Controlling Uncertainty in PDE-Constrained Optimization

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Drew Kouri

Optimization and Uncertainty Quantification
Sandia National Laboratories, Albuquerque, New Mexico
dpkouri@sandia.gov

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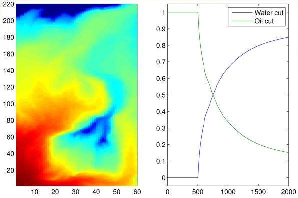
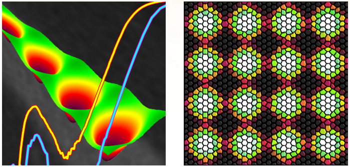
Motivation

Reservoir Optimization



$$v = -\mathbf{K}\lambda(s)\nabla p, \quad \nabla\cdot v = q$$
$$\phi\, \partial_t s + \nabla\cdot\left(f(s)v\right) = \widehat{q}$$

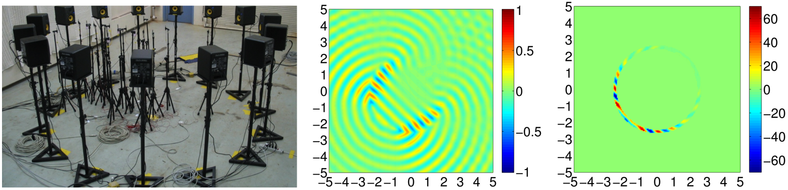
Superconductor Vortex Pinning



Courtesy Argonne National Laboratory

$$\gamma(\partial_t + i\mu)\psi = \epsilon\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi$$
$$\mathbf{J} = \mathrm{Im}(\bar{\psi}(\nabla - i\mathbf{A})\psi) - (\partial_t\mathbf{A} + \nabla\mu), \quad \nabla\cdot\mathbf{J} = 0$$

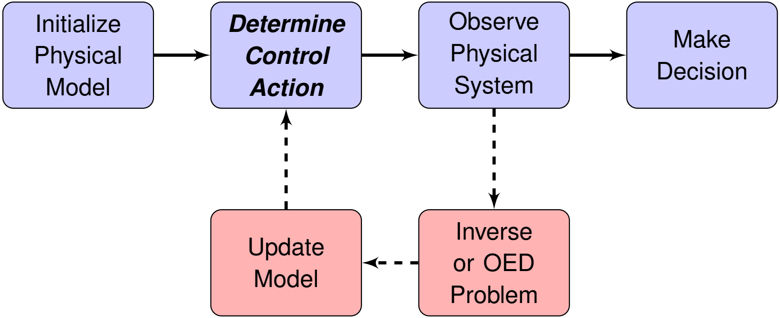
Direct Field Acoustic Testing



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

Optimization Problem Formulation

Goal: Control uncertainty rather than quantify uncertainty.



We implement the control prior to observing the state.
Control is deterministic.

Optimization of PDEs with Random Inputs

Given $\alpha > 0$, $\Omega_o \subseteq \Omega$, $\Omega_c \subseteq \Omega$, and $w \in L^2(\Omega;\mathbb{C})$, we consider

$$\min_{z\in\mathcal{Z}} J(z) \equiv \frac{1}{2}\sigma\left[\int_{\Omega_o}(u(\cdot,x\,;z)-w(x))\overline{(u(\cdot,x\,;z)-w(x))}\,\mathrm{d}x\right]+\frac{\alpha}{2}\int_{\Omega_c} z(x)\overline{z(x)}\,\mathrm{d}x$$

where $u(z) = u \in L^{2p}_\rho(\Xi; H^1(\Omega;\mathbb{C}))$ solves the **weak form** of

$$-\Delta u(\xi,x) - \kappa^2(1+\sigma\epsilon(\xi,x))^2 u(\xi,x) = z(x), \qquad x\in\Omega,\ \xi\in\Xi$$

$$\frac{\partial u}{\partial n}(\xi,x) = i\,\kappa\, u(\xi,x), \qquad x\in\partial\Omega,\ \xi\in\Xi.$$

