Tutorial I PDE-Constrained Optimization Under Uncertainty

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- PDE-constrained optimization arises in many engineering and science applications.
- Important task in digital-twins.





Reservoir management





(Thanks to Drew Kouri, Sandia National Labs)

Direct field acoustic testing



PDE-Constrained Optimization

- Physics, ... described by systems of partial differential equations.
- Uncertainties in system.
- Optimization problems difficult to formulate and expensive to solve
 - Modeling of optimization problem (what is the objective, what are the controls, what physics need to be included, what is the decision time horizon,...)
 - Infinite dimensional problem structure impacts solution f discretized problem.
 - Expensive simulation.
 - ▶ Many control/design variables → derivative based methods
 - Optimize across all realizations of uncertainties in coefficients.
- Applications to design, control, parameter identification.
- Important task in digital twins.
- (First part of) Tutorial based on upcoming paper [Heinkenschloss and Kouri, 2025].

Outline

Examples

Elliptic Optimal Control Problem Optimal Control of Navier-Stokes Topology Optimization

Elliptic Model Problem

Elliptic Model Problems Elliptic Model Problem - Well-Posedness Elliptic Model Problem - Discretization

Elliptic Optimal Control Problem

- ▶ $D = (0, 1) \times (0, 1)$, control boundary $\partial D_c = \{0\} \times [0, 1]$ and Neumann boundary $\partial D_n = \partial D \setminus \partial D_c$.
- Given parameterized coefficient functions

$$\kappa(x,\xi) = \begin{cases} \xi^{(1)}, & x \in [0,1] \times [0,0.6), \\ \xi^{(2)}, & x \in [0,1] \times [0.6,1], \end{cases} \quad c(x) = \begin{pmatrix} 1\\ \xi^{(3)} \end{pmatrix}, \\ f(x,\xi) = 20 \exp\left(-\frac{(x_1 - \xi^{(4)})^2}{0.1}\right) \exp\left(-\frac{(x_2 - \xi^{(5)})^2}{0.1}\right) \end{cases}$$

with
$$\xi = (\xi^{(1)}, \xi^{(2)}, \xi^{(3)}, \xi^{(4)}, \xi^{(5)})^{\top}$$

Consider the linear elliptic PDE

$$\begin{split} -\nabla \cdot \left(\kappa(x,\xi)\nabla y(x,\xi)\right) + c(x,\xi) \cdot \nabla y(x,\xi) &= f(x,\xi), \qquad x \in D, \\ y(x,\xi) &= u(x), \qquad x \in \partial D_c, \\ \left(\kappa(x,\xi)\nabla y(x,\xi)\right) \cdot n(x) &= 0, \qquad x \in \partial D_n. \end{split}$$

Initially set

$$\xi^{(1)} = 0.3, \quad \xi^{(2)} = 0.8, \quad \xi^{(3)} = 0.1, \quad \xi^{(4)} = 0.25, \quad \xi^{(5)} = 0.45$$

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No-control (u = 0) PDE solution y and slices y(x₁, x₂) of solution at x₂ = 0.4, 0.5, 0.6.



▶ Want control $u \in H^1(\partial D_c)$ such that PDE solution $y(u; \cdot, \xi)$ ideally is below a target, here 1, in obs. region $D_o = [0.4, 0.6] \times [0.4, 0.6]$.

Optimal control problem

$$\min_{u \in H^1(\partial D_c)} \frac{1}{2} \int_{D_o} \left(y(u; x, \xi) - 1 \right)_+^2 \mathsf{d}x + \frac{10^{-2}}{2} \|u\|_{H^1(\partial D_c)}^2, \quad (1)$$

where $y(u; \cdot, \xi)$ is the PDE solution given u and ξ . $z_+ = \max\{z, 0\}$.

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• Optimal state $y(u_*; \cdot, \xi)$



- Improves performance a lot at given parameter, but
- What if optimal control is applied with different parameters ξ?
- ▶ Interested in case where params. are not deterministic but are a realization of random variable (r.v.) $\boldsymbol{\xi} = (\boldsymbol{\xi}^{(1)}, \boldsymbol{\xi}^{(2)}, \boldsymbol{\xi}^{(3)}, \boldsymbol{\xi}^{(4)}, \boldsymbol{\xi}^{(5)})^{\top}$,

$$\begin{split} \boldsymbol{\xi}^{(1)} &\sim U(0.2, 0.4), \quad \boldsymbol{\xi}^{(2)} \sim U(0.7, 0.9), \quad \boldsymbol{\xi}^{(3)} \sim U(0.0, 0.2), \\ \boldsymbol{\xi}^{(4)} &\sim U(0.1, 0.4), \quad \boldsymbol{\xi}^{(5)} \sim U(0.3, 0.6). \end{split}$$





- What if optimal control is applied with different parameters ξ?
- Select 10 samples ξ_i of $\boldsymbol{\xi}$, compute $y(u_*; \cdot, \xi_i)$.
- Optimal control computed with fixed ξ can perform poorly if applied with different parameter values.
- Incorporate randomness in params. into computation of control.
- Interested in one control that is applied to all possible outcomes of *ξ*. Must decide on control before uncertainty is revealed.



• Given a control $u \in H^1(\partial D_c)$, consider objective function

$$\frac{1}{2} \int_{D_o} \left(y(u; x, \xi) - 1 \right)_+^2 \mathsf{d}x + \frac{10^{-2}}{2} \|u\|_{H^1(\partial D_c)}^2, \tag{2}$$

where $y(u; \cdot, \xi)$ solves PDE for $\xi \in \Xi$.

