

Optimal control of systems governed by PDEs with uncertain parameters

Three examples

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Outline

Optimal control under uncertainty

Example I: Coil optimization for magnetic confinement

Example II: Porous medium flow

Example III: Sparse stochastic optimal control

Optimal control under uncertainty

PDE-constrained control objective

$$J(y(u, m))$$

where

$$\mathcal{A}(y, m) = f(u)$$

- ▶ $J(\cdot)$: control objective
- ▶ \mathcal{A} : forward (PDE) operator
- ▶ y : state variable
- ▶ m : uncertain parameter (field)
- ▶ u : control function

Two main formulations:

1. *Deterministic control*: One u for all m
2. *Stochastic control*: $u = u(m)$ depends on m

Optimal control under uncertainty

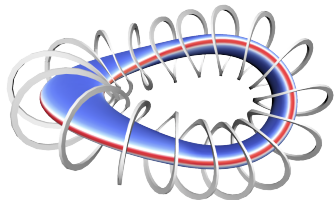
Deterministic control case

$$\min_u E_m \{J(y(u, m))\} + R(y, u, m)$$

where

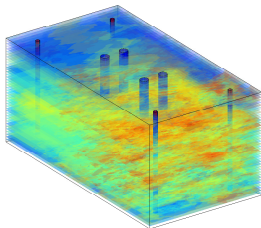
$$\mathcal{A}(y, m) = f(u)$$

Example I: Design of magnetic coils for plasma confinement in fusion



- ▶ One control for all m
- ▶ May include risk measure $R(\cdot)$ (e.g., variance or CVaR)
- ▶ Challenges: Integration over high-dimensional m , PDE forward model

Example II: Optimal fluid insertion in subsurface with uncertain permeability



Optimal control under uncertainty

Stochastic/Adjustable control case

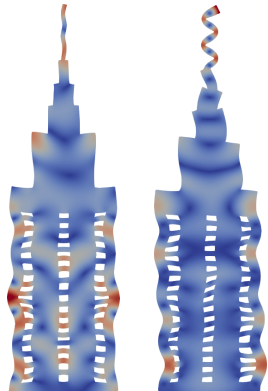
$$\min_{u(m)} J(y(u, m)) + Q(y, u, m)$$

where

$$\mathcal{A}(y, m) = f(u)$$

- ▶ Control u depends on m
- ▶ Includes coupling term $Q()$ for distribution (e.g., $\text{Var}_m(y)$ or joint support term for u)
- ▶ Challenges: Many coupled PDE forward problems, dimension of uncertain parameters

Example III: Optimal placement of active dampers for uncertain vibration/earthquake forces



(Incomplete) literature for PDE-constrained OUU

- ▶ Schulz & Schillings, *Problem formulations and treatment of uncertainties in aerodynamic design*, AIAA J, 2009.
- ▶ Borzi & von Winckel, *A POD framework to determine robust controls in PDE optimization*, Computing and Visualization in Science, 2011.
- ▶ Gunzburger & Ming, *Optimal control of stochastic flow over a backward-facing step using reduced-order modeling*, SISC 2011.
- ▶ Gunzburger, Lee, & Lee, *Error estimates of stochastic optimal Neumann boundary control problems*, SINUM, 2011.
- ▶ Kunoth & Schwab, *Analytic Regularity and GPC Approximation for Control Problems Constrained by Linear Parametric Elliptic and Parabolic PDEs*, SICON, 2013.
- ▶ Tiesler, Kirby, Xiu, & Preusser, *Stochastic collocation for optimal control problems with stochastic PDE constraints*, SICON, 2012.
- ▶ Kouri, Heinkenschloss, Ridzal, & Van Bloemen Waanders, *A trust-region algorithm with adaptive stochastic collocation for PDE optimization under uncertainty*, SISC, 2013.
- ▶ Chen, Quarteroni, & Rozza, *Stochastic optimal Robin boundary control problems of advection-dominated elliptic equations*, SINUM, 2013.
- ▶ Kouri, *A multilevel stochastic collocation algorithm for optimization of PDEs with uncertain coefficients*, JUQ, 2014.
- ▶ Chen, Quarteroni, & Rozza, *Multilevel and weighted reduced basis method for stochastic optimal control problems constrained by Stokes equations*, Num. Math. 2015.
- ▶ Kouri & Surowiec, *Risk-averse PDE-constrained optimization using the conditional value-at-risk*, SIOPT, 2016.