- **Random parameters** ξ**:**
  - Image space: $\Xi \equiv \Xi_1\times\cdots\times\Xi_M$ with $\Xi_k\subseteq\mathbb{R}$
  - Probability law: $\rho\equiv\rho_1\otimes\cdots\otimes\rho_M$ with $\rho_k:\Xi_k\to[0,\infty)\cup\{+\infty\}$
- **Control space:** $\mathcal{Z}\equiv L^2(\Omega_c;\mathbb{C})$ Deterministic
- **State space:** $\mathcal{U}\equiv L^{2p}_\rho(\Xi;H^1(\Omega;\mathbb{C}))$ Stochastic
- **Risk Measure:** $\sigma : L^p_\rho(\Xi)\to\mathbb{R}\cup\{+\infty\}\cup\{-\infty\}$
  see, Rockafellar, Uryasev, Shapiro, Dentcheva, Ruszczynski, . . .

Motivation - Control Uncertainty

Optimal control should be **"risk averse."** For example:

- Reduce **variance** or **deviation**

$$\mathbb{E}[(X - \mathbb{E}[X])^2] \qquad \text{or} \qquad \mathbb{E}[(X - \mathbb{E}[X])_+^q]^{\frac{1}{q}}$$

  e.g. *reduce uncertainty and variability in controlled system.*

- Control **rare events**, **tail probabilities**, or **quantiles**

$$\Pr[X \leq t] \qquad \text{or} \qquad \mathrm{VaR}_\beta[X] = \inf\{\, t \in \mathbb{R} \,:\, \Pr[X \leq t] \geq \beta \,\}$$

  e.g. *reduce failure regions and certify reliability.*

- Minimize over **quantiles**

$$\mathrm{CVaR}_\beta[X] = \frac{1}{1-\beta} \int_{X \geq \mathrm{VaR}_\beta[X]} X(\xi)\rho(\xi)\,\mathrm{d}\xi = \mathbb{E}[X \,|\, X \geq \mathrm{VaR}_\beta[X]]$$

  e.g. *minimize over undesirable events.*

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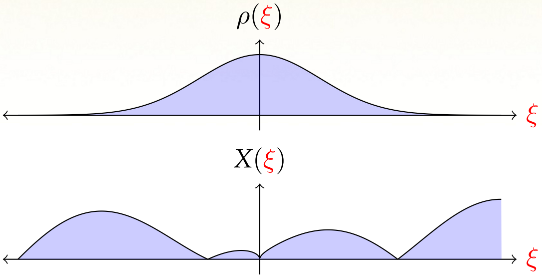
Risk Measures

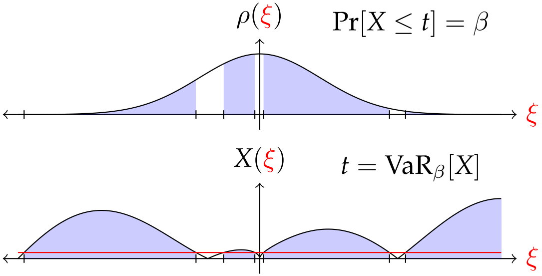
Risk Neutral:

$\sigma[X] = \mathbb{E}[X]$



Conditional Value-at-Risk:

$\sigma[X] = \mathrm{CVaR}_\beta[X]$



Risk Measures

Shapiro, Dentcheva, Ruszczynski, Rockafellar, Uryasev, . . .

We consider the risk measures ($X \in L^1_\rho(\Xi)$):

- Risk Neutral: $\sigma[X] = \mathbb{E}[X]$
- Mean Plus Semideviation: $\sigma[X] = \mathbb{E}[X] + c\mathbb{E}[(X - \mathbb{E}[X])_+], \; c \in (0,1)$
- Conditional Value-at-Risk: $\sigma[X] = \inf\{\, t + c\mathbb{E}[(X-t)_+] \; : \; t \in \mathbb{R}\,\}, \; c > 1$

These σ are **coherent** (Artzner, Delbaen, Eber, Heath): $X, Y \in L^1_\rho(\Xi)$