▶ Want control u that makes (2) small in some sense for all $\xi \in \Xi$.

▶ (2) is a function in $\xi \in \Xi$, need to quantify its size.

One possibility is to take its expected value.:

$$\min_{u \in H^1(\partial D_c)} \int_{\Xi} \rho(\xi) \left[\frac{1}{2} \int_{D_o} \left(y(u; x, \xi) - 1 \right)_+^2 \mathsf{d}x \right] \mathsf{d}\xi + \frac{10^{-2}}{2} \|u\|_{H^1(\partial D_c)}^2.$$

- Compute control u_* as solution of expected value min. problem.
- Compute corresponding state y(u_{*}; x₁, x₂, ξ) at same 10 samples of ξ used before.
- Results in



- Samples y(u_{*}; ·, ξ) of the corresponding state can be significantly larger than target.
- Expected value minimization problem is called risk-neutral problem.

- It may be more harmful if y(u; ·, ξ) exceeds the target by a lot, than if y(u; ·, ξ) barely exceeds the target.
- Minimize (in some sense) $(1 \beta) \times 100\%$ of worst cases.
- Quantified using the average value-at-risk (AVaR).
- For a r.v. $X \in L^1$ and confidence level $\beta \in (0, 1)$,

$$\mathsf{AVaR}_{\beta}(X) := \min_{t \in \mathbb{R}} \left\{ t + \frac{1}{1-\beta} \mathbb{E}[\max\{0, X-t\}] \right\}.$$

For continuous r.vs. X, AVaR_β(X) is average of (1 − β) × 100% largest outcomes of X. Provides measure of distribution tail weight



Set $\beta=0.95,$ concerned with mitigating highest 5% of outcomes.

Risk-averse AVaR optimization problem

$$\min_{u \in H^1(\partial D_c)} \operatorname{AVaR}_{\beta} \left[\frac{1}{2} \int_{D_o} \left(y(u; x, \boldsymbol{\xi}) - 1 \right)_+^2 \mathrm{d}x \right] + \frac{10^{-2}}{2} \|u\|_{H^1(\partial D_c)}^2.$$

Solve AVaR problem. Evaluate solution of state equation with AVaR control at same 10 samples of ξ used before.





 Incorporating uncertainties in parameters into computation of control matters.

▶ Choice of problem formulation (risk-measure) application dependent.

Optimal Control of Boussinesq Flow Equations

Motivated by transport process in high pressure chemical vapor deposition (CVD) reactors



Optimal Control Problem

Boussinesq flow equations on this domain are

$$\begin{split} -\mu\Delta v + (v\cdot\nabla)v + \nabla p + \eta Tg &= 0, & \text{ in } D, \\ \nabla\cdot v &= 0, & \text{ in } D, \\ -\kappa\Delta T + v\cdot\nabla T &= 0, & \text{ in } D, \\ v - v_i &= 0, & T = 0, & \text{ on } \Gamma_i, \\ v - v_o &= 0, & \kappa\nabla T \cdot n = 0, & \text{ on } \Gamma_o, \\ v &= 0, & T - T_b &= 0, & \text{ on } \Gamma_b, \\ v &= 0, & \kappa\nabla T \cdot n + h(u - T) &= 0, & \text{ on } \Gamma_c, \end{split}$$

Re is Reynolds number, Gr is Grashof number, Pr is Prandtl number

$$\mu = \frac{1}{\text{Re}}, \quad \eta = \mu^2 \text{Gr}, \quad \text{and} \quad \kappa = \frac{\mu}{\text{Pr}}$$

- Re, Gr, and Pr random variables, uncertainty in h and T_b modeled using products of truncated KL. 53-dimensional random vector ξ.
- Optimal Control Problem

$$\min_{u\in\mathcal{U}}\ \mathcal{R}\left(\frac{1}{2}\int_D(\nabla\times v(u;\cdot,\pmb{\xi}))(x)\ \mathrm{d}x\right)+\frac{\alpha}{2}\int_{\Gamma_c}|u(x)|^2\ \mathrm{d}x,$$

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Optimal Control Results



• Entropic risk measure with $\sigma = 2$ used

$$\mathcal{R}(X) = \sigma^{-1} \log \mathbb{E}[\exp(\sigma X)], \quad \sigma > 0,$$

Risk-neutral and entropic risk significantly reduce the magnitude of the vorticity by approximately 2.3-fold.

Topology Optimization

 \blacktriangleright u material distribution. y displacement solve linear elasticity eqn.

$$\begin{aligned} -\nabla \cdot (\mathbf{E}(u):\varepsilon) &= f, & \text{in } D, \\ \varepsilon &= \frac{1}{2}(\nabla y + \nabla y^{\top}), & \text{in } D, \\ \varepsilon &n &= T, & \text{on } \Gamma_t, \\ y &= 0, & \text{on } \Gamma_d. \end{aligned}$$

• (f = 0) Traction force $(\boldsymbol{\xi} = (\boldsymbol{\xi}^{(1)}, \boldsymbol{\xi}^{(2)}, \boldsymbol{\xi}^{(3)}, \boldsymbol{\xi}^{(4)})$ uniformly distr.)

$$T(x,\xi) = \begin{cases} \left(\xi^{(1)}\cos(\xi^{(2)}),\xi^{(1)}\sin(\xi^{(2)})\right)^{\top}, & \text{if } x_1 \in [0,1/8] \text{ and } x_2 = 2, \\ \left(\xi^{(3)}\cos(\xi^{(4)}),\xi^{(3)}\sin(\xi^{(4)})\right)^{\top}, & \text{if } x_1 \in [7/8,1] \text{ and } x_2 = 2, \\ \left(0,0\right)^{\top}, & \text{otherwise.} \end{cases}$$