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Fusion: Tokamaks and Stellarators

with: A. Giuliani, F. Wechsung, A. Cerfon, M. Landreman; funded by Simons Foundation

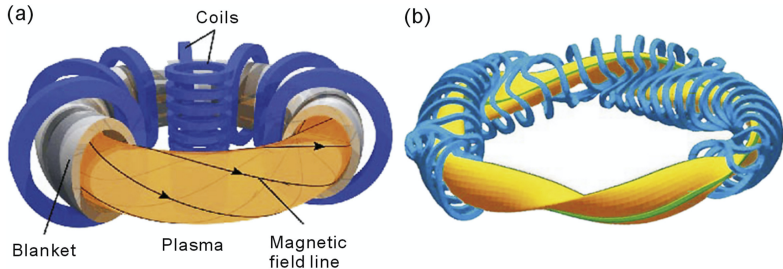


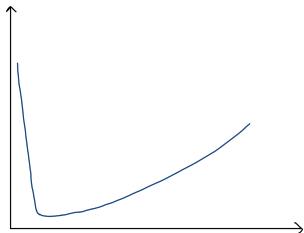
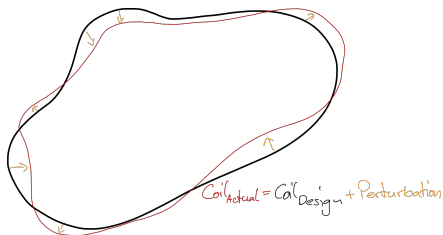
Figure: a) A tokamak creates rotational transform (RT) by running current through the plasma. b) A stellarator creates RT by *twisting* the magnetic field. [Figure: Xu]

- ▶ Tokamak: how do we deal with MHD instabilities triggered by the current in the plasma?
- ▶ Stellarator: how do we design coils to create a field with appropriate rotational transform and particle confinement?
- ▶ W7-X youtube video

Coil errors — motivation

Problem

In practice, we can not precisely build the coils we designed.



Conclusion

We have to find minima that are robust to small perturbations of the design.

National Compact Stellarator Experiment (NCSX)

The assembly tolerances were very tight and required state of the art use of metrology systems [...] \$50 million of additional funding was needed [...] The required tolerances could not be achieved; As the modules were assembled, parts were found to be in contact, would sag once installed, and other unexpected effects made alignment very difficult.[...] Fixes were worked into the design, but each one further delayed the completion and required more funding.[...] when the goal was not met on budget, the project was cancelled.

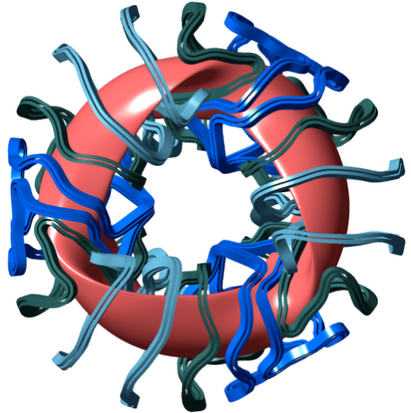


Figure: NCSX Stellarator [Figure: wiki].

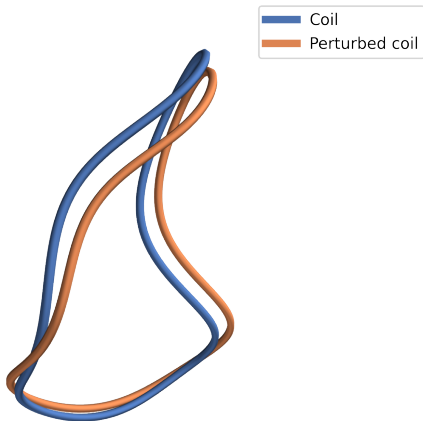


Figure: We model coil errors m with a Gaussian process.