- **Convexity:** $\sigma[tX + (1-t)Y] \le t\sigma[X] + (1-t)\sigma[Y], \quad \forall t \in [0,1]$
- **Monotonicity:** $X \ge Y$ a.e. $\implies \sigma[X] \ge \sigma[Y]$
- **Translation Equivariance:** $\sigma[X + t] = \sigma[X] + t, \quad \forall t \in \mathbb{R}$
- **Positive Homogeneity:** $\sigma[tX] = t\sigma[X], \quad \forall t > 0.$

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Infinite-Dimensional Results

Existence of Optimal Controls: Assume Helmholtz equation is uniquely solvable, then there exists a unique minimizer of

$$J(z) \equiv \frac{1}{2}\sigma\left[\int_{\Omega_o}(u(\cdot,x;z)-w(x))\overline{(u(\cdot,x;z)-w(x)))}\,\mathrm{d}x\right]+\frac{\alpha}{2}\int_{\Omega_c} z(x)\overline{z(x)}\,\mathrm{d}x$$

Differentiability: $J(z)$ is Hadamard differentiable

- **State Equation:** Find $u(\xi)=u(\xi;z)\in H^1(\Omega;\mathbb{C})$ a.e. in Ξ solving

$$-\Delta u(\xi,x)-\kappa^2(1+\sigma\epsilon(\xi,x)))^2u(\xi,x)=z(x), \qquad \xi\in\Xi,\ x\in\Omega$$

$$\frac{\partial u}{\partial n}(\xi,x)=i\,\kappa\,u(\xi,x), \qquad \xi\in\Xi,\ x\in\partial\Omega.$$

- **Adjoint Equation:** Find $\lambda(\xi)=\lambda(\xi;z)\in H^1(\Omega;\mathbb{C})$ a.e. in Ξ solving

$$-\Delta\lambda(\xi,x)-\kappa^2(1+\sigma\epsilon(\xi,x)))^2\lambda(\xi,x)=\ -(u(\xi,x)-w(x)), \qquad \xi\in\Xi,\ x\in\Omega$$

$$\frac{\partial\lambda}{\partial n}(\xi,x)=i\,\kappa\,\lambda(\xi,x), \qquad \xi\in\Xi,\ x\in\partial\Omega.$$

- **Gradient:**

$$\nabla J(z)=\alpha z-\underbrace{\mathbb{E}\left[\nabla\sigma\left[\int_{\Omega_o}(u(\cdot,x;z)-w(x))\overline{(u(\cdot,x;z)-w(x)))}\,\mathrm{d}x\right]\ \lambda\right]}_{\text{INTEGRATION}}.$$

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Discretization of Optimization Problem

Replace all expected values with quadrature approximations

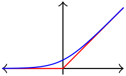
- Risk Neutral: $\sigma_Q[X] = \mathbb{E}_Q[X] = \sum_{k=1}^{Q} \omega_k X(\xi_k)$
- Mean Plus Semideviation: $\sigma_Q[X] = \mathbb{E}_Q[X] + c\mathbb{E}_Q[\wp(X - \mathbb{E}_Q[X], \gamma)],\ c \in (0,1)$
- Conditional Value-at-Risk: $\sigma_Q[X] = \inf \{\, t + c\mathbb{E}_Q[\wp(X - t, \gamma)] \ :\ t \in \mathbb{R} \,\},\ c > 1$

Require the solutions $u(\xi_k) = u_k \in H^1(\Omega; \mathbb{C})$, $k = 1, \ldots, Q$, solves the **weak form** of

$$-\Delta u_k(x) - \kappa^2(1 + \sigma\epsilon(\xi_k, x))^2 u_k(x) = z(x), \qquad x \in \Omega$$

$$\frac{\partial u_k}{\partial n}(x) = i\,\kappa\, u_k, \qquad x \in \partial\Omega.$$

- Decoupled PDE system is equivalent to **stochastic collocation** for a single PDE
- Use favorite numerical PDE technique to solve deterministic PDEs
- For convergence, must **smooth** plus function (Chen and Mangasarian 1994)



$$(x)_+ \approx \wp(x, \gamma) \equiv x + \gamma^{-1}\log(1 + \exp(-\gamma x))$$

- Convergence depends on quad. rule and regularity of state and adjoint w.r.t. ξ.