Optimization problem

$$\begin{split} \min_{u\in L^2(D)} \int_D f(x)\cdot y(u;x)\,\mathrm{d}x + \int_{\Gamma_t} T(x)\cdot y(u;x)\,\mathrm{d}x\\ \text{subject to} \quad \int_D u(x)\,\mathrm{d}x \leq v_0 |D|, \qquad 0\leq u\leq 1 \ \text{a.e.} \end{split}$$

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Topology Optimization Results



- Intuitively, deterministic design places material in direction of the single deterministic load given by mean 𝔼[𝔅] = (1, 270°, 1, 270°) of uncertain parameters 𝔅.
- Risk-neutral and risk-averse designs differ considerably from deterministic mean-value design, accounting for various loading scenarios modelled by traction load T(·, ξ).

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Elliptic Model Problems

Mathematical formulation of problem is foundation for reliable and efficient solution.

Discuss statement of and well-posedness results for elliptic model problems.

Begin with formal statement of two linear-quadratic elliptic optimal control problems.

Elliptic Model Problem - Deterministic

▶ Bounded domain $D \subset \mathbb{R}^n$ with boundary ∂D , given functions

$$f \in L^2(D), \ \kappa \in L^\infty(D),$$

such that

$$\kappa_{\max} \ge \kappa(x) \ge \kappa_{\min} > 0$$
 a.e. in D ,

and given $u \in L^2(D)$, consider the elliptic PDE

$$\begin{aligned} -\nabla\cdot(\kappa(x)\nabla y(x)) &= f(x) + u(x), & x \in D, \quad \text{(3a)} \\ y(x) &= 0, & x \in \partial D. \quad \text{(3b)} \end{aligned}$$

Want to find u ∈ L²(D) such that solution y(u; ·) of (3) is close to desired state ŷ a domain D_o ⊂ D in the L² sense.

Optimal control problem

$$\min_{u\in L^2(D)} \ \frac{1}{2} \int_{D_o} \left(y(u;x) - \widehat{y}(x)\right)^2 \mathsf{d}x + \frac{\alpha}{2} \int_D u(x)^2 \,\mathsf{d}x,$$

where $y(u; \cdot) \in H_0^1(D)$ is the solution of (3) given $u \in L^2(D)$.

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Elliptic Model Problem - Random

 $\blacktriangleright \ (\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space. State equation

$$-\nabla \cdot \left(\kappa(x,\omega)\nabla y(x,\omega)\right) = f(x,\omega) + u(x), \quad x \in D, \omega \in \Omega, \quad \text{(4a)} \\ y(x,\omega) = 0, \quad x \in \partial D, \omega \in \Omega, \quad \text{(4b)}$$

where $u \in L^2(D)$, $f \in L^2_{\mathbb{P}}(\Omega, L^2(D))$, $\kappa \in L^\infty_{\mathbb{P}}(\Omega, L^\infty(D))$, and there exist measurable functions κ_{\min} and κ_{\max} such that

 $\kappa_{\max}(\omega) \geq \kappa(x,\omega) \geq \kappa_{\min}(\omega) > 0, \quad x \in D, \text{a.a. } \omega \in \Omega.$

- Solution $\Omega \ni \omega \mapsto y(u; \omega; \cdot) \in H^1_0(D)$ of (4) is random field.
- Objective function

$$\Omega \ni \omega \mapsto \frac{1}{2} \int_{D_o} \left(y(u;\omega;x) - \widehat{y}(x) \right)^2 \mathrm{d}x + \frac{\alpha}{2} \int_D u(x)^2 \, \mathrm{d}x,$$

is random variable.

Risk neutral (expected value) optimal control problem

$$\min_{u \in L^2(D)} \int_{\Omega} \frac{1}{2} \int_{D_o} \left(y(u;\omega;x) - \widehat{y}(x) \right)^2 \mathrm{d}x \mathrm{d}\mathbb{P} + \frac{\alpha}{2} \int_D u(x)^2 \, \mathrm{d}x,$$

where $y(u;\omega;\cdot) \in H^1_0(D)$ is the solution of (4) given $u \in L^2(D)$.

Elliptic Model Problem - Determinstic

- Well-posedness of elliptic model problem.
- Literature: Books by [Lions, 1971], [Hinze et al., 2009], [Tröltzsch, 2010], [Manzoni et al., 2021].

State Equation

- Hilbert space \mathcal{U} is control space; Hilbert space \mathcal{V} is state space.
- Given a control $u \in U$, state $y \in V$ satisfies variational equation

$$a(y,\varphi) + b(u,\varphi) = \ell(\varphi) \quad \forall \varphi \in \mathcal{V},$$
(5)

where

▶ $a: \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ is a \mathcal{V} -coercive and continuous bilinear form, i.e., there exist $0 < a_{\min} \leq a_{\max}$ such that

 $a_{\min} \|y\|_{\mathcal{V}}^2 \leq a(y,y) \quad \text{ and } \quad |a(y,\varphi)| \leq a_{\max} \, \|y\|_{\mathcal{V}} \|\varphi\|_{\mathcal{V}} \quad \forall y,\varphi \in \mathcal{V},$

▶ $b: U \times V \to \mathbb{R}$ is a continuous bilinear form, i.e., there exists $0 < b_{\max}$ such that

 $|b(u,\varphi)| \le b_{\max} \|u\|_{\mathcal{U}} \|\varphi\|_{\mathcal{V}} \quad \forall u \in \mathcal{U}, \varphi \in \mathcal{V},$

• $\ell \in \mathcal{V}^*$ is a bounded linear form on \mathcal{V} .