Now take a function that maps a control u and a random variable m to a quantity of interest:

$$(u, m) \mapsto f(u, m)$$

- Deterministic

$$\min_u f(u, 0)$$

- Risk-Neutral

$$\min_u \mathbb{E}_m[f(u, m)]$$

- Robust

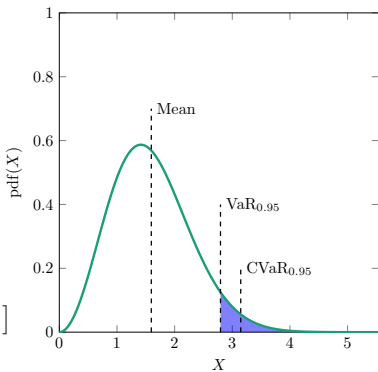
$$\min_u \max_m f(u, m)$$

- Risk-Averse, e.g.

$$\min_u \mathbb{E}[f(u, m)] + \gamma \text{Var}[f(u, m)]$$

$$\min_u \text{VaR}_\alpha[f(u, m)]$$

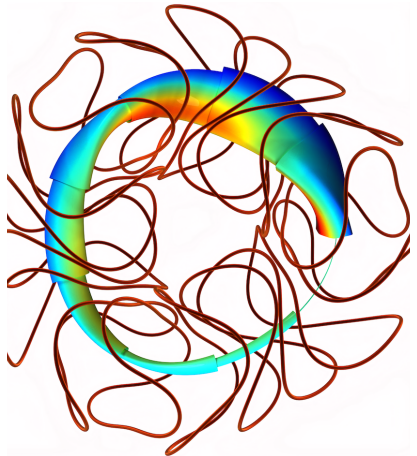
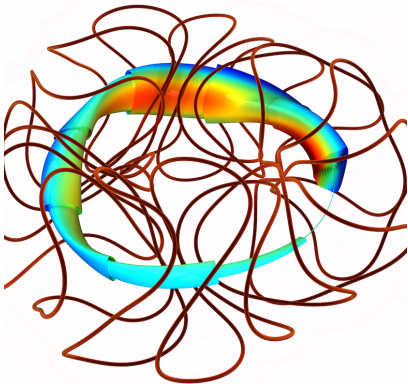
$$\min_u \text{CVaR}_\alpha[f(u, m)]$$



- Using Monte Carlo sampling, the optimisation problem becomes

$$\min_u \mathbb{E}_m[f(u, m)] \approx \min_u \frac{1}{N} \sum_{k=1}^{N_{\text{MC}}} f(u, m^{(k)}).$$

Typical coils:



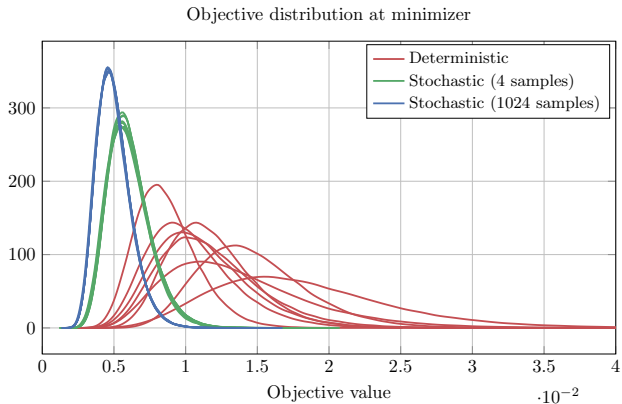


Figure: Distribution of the objective value evaluated at minimizers for 8 different initial guesses.

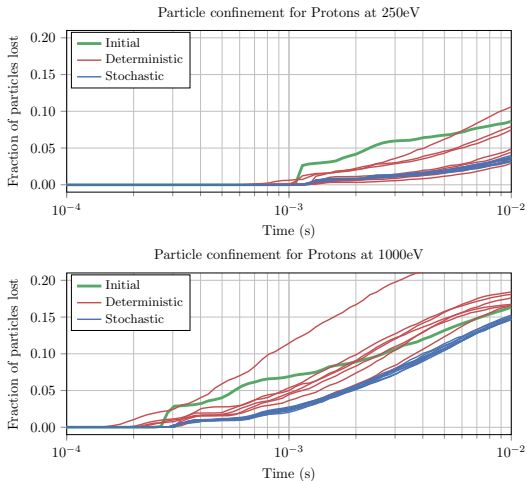


Figure: Particle losses over time for protons spawned on axis at 250eV and 1000eV for perturbations of configurations obtained from stochastic and deterministic optimization.

