $Z = Z_{\text{ad}} = L^2(D)$

$$\min_{z \in Z_{\text{ad}}} \mathcal{R} \left(\frac{1}{2} \int_D (S(z) - 1)^2 \, dx \right) + \frac{\alpha}{2} \int_D z^2 \, dx$$

where $u = S(z)$ solves

$$\begin{aligned} -\nu(\xi) \partial_{xx} u(\xi) + u(\xi) \partial_x u(\xi) &= f(\xi) + z && \text{in } D \text{ a.s.} \\ [u(\xi)](0) = d_0(\xi), \quad [u(\xi)](1) &= d_1(\xi) && \text{a.s.} \end{aligned}$$

Risk Measures:

Mean-Plus-Semideviation

$$\mathcal{R}(X) = \mathbb{E}[X] + c \mathbb{E}[\max\{0, X - \mathbb{E}[X]\}]$$

Mean-Plus-Semideviation-From-Target

$$\mathcal{R}(X) = \mathbb{E}[X] + c \mathbb{E}[\max\{0, X - t\}]$$

Average Value-at-Risk

$$\mathcal{R}(X) = \lambda \mathbb{E}[X] + (1 - \lambda) \text{AVaR}_\beta(X)$$

Buffered Probability

$$\mathcal{R}(X) = \inf_{t \geq 0} \mathbb{E}[\max\{0, t(X - x) + 1\}]$$



example	risk	PD Algorithm				Bundle	
		iter	nfval	ngrad	subiter	iter	neval
elliptic 1d	MPSD	7	14	14	7	37	530
	MPSDFT	7	11	11	4	28	427
	CVAR	7	23	23	16	37	240
	BPOE	7	66	59	33	---	---
elliptic 2d	MPSD	5	15	15	5	---	---
	MPSDFT	6	21	20	8	---	---
	CVAR	9	99	57	31	---	---
	BPOE	10	123	72	47	---	---
burgers	MPSD	14	35	30	21	362	395
	MPSDFT	11	23	23	12	329	361
	CVAR	11	63	63	52	369	466
	BPOE	11	179	129	76	---	---

Between 7 and 38 fold reduction in computational work!

Conclusions:

- ▶ **Numerical solution** of risk-averse simulation-constrained optimization is **expensive**
- ▶ Most **coherent risk measures** are **not** continuously differentiable
- ▶ We can use the **infimal convolution** to **smooth** risk measures
- ▶ Appropriate assumptions ensure smoothed risk **is** continuously differentiable
- ▶ Generalized method of multipliers solves a sequence of **smooth, epi-regularized** subproblems
- ▶ Proved **convergence** of approximate minimizers and first-order stationary points
- ▶ Numerical examples suggest **$\sim 10\text{--}40\times$ improvement** compared to bundle method

References:

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