By Lax-Milgram Theorem: For every u ∈ U, state equation (5) has a unique solution y(u) ∈ V with satisfies

$$\|y(u)\|_{\mathcal{V}} \le a_{\min}^{-1} \left(\|\ell\|_{\mathcal{V}^*} + b_{\max} \|u\|_{\mathcal{U}} \right) \quad \forall u \in \mathcal{U}.$$

State Equation (cont.)

Variational equation (5) equivalent to linear operator equation

$$Ay + Bu = \ell$$
 in \mathcal{V}^* ,

where $A \in \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ and $B \in \mathcal{L}(\mathcal{U}, \mathcal{V}^*)$ are defined by

$$\langle Ay, \varphi \rangle_{\mathcal{V}^*, \mathcal{V}} = a(y, \varphi), \quad \langle Bu, \varphi \rangle_{\mathcal{V}^*, \mathcal{V}} = b(u, \varphi) \quad \forall y, \varphi \in \mathcal{V}, u \in \mathcal{U}.$$

> Because a is \mathcal{V} -coercive, linear operator A is continuously invertible,

$$A^{-1} \in \mathcal{L}(\mathcal{V}^*, \mathcal{V}).$$

Optimal Control Problem

Consider quadratic objective functional

$$\frac{1}{2}q(y,y)+c(y)+\frac{1}{2}r(u,u),$$

where

▶ $q: \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ is symmetric, non-negative, continuous bilinear form, i.e., $q(y, \varphi) = q(\varphi, y)$ for all $y, \varphi \in \mathcal{V}$,

 $0 \leq q(y,y) \quad \text{ and } \quad |q(y,\varphi)| \leq q_{\max} \, \|y\|_{\mathcal{V}} \|\varphi\|_{\mathcal{V}} \quad \forall y,\varphi \in \mathcal{V},$

▶ $r: \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ is a symmetric, \mathcal{U} -coercive and continuous bilinear form, i.e., $r(u, \psi) = r(\psi, u)$ for all $u, \psi \in \mathcal{U}$, and

 $\|r_{\min}\|u\|_{\mathcal{U}}^2 \leq r(u, u)$ and $\|r(u, \psi)\| \leq r_{\max}\|u\|_{\mathcal{U}}\|\psi\|_{\mathcal{U}} \quad \forall u, \psi \in \mathcal{U},$

• $c \in \mathcal{V}^*$ is a bounded linear form on \mathcal{V} .

Optimal control problem

$$\min_{u \in \mathcal{U}} \frac{1}{2}q(y(u), y(u)) + c(y(u)) + \frac{1}{2}r(u, u),$$

where $y(u) \in \mathcal{V}$ is solution of state equation (5) given $u \in \mathcal{U}$.

Optimal Control Problem (Cont.)

Optimal control problem

$$\min_{u \in \mathcal{U}} \frac{1}{2} q(y(u), y(u)) + c(y(u)) + \frac{1}{2} r(u, u),$$

where $y(u) \in \mathcal{V}$ is solution of state equation (5) given $u \in \mathcal{U}$.

- Is a convex, elliptic, linear-quadratic optimal control problem.
- Objective function

$$f: \mathcal{U} \to \mathbb{R}, \quad u \mapsto f(u) := \frac{1}{2}q(y(u), y(u)) + c(y(u)) + \frac{1}{2}r(u, u),$$

is Fréchet differentiable

Fréchet derivative applied to δu is

$$f'(u)\delta u = r(u,\delta u) + b(\delta u,\lambda),$$

where $\lambda \in \mathcal{V}$ solves adjoint equation

$$a(\varphi,\lambda)+q(u,\varphi)=-c(\varphi), \qquad \qquad \forall \varphi\in \mathcal{V}.$$

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Optimal Control Problem - Optimality Conditions

Optimal control problem

$$\min_{u \in \mathcal{U}} \frac{1}{2}q(y(u), y(u)) + c(y(u)) + \frac{1}{2}r(u, u),$$

where $y(u) \in \mathcal{V}$ is solution of state equation (5) given $u \in \mathcal{U}$.

- Is a convex, elliptic, linear-quadratic optimal control problem.
- Has a unique solution $u \in \mathcal{U}$.
- $u \in \mathcal{U}$ solves optimal control problem if and only if there exist $y \in \mathcal{V}$ and $\lambda \in \mathcal{V}$ such that y, u, λ solve

$$\begin{aligned} a(\varphi,\lambda) + q(y,\varphi) &= -c(\varphi) & \forall \varphi \in \mathcal{V}, \\ r(u,\psi) + b(\psi,\lambda) &= 0 & \forall \psi \in \mathcal{U}, \\ a(y,\varphi) + b(u,\varphi) &= \ell(\varphi) & \forall \varphi \in \mathcal{V}. \end{aligned}$$

Example Optimal Control Problem - Optimality Conditions

Optimal control problem

$$\min_{u\in L^2(D)} \ \frac{1}{2} \int_{D_o} \left(y(u;x) - \widehat{y}(x)\right)^2 \mathsf{d}x + \frac{\alpha}{2} \int_D u(x)^2 \,\mathsf{d}x,$$

where $y(u) \in H_0^1(D)$ is solution of state equation

$$\int_D \kappa(x) \nabla y(x) \nabla \varphi(x) \, \mathrm{d} x = \int_D \left(f(x) + u(x) \right) \varphi(x) \, \mathrm{d} x \quad \forall \varphi \in H^1_0(D).$$