Outline

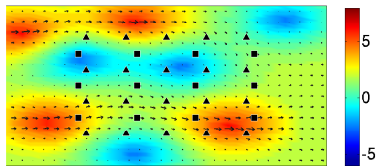
Optimal control under uncertainty

Example I: Coil optimization for magnetic confinement

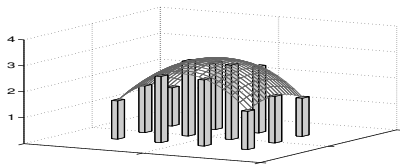
Example II: Porous medium flow

Example III: Sparse stochastic optimal control

Deterministic control: Injection in a porous medium flow



\bar{m} = mean of log permeability field



- State PDE: single phase flow in a porous medium

$$-\nabla \cdot (\exp(\mathbf{m}) \nabla y) = \sum_i \mathbf{u}_i f_i(\vec{x})$$

with Dirichlet lateral & Neumann top/bottom BCs

- Uncertain parameter: log permeability field \mathbf{m}
- Controls: \mathbf{u}_i , mass source at wells; f_i , mollified Dirac deltas
- Objective: $J(\mathbf{u}, \mathbf{m}) := \frac{1}{2} \|y(\mathbf{u}, \mathbf{m}) - y_d\|^2$, y_d ... target

Porous medium with random permeability field

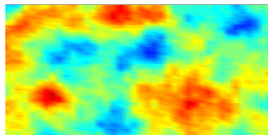
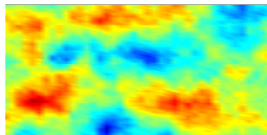
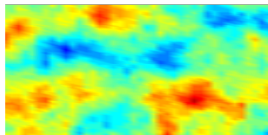
- ▶ Law of m :

$$\mu = \mathcal{N}(\bar{m}, \mathcal{C}) \quad (\text{Gaussian measure on Hilbert space } L_2)$$

- ▶ Take covariance operator as square of inverse of Poisson-like operator:

$$\mathcal{C} = (-\kappa\Delta + \alpha I)^{-2} \quad \kappa, \alpha > 0$$

- ▶ \mathcal{C} is positive, self-adjoint, of trace-class; μ well-defined on L_2 (Stuart '10)
- ▶ $\frac{\kappa}{\alpha} \propto$ correlation length; the larger α , the smaller the variance



Random draws for $\kappa = 2 \times 10^{-2}$, $\alpha = 4$

O UU with quadratic approximation of J

- ▶ Risk-averse optimal control problem (including cost of controls)

$$\min_u \mathbb{E}_m \{ J(u, m) \} + \beta \text{Var}_m \{ J(u, m) \} + \gamma \|u\|^2$$

- ▶ Quadratic approximation to parameter-to-objective map

$$\begin{aligned} J_{\text{quad}}(u, m) &= J(u, \bar{m}) + \langle g_m(u, \bar{m}), m - \bar{m} \rangle \\ &\quad + \frac{1}{2} \langle H_m(u, \bar{m})(m - \bar{m}), m - \bar{m} \rangle \end{aligned}$$

- ▶ g_m and H_m are the gradient of J with respect to m

O UU with quadratic approximation of J

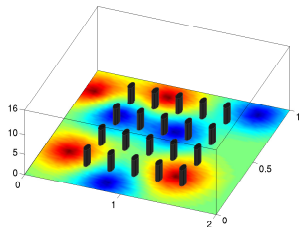
Observations:

- ▶ Expansion does not lead to a quadratic control objective
- ▶ However, can derive analytic formulas for the moments of J_{quad} in the infinite-dimensional Hilbert space setting.