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Smoothed, Semi-Discretized Results

Existence of Optimal Controls: There exists a minimizer of

$$J_Q(z) \equiv \frac{1}{2}\sigma_Q \left[\int_{\Omega_o} (u(\cdot, x; z) - w(x))\overline{(u(\cdot, x; z) - w(x))}\, \mathrm{d}x \right] + \frac{\alpha}{2} \int_{\Omega_c} z(x)\overline{z(x)}\, \mathrm{d}x$$

in the set $\{ \, z \in \mathcal{Z} \; : \; \|z\|_{L^2(\Omega_c;\mathbb{C})} \leq K \, \}$ for any $K > 0$.
Add constraint because quadrature weights may be **negative**!

Differentiability: $J_Q(z)$ is Fréchet differentiable with gradient computed as

- **State Equation:** Find $u_k = u(\xi_k; z) \in H^1(\Omega; \mathbb{C})$, $k = 1, \ldots, Q$, solving

$$\begin{aligned} -\Delta u_k(x) - \kappa^2(1 + \sigma\epsilon(\xi_k, x))^2 u_k(x) &= z(x), & x \in \Omega \\ \frac{\partial u_k}{\partial n}(x) &= i\,\kappa\, u_k, & x \in \partial\Omega. \end{aligned}$$

- **Adjoint Equation:** Find $\lambda_k = \lambda(\xi_k; z) \in H^1(\Omega; \mathbb{C})$, $k = 1, \ldots, Q$, solving

$$\begin{aligned} -\Delta\lambda_k(x) - \kappa^2(1 + \sigma\epsilon(\xi_k, x)))^2\lambda_k &= -(u_k(x) - w(x)), & x \in \Omega \\ \frac{\partial \lambda_k}{\partial n}(x) &= i\,\kappa\,\lambda_k(x), & x \in \partial\Omega. \end{aligned}$$

- **Gradient:** $\nabla J_Q(z) =$

$$\alpha z - \underbrace{\sum_{k=1}^{Q} \omega_k \nabla\sigma_Q \left[\int_{\Omega_o} (u(\cdot, x; z) - w(x))\overline{(u(\cdot, x; z) - w(x)))}\, \mathrm{d}x \right] (\xi_k)\, \lambda_k}_{\text{QUADRATURE}} .$$

Adaptivity and Optimization

- Efficient Numerical Method
  - Gradient computation requires two PDE solves per quad. point;
  - High accuracy or large $\dim(\Xi) \implies$ large Q;
  - In optimization, accuracy **not** required far from a solution.
- Accurate Characterization of the Random Field
  - Use adaptive sparse grids to exploit anisotropy in random fields (Gerstner and Griebel 1998, Ma and Zabaras 2009, Agarwal and Aluru 2009, Webster et al.);
  - Use adaptive finite elements to accurately resolve PDE solution (Carstensen 2005, Becker et al. 2007).
- Trust Region Methods
  - Globally convergent opt. algorithm (Powell 1975, Sorensen 1982);
  - Allows for inexact gradients and objective functions (Carter 1989, Heinkenschloss and Vicente 2001, Ziems and Ulbrich 2011);
  - Natural framework for model management (Alexandrov et al. 1998, Dennis and Torczon 1996).

Trust-Region Algorithm

Given: z_0, $m_0(s) \approx J(z_0 + s)$, $J_0 \approx J$, $\Delta_0 \geq 0$, and $\mathrm{gtol} > 0$.
While $\|\nabla m_k(s)\|_{\mathcal{Z}} > \mathrm{gtol}$

1. **Model Update:** Choose a new $m_k(s) \approx J(z_k + s)$.
2. **Step Computation:** Approximate a solution, s_k, to the subproblem

$$\min_{s \in \mathcal{Z}} \; m_k(s) \quad \text{subject to} \quad \|s\|_{\mathcal{Z}} \leq \Delta_k.$$

3. **Objective Update:** Choose a new $J_k(z) \approx J(z)$.
4. **Step Acceptance:** Compute

$$\rho_k = \frac{J_k(z_k) - J_k(z_k + s_k)}{m_k(0) - m_k(s_k)}.$$

   If $\rho_k \geq \eta \in (0, 1)$, then $z_{k+1} = z_k + s_k$ else $z_{k+1} = z_k$.