Has a unique solution u ∈ L²(D).
 u ∈ L²(D) solves optimal control problem if and only if there exist y ∈ H¹₀(D) and λ ∈ H¹₀(D) such that y, u, λ solve

$$-\nabla \cdot (\kappa(x)\nabla\lambda(x)) = -(y(x) - \hat{y}(x)), \qquad x \in D,$$

$$\lambda(x) = 0, \qquad x \in \partial D,$$

$$\alpha u(x) - \lambda(x) = 0, \qquad \qquad x \in D,$$

$$-\nabla \cdot \left(\kappa(x)\nabla y(x)\right) = f(x) + u(x), \qquad x \in D,$$

y(x) = 0, $x \in \partial D.$

Elliptic Model Problem - Uncertainties in PDE

- Well-posedness of elliptic model problem.
- Conditions for almost all (a.a.) samples ω ∈ Ω not enough for well-posedness, differentiabilty.
- Literature: [Heinkenschloss and Kouri, 2025].

Bochner Spaces

- $\blacktriangleright~(\Omega,\mathcal{F},\mathbb{P})$ be a complete probability space, where
 - Ω is the set of outcomes,
 - $\mathcal{F} \subset 2^{\Omega}$ is σ -algebra of events, and
 - $\mathbb{P}: \mathcal{F} \to [0,1]$ is a probability measure.
- Given Banach space \mathcal{Y} , we define the Bochner spaces

$$L^q_{\mathbb{P}}(\Omega, \mathcal{Y}) := \Big\{ v : \Omega o \mathcal{Y} \mid v \text{ is strongly measurable and} \\ \int_{\Omega} \|y(\omega)\|^q_{\mathcal{Y}} \ \mathrm{d}\mathbb{P}(\omega) < \infty \Big\},$$

for $q\in [1,\infty),$ and

 $L^{\infty}_{\mathbb{P}}(\Omega, \mathcal{Y}) := \Big\{ v : \Omega \to \mathcal{Y} \mid v \text{ is strongly measurable and} \\ \mathbb{P} - \operatorname{ess\,sup}_{\omega \in \Omega} \|y(\omega)\|_{\mathcal{Y}} < \infty \Big\}.$

When $\mathcal{Y} = \mathbb{R}$, we simplify notation to $L^p_{\mathbb{P}}(\Omega, \mathbb{R}) = L^p_{\mathbb{P}}(\Omega)$.

State Equation

- Hilbert space U is control space; separable Hilbert space V related to state space.
- $(\Omega, \mathcal{F}, \mathbb{P})$ complete probability space; \mathcal{B} Borel σ -algebra on \mathbb{R} .
- Given a control $u \in \mathcal{U}$ and realization $\omega \in \Omega$, consider

$$a(y,\varphi,\omega) + b(u,\varphi,\omega) = \ell(\varphi,\omega) \quad \forall \varphi \in \mathcal{V},$$
(6)

Assume (pointwise a.a. $\omega \in \Omega$ assumptions)

- $\blacktriangleright \ a(\cdot,\cdot,\omega): \mathcal{V} \times \mathcal{V} \to \mathbb{R}, \quad b(\cdot,\cdot,\omega): \mathcal{U} \times \mathcal{V} \to \mathbb{R}, \quad \ell(\cdot,\omega) \in \mathcal{V}^*.$
- For each $y, \varphi \in \mathcal{V}$, $u \in \mathcal{U}$, the functions

 $a(y,\varphi,\cdot), b(u,\varphi,\cdot):\Omega\to\mathbb{R} \text{ are } (\mathcal{F},\mathcal{B}) \text{ measurable}.$

• There exist measurable functions $0 < a_{\min}(\omega) \le a_{\max}(\omega)$ and $0 < b_{\max}(\omega)$ such that for a.a. $\omega \in \Omega$,

$$\begin{aligned} a(y, y, \omega) &\geq a_{\min}(\omega) \|y\|_{\mathcal{V}}^{2} & \forall y \in \mathcal{V}, \\ |a(y, \varphi, \omega)| &\leq a_{\max}(\omega) \|y\|_{\mathcal{V}} \|\varphi\|_{\mathcal{V}} & \forall y, \varphi \in \mathcal{V}, \\ |b(u, \varphi, \omega)| &\leq b_{\max}(\omega) \|u\|_{\mathcal{U}} \|\varphi\|_{\mathcal{V}} & \forall u \in \mathcal{U}, \varphi \in \mathcal{V}. \end{aligned}$$

a: V×V×Ω → ℝ is a Carathéodory function; for every u ∈ U, b(u, ·, ·): V×Ω → ℝ is a Carathéodory function. Composition of a, b with Lebesque meas. function is Lebesque meas.

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State Equation (cont.)

For every control $u \in \mathcal{U}$ and a.a. realizations $\omega \in \Omega$ the parameterized state equation

$$a(y,\varphi,\omega) + b(u,\varphi,\omega) = \ell(\varphi,\omega) \quad \forall \varphi \in \mathcal{V},$$

has a unique solution $y(u; \omega) \in \mathcal{V}$.

However, need measurability and integrability properties of the function y(u; ·) : Ω → V.

Two possible routes:

- 1. Formulate state equation as variational equation in $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$.
- Prove that ω → y(u,ω) is measurable by showing it is the limit of measurable functions. Then use properties of a_{min}(ω), a_{max}(ω), b_{max}(ω), l(ω) to establish integrability result of ω → y(u,ω).