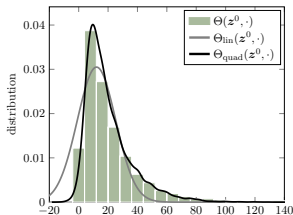
These expressions involve:

- ▶ Matrix/operator traces
- ▶ For PDE-constrained O UU, their approximation requires repeated forward and adjoint PDE solves

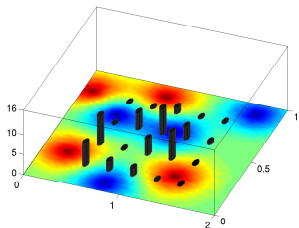
Risk-averse optimal control with quadratized objective



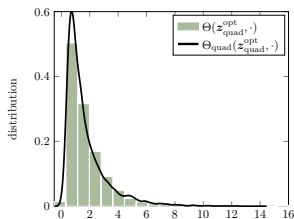
initial (suboptimal) control u^0



distrib. of exact & approx objectives at u^0



optimal control $u_{\text{quad}}^{\text{opt}}$ based on J_{quad}



distrib. of exact & approx objectives at $u_{\text{quad}}^{\text{opt}}$

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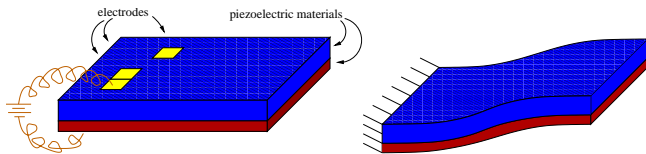
Example III: Sparse stochastic optimal control

Sparse distributed control

with C. Li

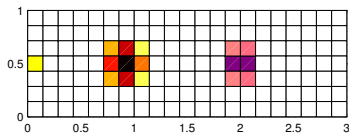
Optimal actuator placement problem:

Place (few) electrodes optimal to achieve desired displacement



Approach III: Optimal control with L^1 cost

- + Continuous, efficient solution, (sub-)optimal
- (-) might need several tries to find desired structure



Elliptic sparse optimal control

Minimize over $(y, u) \in H_0^1(\Omega) \times L^2(\Omega)$:

$$\min_{y,u} \frac{1}{2} \int_{\Omega} |y - y_d|^2 + \alpha |u|^2 dx + \beta \int_{\Omega} |u| dx$$

subject to $Ay = u + f \in \Omega$,

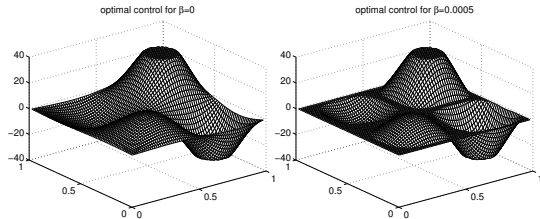
$$a \leq u \leq b \text{ a. e. in } \Omega$$

Numerical solution:

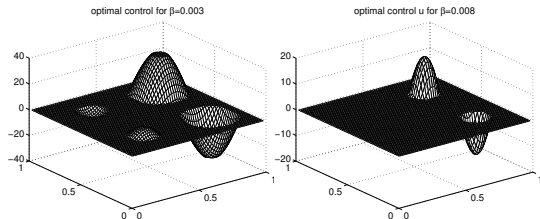
- ▶ That's a nonsmooth and inequality-constraint optimization problem.
- ▶ However, the problem can be reformulated using Lagrange multipliers.
- ▶ Thus, we can use a (discretized) function-space Newton-type algorithms for its solution.

Sparsening effect of L^1 -regularization

Optimal controls for changing β :



Solutions for $\beta = 0$ and
 $\beta = 0.0005$



Solutions for $\beta = 0.003$
 $\beta = 0.008$

Optimal control governed by PDEs

Sparse Control under uncertainty

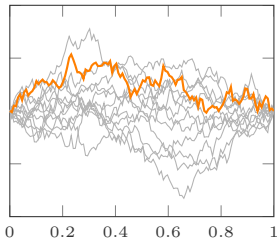
Let $\mathcal{D} \subset \mathbb{R}^n$, $n \leq 3$ bounded, $A : H^1(\mathcal{D}) \rightarrow H^{-1}(\mathcal{D})$ invertible, f, y^d given, $\alpha > 0$.

$$\min_{y(\omega), u(\omega)} \frac{1}{2} \int_{\Omega} \int_{\mathcal{D}} |y(\omega) - y^d|^2 + \alpha |u(\omega)|^2 dx d\mu + \beta \int_{\mathcal{D}} \left[\int_{\Omega} |u(\omega)|^2 d\mu \right]^{1/2} dx$$

subject to

$$Ay(\omega) = u(\omega) + f + Bm(\omega)$$

- ▶ $u \in U_{\text{ad}} \subset L^2(\mathcal{D})$... control
- ▶ $y \in Y \subset H^1(\mathcal{D})$ state.
- ▶ Interpretation for placement of controllers, $\beta > 0$.
- ▶ $m = m(\omega) \in \mathcal{H}$ random variable over Ω , law μ , $B : \mathcal{H} \mapsto H^{-1}(\mathcal{D})$.