5. **Trust Region Update:** Choose a new trust region radius, Δ_{k+1}.

EndWhile

Trust-Region Algorithm

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While $\|\nabla m_k(s)\|_{\mathcal{Z}} > \mathrm{gtol}$

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Inexact Gradients and Objective Functions

Kouri, Heinkenschloss, Ridzal, and van Bloemen Waanders

Inexact Gradients

There exists $c > 0$ independent of k such that

$$\|\nabla m_k(0) - \nabla J(z_k)\|_{\mathcal{Z}} \leq c \min\{\|\nabla m_k(0)\|_{\mathcal{Z}}, \Delta_k\}$$

(Carter 1989, Heinkenschloss and Vicente 2001).

Inexact Objective Functions

There exists $K > 0$, $\omega \in (0, 1)$, and $\theta(z, s) \to 0$ as $r \to 0$ such that

$$|(J(z_k) - J(z_k + s_k)) - (J_k(z_k) - J_k(z_k + s_k))| \leq K\theta(z_k, s_k)$$
$$\theta(z_k, s_k)^\omega \leq \eta \min\{(m_k(0) - m_k(s_k)), r_k\}.$$

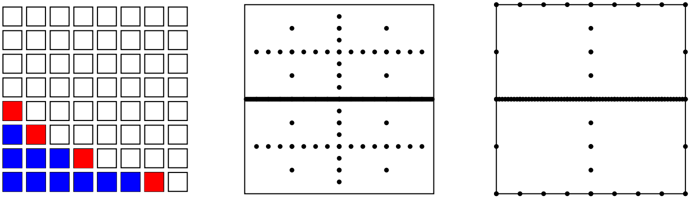
Here, $\eta > 0$ is tied to algorithmic parameters and $\lim_{k\to\infty} r_k = 0$.
(Carter 1989, Ziems and Ulbrich 2013).

- **Cannot** compute $J(z_k)$ and $\nabla J(z_k)$;
- Control *a posteriori* errors using **adaptive sparse grids**.

Sparse Grids and Adaptivity

Gerstner and Griebel 2003

- **1D Operators:** For $k = 1, \dots, M$, $\mathbb{E}_k^0 \equiv 0$ and
$$\Delta_k^i \equiv \mathbb{E}_k^i - \mathbb{E}_k^{i-1} \quad \text{where} \quad \mathbb{E}_k^i(g) \xrightarrow{i \to \infty} \int_{\Xi_k} \rho_k(\xi) g(\xi) \mathrm{d}\xi$$
- **Sparse-Grid Operator:** For an index set $\mathcal{I} \subset \mathbb{N}^M$,
$$\mathbb{E}_{\mathcal{I}} \equiv \sum_{\mathbf{i} \in \mathcal{I}} (\Delta_1^{i_1} \otimes \cdots \otimes \Delta_M^{i_M})$$
- **Admissibility:** $\mathbf{i} \in \mathcal{I}$ and $\mathbf{i} \geq \mathbf{j} \implies \mathbf{j} \in \mathcal{I}$
- **Error:** Given the index set $\mathcal{I} \subset \mathbb{N}^M$, the error is
$$\mathbb{E} - \mathbb{E}_{\mathcal{I}} = \sum_{\mathbf{i} \notin \mathcal{I}} (\Delta_1^{i_1} \otimes \cdots \otimes \Delta_M^{i_M})$$
- **Adaptivity:** Pick $\mathbf{i} \notin \mathcal{I}$ s.t. $\mathcal{I} \cup \{\mathbf{i}\}$ admissible and $\Delta_1^{i_1} \otimes \cdots \otimes \Delta_M^{i_M}$ “large”



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1. **Model Update:** Choose a new $m_k(s) \approx J(z_k + s)$.