1. State Equation in $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$.

• Use variational theory (Lax Milgram) in Hilbert space $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$.

▶ For every control $u \in U$ state equation

$$\begin{split} &\int_{\Omega} a(y(\omega),\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega) + \int_{\Omega} b(u,\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega) \\ &= \int_{\Omega} \ell(\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega), \quad \forall \varphi \in L^2_{\mathbb{P}}\big(\Omega,\mathcal{V}\big). \end{split}$$

$$a(y, y, \omega) \ge a_{\min}(\omega) \|y\|_{\mathcal{V}}^2 \qquad \forall y \in \mathcal{V},$$

with

$$\begin{split} & \operatorname*{ess\,inf}_{\omega\in\Omega} a_{\min}(\omega) > 0,\\ & \text{and} \ a_{\max}\in L^\infty_{\mathbb{P}}(\Omega), \quad b_{\max}\in L^2_{\mathbb{P}}(\Omega), \quad \ell\in L^2_{\mathbb{P}}(\Omega,\mathcal{V}^*). \end{split}$$

1. State Equation in $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$ (cont.).

State equation

$$\begin{split} &\int_{\Omega} a(y(\omega),\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega) + \int_{\Omega} b(u,\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega) \\ &= \int_{\Omega} \ell(\varphi(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega), \quad \forall \varphi \in L^2_{\mathbb{P}}\big(\Omega,\mathcal{V}\big). \end{split}$$

▶ Use variational theory (Lax Milgram) in Hilbert space $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$: $\forall u \in \mathcal{U}$, state equation has a unique solution $y(u) \in L^2_{\mathbb{P}}(\Omega, \mathcal{V})$, and

$$\|y(u)\|_{L^2_{\mathbb{P}}(\Omega,\mathcal{V})} \leq \frac{1}{\operatorname{ess\,inf}_{\omega\in\Omega} a_{\min}} \big(\|\ell\|_{L^2_{\mathbb{P}}(\Omega,\mathcal{V}^*)} + \|b_{\max}\|_{L^\infty_{\mathbb{P}}(\Omega)} \|u\|_{\mathcal{U}} \big).$$

1. State Equation in $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$ (cont.).

Apply to

$$\begin{split} -\nabla\cdot \left(\kappa(x,\omega)\nabla y(x,\omega)\right) &= f(x,\omega) + u(x), \qquad x \in D, \omega \in \Omega, \\ y(x,\omega) &= 0, \qquad \qquad x \in \partial D, \omega \in \Omega, \end{split}$$

where $\kappa \in L^{\infty}_{\mathbb{P}}(\Omega, L^{\infty}(D))$ such that

 $\kappa_{\max}(\omega) \geq \kappa(x,\omega) \geq \kappa_{\min}(\omega) > 0, \quad x \in D, \text{a.a. } \omega \in \Omega.$

For lognormally distributed

$$\kappa(x,\omega) = \exp\bigg(\sum_{m=1}^{M} b^{(m)}(x) \boldsymbol{\xi}^{(m)}(\omega)\bigg),$$

 $b^{(m)} \in L^{\infty}(D)$, $\boldsymbol{\xi}^{(m)} \sim N(0,1)$, $m = 1, \dots, M$, i.i.d.,

 κ not uniformly bded away from zero \Rightarrow variational theory doesn't apply! \blacktriangleright Can select the lower bound

$$\kappa_{\min}(\omega) = \exp\bigg(-\sum_{m=1}^{M} \|b^{(m)}\|_{L^{\infty}(D)} |\boldsymbol{\xi}^{(m)}(\omega)|\bigg),$$

Satisfies $\kappa_{\min}^{-1} \in L^{kq}_{\mathbb{P}}(\Omega) \ \forall k \in \mathbb{N}$, $1 < q < \infty$. [Babuška et al., 2007]
2. State Equation in $L^2_{\mathbb{P}}(\Omega, \mathcal{V})$ (cont.).

• $\omega \mapsto y(u,\omega)$ is the limit of the solutions $y_n \in L^2_{\mathbb{P}}(\Omega,\mathcal{V})$ of

$$a(y,\varphi,\omega) + \frac{1}{n} \langle y,\varphi \rangle_{\mathcal{V}} + b(u,\varphi,\omega) = \ell(\varphi,\omega) \quad \forall \varphi \in \mathcal{V},$$

- ▶ Use properties of $a_{\min}(\omega), a_{\max}(\omega), b_{\max}(\omega), l(\omega)$ to establish integrability result of $\omega \mapsto y(u, \omega)$.
- ▶ Existence and Uniqueness: Let $p, q \ge 1$ with 1/p + 1/q = 1 and $k \in \mathbb{N}$. If $\ell \in L^{kp}_{\mathbb{P}}(\Omega, \mathcal{V}^*)$, $b_{\max} \in L^{kp}_{\mathbb{P}}(\Omega)$, and $a^{-1}_{\min} \in L^{kq}_{\mathbb{P}}(\Omega)$, then unique solution $y(u; \cdot)$ of (6) satisfies $y(u; \cdot) \in L^k_{\mathbb{P}}(\Omega, \mathcal{V})$ and

$$\begin{split} \int_{\Omega} \|y(u;\omega)\|_{\mathcal{V}}^{k} \, \mathrm{d}\mathbb{P}(\omega) &\leq \Bigl(\int_{\Omega} \Bigl(\frac{1}{a_{\min}(\omega)}\Bigr)^{kq} \, \mathrm{d}\mathbb{P}(\omega)\Bigr)^{1/q} \\ &\times \Bigl(\int_{\Omega} \Bigl(\|\ell(\omega)\|_{\mathcal{V}^{*}} + b_{\max}(\omega)\|u\|_{\mathcal{U}}\Bigr)^{kp} \, \mathrm{d}\mathbb{P}(\omega)\Bigr)^{1/p}. \end{split}$$

 Special case of variational result if one chooses p = 1, q = ∞, k = 2.
 Applies to problem with lognormally distributed coeff. If, for some ε > 0, f ∈ L^{k(1+ε)}_P(Ω, L²(D)), solution y(u; ·) ∈ L^k_P(Ω, H¹₀(Ω)).