Sparse stochastic control under uncertainty

$$\min_{y(\omega), u(\omega)} \frac{1}{2} \int_{\Omega} \int_{\mathcal{D}} |y(\omega) - y^d|^2 + \alpha |u(\omega)|^2 dx d\mu + \beta \int_{\mathcal{D}} \left[\int_{\Omega} |u(\omega)|^2 d\mu \right]^{1/2} dx$$

subject to

$$Ay(\omega) = u(\omega) + f + Bm(\omega).$$

Observations:

- ▶ Control $u(\omega)$ depends on $\omega \in \Omega$. . . stochastic optimal control.
- ▶ Problems for different ω are coupled through **sparsity term**
- ▶ All controls have the same sparsity pattern—place controllers where $u(\omega) \neq 0$ (independent from ω)
- ▶ Two stage problem: Decide on controller placement (offline) and compute optimal control (online).

Sparse stochastic control under uncertainty

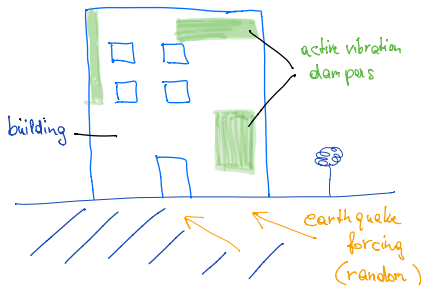
$$\min_{y(\omega), u(\omega)} \frac{1}{2} \int_{\Omega} \int_{\mathcal{D}} |y(\omega) - y^d|^2 + \alpha |u(\omega)|^2 dx d\mu + \beta \int_{\mathcal{D}} \left[\int_{\Omega} |u(\omega)|^2 d\mu \right]^{1/2} dx$$

subject to

$$Ay(\omega) = u(\omega) + f + Bm(\omega).$$

Application:

- ▶ Place active (e.g., piezoelectric) dampers
- ▶ Placement optimal for range of earthquakes
- ▶ For each earthquake forcing $\omega \in \Omega$, control computed in real time



Sparse stochastic control under uncertainty

$$\min_{y(\omega), u(\omega)} \frac{1}{2} \int_{\Omega} \int_{\mathcal{D}} |y(\omega) - y^d|^2 + \alpha |u(\omega)|^2 dx d\mu + \beta \int_{\mathcal{D}} \left[\int_{\Omega} |u(\omega)|^2 d\mu \right]^{1/2} dx$$

subject to

$$Ay(\omega) = u(\omega) + f + Bm(\omega).$$

Mathematical structure

- ▶ **Nondifferentiable L_1/L_2 -type sparse** optimal control problem
 - ▶ Literature: Borzi, Casas, Clason, Herzog, Ito, Kunisch, S., Pieper, Rozza, Troltsch, Vexler, Wachsmuth D, Zuazua, ...
- ▶ **High-dimensional:** physical space ($\mathcal{D}, n \leq 3$) and random space Ω , possibly infinite-dimensional.
 - ▶ Literature: Alexanderian, Borzi, Chen, Ghattas, Heinkenschloss, Kouri, Quarteroni, Ridzal, Rozza, Schulz, Surowiec, Ulbrich M, Ullmann, Xiu, ...