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EndWhile

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Hierarchical Sparse Grids and TR Subproblems

Nash 2001, Kouri 2013

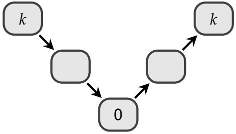
Hierarchy of Optimization Problems

Let $\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \ldots \subseteq \mathcal{I}_k$ denote a sequence of *gradient-adapted* sparse grid index sets and consider the hierarchy of TR subproblems

$$\min_{s \in \mathcal{Z}} \; \widehat{q}_{k,\ell}(s) \equiv q_{k,\ell}(s) - \langle v_\ell, s \rangle_{\mathcal{Z}} \quad \text{subject to} \quad \|s\|_{\mathcal{Z}} \leq \Delta_k$$

where $v_k = 0$, $v_\ell = v_{\ell+1} + (\nabla q_{k,\ell}(s_{\ell+1}) - \nabla q_{k,\ell+1}(s_{\ell+1}))$, and

$$q_{k,\ell}(s) \equiv \frac{1}{2}\langle \nabla^2 J_{\mathcal{I}_\ell}(z_k)s, s\rangle_{\mathcal{Z}} + \langle \nabla J_{\mathcal{I}_k}(z_k), s\rangle_{\mathcal{Z}}.$$



Modified MG/OPT

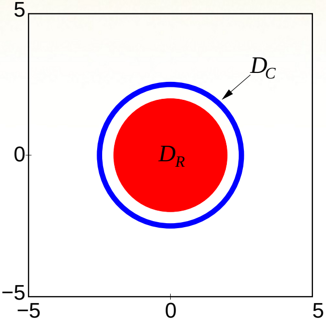
- Existing TR subproblem solver $\texttt{OPT}$
- **Pre-Smoothing:** $T_{1,\ell}$ its. of $\texttt{OPT}$ to $\widehat{q}_{k,\ell}(s_{\ell+1} + s)$
- **Step Acceptence:** $\widehat{q}_{k,\ell+1}(s_\ell) \geq \eta\, \widehat{q}_{k,\ell}(s_\ell)$
- **Post-Smoothing:** $T_{2,\ell}$ its. of $\texttt{OPT}$ to $\widehat{q}_{k,\ell}(s_\ell + s)$

$\texttt{OPT}$ steps increase / satisfy FCD $\implies$ so do modifed MG/OPT steps.

Direct Field Acoustic Testing (DFAT)

Larkin and Whalen

- **Physical Domain:** $D = (-5,5)^2$
- **Parameter Space:** $\Xi = [-\sqrt{3}, \sqrt{3}]^M$
- **Probability Measure:**
  $\rho(\xi)\mathrm{d}\xi = \left(2\sqrt{3}\right)^{-M}\mathrm{d}\xi$
- **Stochastic Material:** $\epsilon(\xi, x)$
  KL expansion of Matérn covariance
- **Desired State:** $\theta = \frac{\pi}{4}$, $k = 10$
  $\bar{w}(x) = \exp\left(i\left((k\cos\theta)x_1 + (k\sin\theta)x_2\right)\right)$



Let $\alpha > 0$ and $\vartheta = 0.1$. Consider the optimal control problem

$$\min_{z\in L^2(D;\mathbb{C})} \frac{1}{2}\sigma\left[\int_{D_R}(u(z;\xi,x)-\bar{w}(x))\overline{(u(z;\xi,x)-\bar{w}(x))}\,\mathrm{d}x\right] + \frac{\alpha}{2}\int_{D_c} z(x)\overline{z(x)}\,\mathrm{d}x$$

where $u = u(z) \in L^2_\rho(\Xi; H^1(D;\mathbb{C}))$ solves

$$\begin{aligned} -\Delta u(\xi,x) - k^2(1+\vartheta\epsilon(\xi,x))^2 u(\xi,x) &= z(x) & \forall\ (\xi,x) \in \Xi\times D \\ \frac{\partial u}{\partial n}(\xi,x) &= iku(\xi,x) & \forall\ (\xi,x)\in \Xi\times\partial D. \end{aligned}$$