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Optimal Control Problem

We consider a quadratic fiunction

$$\frac{1}{2}q(y,y,\omega) + c(y;\omega) + \frac{1}{2}r(u,u),$$

where

▶ For $\omega \in \Omega$, $q(\cdot, \cdot, \omega) : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ is symmetric, non-negative, continuous bilinear form, i.e., $q(y, \varphi, \omega) = q(\varphi, y, \omega)$ for all $y, \varphi \in \mathcal{V}$,

$$\begin{split} & 0 \leq q(y,y,\omega), \quad \text{and} \\ & |q(y,\varphi,\omega)| \leq \!\! q_{\max}(\omega) \, \|y\|_{\mathcal{V}} \|\varphi\|_{\mathcal{V}} \; \; \forall y,\varphi \in \mathcal{V}, \qquad q_{\max} \in L^\infty_{\mathbb{P}}\big(\Omega\big). \end{split}$$

• (as before) $r: \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ is a symmetric, \mathcal{U} -coercive and continuous bilinear form, i.e., $r(u, \psi) = r(\psi, u)$ for all $u, \psi \in \mathcal{U}$, and $r_{\min} \|u\|_{\mathcal{U}}^2 \leq r(u, u)$ and $|r(u, \psi)| \leq r_{\max} \|u\|_{\mathcal{U}} \|\psi\|_{\mathcal{U}} \quad \forall u, \psi \in \mathcal{U}$,

•
$$c \in L^2_{\mathbb{P}}(\Omega, \mathcal{V}^*).$$

• If state $y(u; \cdot) \in L^2_{\mathbb{P}}(\Omega, \mathcal{V})$, then

$$\omega \mapsto \frac{1}{2}q(y(u;\omega), y(u;\omega), \omega) + c(y(u;\omega), \omega) + \frac{1}{2}r(u,u)$$

is integrable

Optimal Control Problem (Cont.)

▶ Risk-neutral optimal control problem: If state $y(u; \cdot) \in L^2_{\mathbb{P}}(\Omega, \mathcal{V})$, can minimize expected cost

$$\min_{u\in\mathcal{U}} \int_{\Omega} \frac{1}{2}q\big(y(u;\omega),y(u;\omega),\omega\big) + c\big(y(u;\omega),\omega\big)\,\mathrm{d}\mathbb{P}(\omega) + \frac{1}{2}r(u,u),$$

- ► Control $u \in \mathcal{U}$ is deterministic because we need to decide on control before uncertainty is revealed, i.e., before outcome $\omega \in \Omega$ is known.
- ▶ If previous existence result holds with k = 2, risk-neutral optimal control problem is convex, has a unique solution $u \in U$.

Three Maps Associated with Objective

Control-to-state map

$$\begin{split} S: \mathcal{U} &\to L^2_{\mathbb{P}}\big(\Omega, \mathcal{V}\big), \\ u &\mapsto y(u; \cdot) \quad (y(u; \omega) \text{ solves (6)}). \end{split}$$

Pointwise

$$\begin{aligned} J: \mathcal{V} \times \Omega \to \mathbb{R}, \\ (y, \omega) \mapsto \frac{1}{2} q(y, y, \omega) + c(y, \omega), \end{aligned}$$

and associated map

$$\begin{split} \mathcal{J} &: L^2_{\mathbb{P}}\big(\Omega, \mathcal{V}\big) \to L^1_{\mathbb{P}}\big(\Omega\big), \\ & y \mapsto [\mathcal{J}(y)](\cdot) = J(y(\cdot), \cdot). \end{split}$$

Expected value (risk measure)

$$egin{aligned} \mathcal{R} &: L^1_\mathbb{P}(\Omega) o \mathbb{R} \ oldsymbol{\xi} &\mapsto \mathbb{E}[oldsymbol{\xi}] = \int_\Omega oldsymbol{\xi}(\omega) \, \mathsf{d}\mathbb{P}(\omega). \end{aligned}$$

• Optimal control problem $\min_{u \in \mathcal{U}} \mathcal{R}[\mathcal{J}(S(u))] + \frac{1}{2}r(u, u).$

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Fréchet Differentiability

Control-to-state map:

- If 'pointwise assumptions' hold, $\mathcal{U} \ni u \mapsto y(u; \omega) \in \mathcal{V}$ is Fréchet diff'bel. a.a. $\omega \in \Omega$.
- If 'existence & uniquess assumptions' hold with k = 2, $S: \mathcal{U} \to L^2_{\mathbb{P}}(\Omega, \mathcal{V})$ is Fréchet diff'bel., Fréchet derivative can be computed pointwise for a.a. $\omega \in \Omega$.
- Objective function maps
 - If 'pointwise assumptions' on q, c hold, $J : \mathcal{V} \times \Omega \rightarrow \mathbb{R}$, is Fréchet diff'bel. in y on $\mathcal{V} \times \Omega$.
 - ▶ If integrability conditions on q_{max} hold, $\mathcal{J} : L^2_{\mathbb{P}}(\Omega, \mathcal{V}) \to L^1_{\mathbb{P}}(\Omega)$ is Fréchet diff'bel.
- ▶ Composition: If all above condition hold, $\mathcal{J} \circ S$ is Fréchet differentiable.