Existence, uniqueness and optimality conditions

Notation: $\|u\|_{\Omega}(x) = \left(\int_{\Omega} u(\omega, x)^2 d\mu\right)^{1/2}$

$$\min_{a \leq u(\omega) \leq b} \frac{1}{2} \int_{\Omega} \int_{\mathcal{D}} |y(\omega) - y^d|^2 + \alpha |u(\omega)|^2 dx d\mu + \beta \int_{\mathcal{D}} \|u\|_{\Omega}(x) dx$$

Theorem: This problem has a unique solution $\bar{u}(\omega)$, characterized by the existence of $\bar{y}(\omega) \in Y$, $\bar{p}(\omega) \in Y$ and $\bar{\lambda}(\omega)$ such that

$$A\bar{y} - \bar{u} - f - Bm = 0,$$

$$A^*\bar{p} - y_d + \bar{y} = 0,$$

$$-\bar{p} + \alpha\bar{u} + \beta\bar{\lambda} + \bar{\mu} = 0,$$

$$\bar{\lambda}(\omega, x) = \frac{\bar{u}(\omega, x)}{\|\bar{u}\|_{\Omega}(x)} \text{ if } \|\bar{u}\|_{\Omega}(x) \neq 0, \text{ or } \|\bar{\lambda}\|_{\Omega}(x) \leq 1 \text{ if } \|\bar{u}\|_{\Omega}(x) = 0$$

$$\bar{\mu} \leq 0 \text{ if } \bar{u} = a, \quad \bar{\mu} \geq 0 \text{ if } \bar{u} = b \quad \text{and} \quad \bar{\mu} = 0 \text{ if } a \leq \bar{u} \leq b.$$

Norm reweighting formulation (IRLS)

Main challenges:

- ▶ All variables defined over physical and random space, e.g., $u = u = u(x, \omega)$.
- ▶ Avoid approximation of random space, try to use Gaussians if possible

Assumptions/limitations:

- ▶ Neglect bound constraints on u
- ▶ Distribution of m is Gaussian, linearity
- ▶ $\alpha > 0$ for regularity and model reduction

Iteratively reweighted least squares (IRLS) algorithm: Classical algorithm; recent finite-dimensional analysis by Daubechies, DeVore, Fornasier, Güntürk, Rauhut, . . .)

Iterates over weight function ν that only depends on x

Norm reweighting formulation

Basic idea: \bar{u} minimizer of

$$\min_{u(\omega)} Q(u, m) + \beta \int_{\mathcal{D}} \left(\|u\|_{\Omega}^2(x) + \varepsilon^2 \right)^{1/2} dx$$

iff it minimizes the quadratic problem

$$\min_{u(\omega)} Q(u, m) + \beta \int_{\mathcal{D}} \nu \left(\|u\|_{\Omega}^2(x) + \varepsilon^2 \right) dx \quad (1)$$

with

$$\nu(x) = \left(\|\bar{u}\|_{\Omega}^2(x) + \varepsilon^2 \right)^{-1/2}. \quad (2)$$

This leads to a **reweighting algorithm**, iterates over $\nu = \nu(x)$ only:

- 1: Initialize $\nu^0 : \mathcal{D} \rightarrow \mathbb{R}$. For $k = 0, 1 \dots$
- 2: Solve (1) with $\nu = \nu^k$.
- 3: Compute ν^{k+1} from (2) and iterate.

Norm reweighting formulation

Theorem: The iterates ν^k satisfy for a non-increasing sequence ε^k :

- ▶ All $u^k = u^k(x, \omega)$ are Gaussian
- ▶ The costs functionals $J(u^k, \nu^k)$ are monotonously decreasing
- ▶ If $\varepsilon^k \rightarrow \bar{\varepsilon} > 0$, then $u^k \rightarrow u_{\bar{\varepsilon}}$ strongly in $L^2(\mathcal{D} \times \Omega)$.

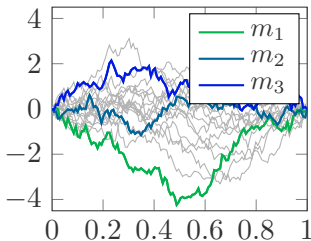
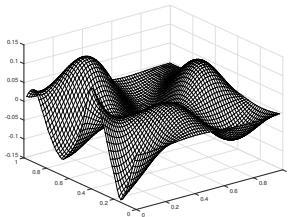
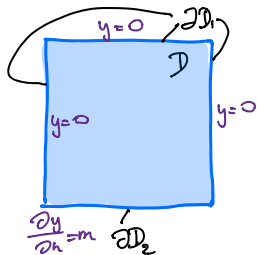
Computing $u = u(x, \omega)$ is still difficult (due to the high dimension!)