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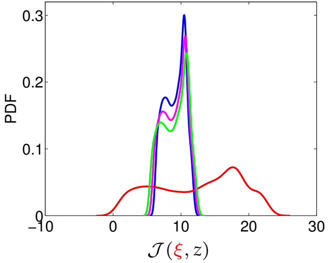
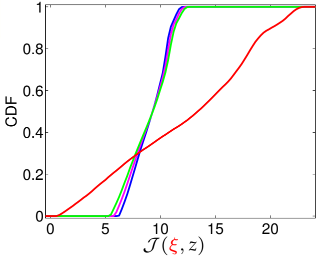
Results: $M = 6$, $\gamma = 5$, and $\alpha = 10^{-4}$

$$\mathcal{J}(\xi, z) = \int_{D_R} (u(z;\xi,x) - \bar{w}(x))\overline{(u(z;\xi,x) - \bar{w}(x))}\,\mathrm{d}x.$$



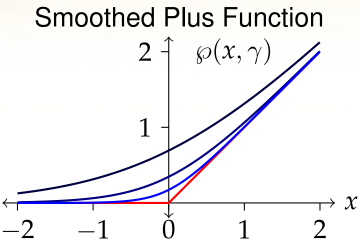


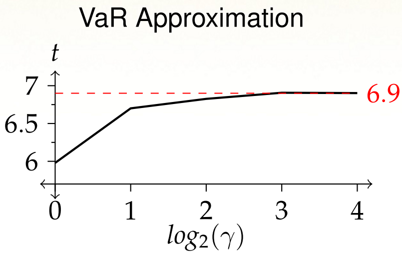
- Mean value: $\xi \leftarrow \mathbb{E}[\xi]$
- Mean plus CVaR: $\sigma[X] = \frac{1}{2}\mathbb{E}[X] + \frac{1}{2}\mathrm{CVaR}_{0.1}[X]$
- Risk neutral: $\sigma[X] = \mathbb{E}[X]$
- CVaR: $\sigma[X] = \mathrm{CVaR}_{0.1}[X]$

Mean plus CVaR Value-at-Risk: $t = 6.59073$

CVaR Value-at-Risk: $t = 6.90629$

Results: The Effect of Smoothing - CVaR





γ	$\|z\|_{\mathcal{Z}}$	Abs. Err.	Rate	t	Abs. Err.	Rate
1	37.8369	-	-	5.9792	-	-
2	37.0495	1.2177	-	6.7004	0.7212	-
4	36.7416	0.7111	0.7760	6.8258	0.1254	2.5239
8	36.6653	0.4396	0.6939	6.9066	0.0808	0.6341

Theoretical convergence rate is $\frac{1}{2}$ (Kouri and Surowiec).

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Results: Risk Neutral

$\alpha = 10^{-4}$

dim	Algorithm	PDE Solves	CP_{grad}	CP_{obj}
20	Grad. Adapt. TR	1,136,784	1,405	120,401
	Obj. Adapt. TR	122,331	1,509	2,933
40	Grad. Adapt. TR	16,327,120	1,445	1,804,001
	Obj. Adapt. TR	128,051	1,549	2,973

Table : Computational cost of the classical trust-region algorithm applied to the Helmholtz example with $M \in \{20, 40\}$ and $\alpha = 10^{-4}$.

$\alpha = 10^{-6}$

dim	Algorithm	PDE Solves	CP_{grad}	CP_{obj}
40	Obj. Adapt. TR	234,411	1,549	1,525
	Mod. MG/OPT	139,039	1,565	2,657

Table : Computational cost of the classical trust-region algorithm applied to the Helmholtz example with $M = 40$ and $\alpha = 10^{-6}$.

Conclusions:

- Objective function and derivative computations are ***expensive***
- Use trust regions to guide sparse-grid adaptivity
- Exploit sparse-grid hierarchy to accelerate TR subproblem solves
- Solve control problem at costs comparable to forward PDE solve of a fixed high-fidelity sparse grid

Future Work:

- **CVaR constraints** to shape the distribution and control *rare events* (Shapiro, Uryasev, Rockafellar, ...)
- **Ambiguous stochastic programming** to incorporate *data* (Shapiro, Bertsimas, Bayraksan, ...)

$$\min_{z \in \mathcal{Z}} \sup_{P \in \mathcal{M}_0} \int_{\Xi} f(u(z;\xi), z, \xi)\, \mathrm{d}P(\xi)$$

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