- ▶ Compute an upfront low-rank approximation (using a rand-SVD) of $A^{-*}A^{-1}$, where the truncation depends on α and the error can be controlled (r basis vectors, $r = O(100)$). Similar to POD/reduced basis method.
- ▶ After this computation, each reweighting step amounts to $O(r)$ inner products and matrix operations of size $r \times r$.

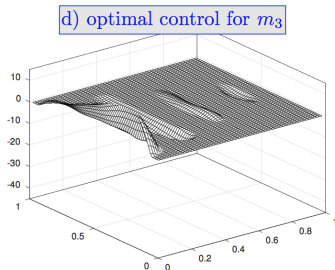
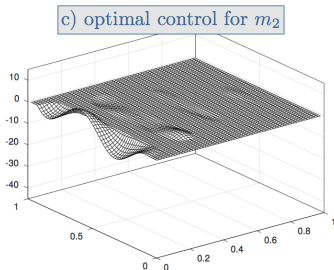
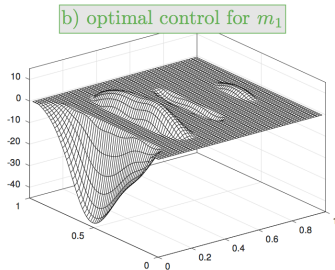
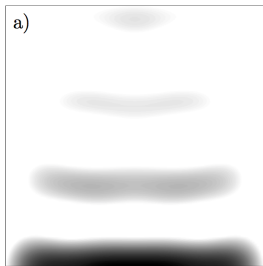
Reweighting is still a slow algorithm (sublinear convergence), but we've a Newton variant of the algorithm that is fast.

Helmholtz equation example

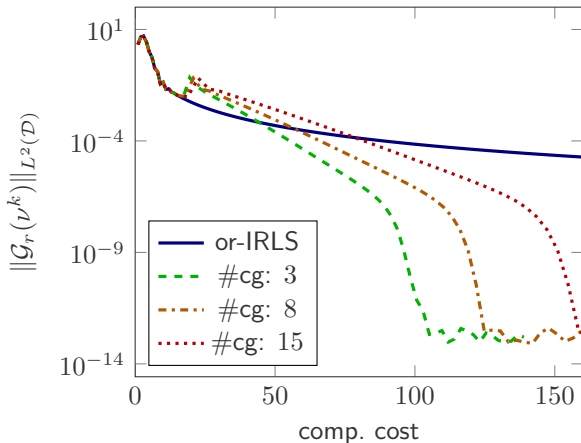
- ▶ $A = -\Delta - \kappa^2 I$, $\kappa = 12 \dots$ indefinite Helmholtz operator
- ▶ Optimization problem is convex
- ▶ Other data: $y_d = 0$, $f \equiv 0$, $\alpha = 5 \times 10^{-5}$ and $\beta = 5 \times 10^{-4}$.
- ▶ Shown below are solution of the Helmholtz equation with boundary forcing only and trajectories of three different random draws



Helmholtz equation example



Preconditioned inexact Newton-CG reweighting



Comparison of performance of or-IRLS and preconditioned Newton-CG (NIRLS) for different numbers of CG iterations per Newton step, $n = 128$, $\varepsilon = 10^{-7}$.

Summary, Discussion, Outlook

Summary

- ▶ Optimization under uncertainty for PDE problem
- ▶ Deterministic control:
 - ▶ Taylor expansion in uncertain parameter
 - ▶ Alternatives: MC sampling, sparse grids, etc
- ▶ Stochastic control:
 - ▶ Sparsification for controller placement
 - ▶ Reduction to algorithms over spatial variable only
 - ▶ Low rank approximations necessary

Main references:

F. Wechsung, A. Giuliani, M. Landreman, A. Cerfon, G. Stadler: Single-stage gradient-based stellarator coil design: stochastic optimization, 2021, arXiv:2106.12137

A. Alexanderian, N. Petra, G. Stadler, O. Ghattas: *Mean-variance risk-averse optimal control of systems governed by PDEs with random parameter fields using quadratic approximations*, SIUQ, 2017.

C. Li, G. Stadler: *Sparse solutions in optimal control of PDEs with uncertain parameters: the linear case*, SICON, 2020, arXiv:1804.05678