Fréchet Differentiability (cont.)

 \blacktriangleright If all above conditions hold, $\mathcal{J} \circ S$ is Fréchet differentiable and the Fréchet derivative is

$$\begin{aligned} [\mathcal{J}_y(S(u))\,S'(u)\delta u](\cdot) &= q\big(y(u;\cdot), y_u(u;\cdot)\delta u,\cdot\big) + c\big(y_u(u;\cdot)\delta u,\cdot\big) \\ &= b(\delta u,\lambda(\cdot),\cdot), \end{aligned}$$

where $\lambda \in L^1_{\mathbb{P}}(\Omega, \mathcal{V})$ is solution of (pointwise) adjoint equation

 $a(\varphi,\lambda(\omega),\omega)+q(y(u;\omega),\varphi,\omega)=-c(\varphi,\omega), \quad \forall \varphi\in\mathcal{V}, \text{ a.a. } \omega\in\Omega.$

If, in addition, $a_{\min}^{-1} \in L^{\infty}_{\mathbb{P}}(\Omega)$, then $\lambda \in L^{2}_{\mathbb{P}}(\Omega, \mathcal{V})$.

▶ If all above conditions hold, $f = \mathbb{E} \circ \mathcal{J} \circ S$ is Fréchet differentiable; Fréchet derivative applied to δu is

$$f'(u)\delta u = \int_{\Omega} b(\delta u, \lambda(\omega), \omega), \, \mathrm{d}\mathbb{P}(\omega) + r(u, \delta u).$$

Optimal Control Problem - Optimality Conditions

▶ Risk-neutral optimal control problem: If state $y(u; \cdot) \in L^2_{\mathbb{P}}(\Omega, \mathcal{V})$, can minimize expected cost

$$\min_{u \in \mathcal{U}} \int_{\Omega} \frac{1}{2} q\big(y(u;\omega), y(u;\omega), \omega\big) + c\big(y(u;\omega), \omega\big) \, \mathrm{d}\mathbb{P}(\omega) + \frac{1}{2} r(u,u).$$

- If state equation existence result holds with k = 2, risk-neutral optimal control problem Is convex. Has a unique solution u ∈ U.
- ▶ $u \in \mathcal{U}$ solves risk-neutral optimal control problem if and only if there exist $y \in L^2_{\mathbb{P}}(\Omega, \mathcal{V})$ and $\lambda \in L^1_{\mathbb{P}}(\Omega, \mathcal{V})$ such that y, u, λ solve

$$\begin{split} a(\varphi,\lambda(\omega),\omega) + q(y(\omega),\varphi,\omega) &= -c(\varphi,\omega) \quad \forall \varphi \in \mathcal{V}, \text{ a.a. } \omega \in \Omega, \\ \int_{\Omega} b(\psi,\lambda(\omega),\omega) \, \mathrm{d}\mathbb{P}(\omega) + r(u,\psi) &= 0 \qquad \qquad \forall \psi \in \mathcal{U}, \\ a(y(\omega),\varphi,\omega) + b(u,\varphi,\omega) &= \ell(\varphi,\omega) \qquad \forall \varphi \in \mathcal{V}, \text{ a.a. } \omega \in \Omega. \end{split}$$

Example Optimal Control Problem - Optimality Conditions • $\eta \in L^{\infty}_{\mathbb{P}}(\Omega, L^{\infty}(D)), \eta \geq 0$ a.e. in $D \times \Omega$. Optimal control problem $\min_{u \in L^2(D)} \int_{\Omega} \frac{1}{2} \int_{D} \eta(x,\omega) \big(y(u;x,\omega) - \widehat{y}(x) \big)^2 \, \mathrm{d}x \, \mathrm{d}\mathbb{P}(\omega) + \frac{\alpha}{2} \int_{\Omega} u(x)^2 \, \mathrm{d}x,$ where for a.a. $\omega \in \Omega$, $y(u, \cdot, \omega) \in H_0^1(D)$ solves $\int_{\Sigma} \kappa(x,\omega) \nabla y(x,\omega) \nabla \varphi(x) \, \mathrm{d}x = \int_{D} \left(f(x,\omega) + u(x) \right) \varphi(x) \, \mathrm{d}x \, \forall \varphi \in H^1_0(D).$ \blacktriangleright $u \in L^2(D)$ solves optimal control problem if and only if there exist $y \in L^2_{\mathbb{P}}(\Omega, H^1_0(D)), \lambda \in L^1_{\mathbb{P}}(\Omega, H^1_0(D))$ such that $-\nabla \cdot (\kappa(x,\omega)\nabla\lambda(x,\omega)) = -\eta(x,\omega)(y(x,\omega)-\widehat{y}(x)), \ x \in D, \text{a.a.} \ \omega \in \Omega,$ $\lambda(x,\omega) = 0.$ $x \in \partial D$, a.a. $\omega \in \Omega$, $\int_{\Omega} \lambda(x,\omega) \, \mathrm{d}\mathbb{P}(\omega) = \alpha u(x),$ $x \in D$, $-\nabla \cdot (\kappa(x,\omega)\nabla y(x,\omega)) = f(x,\omega) + u(x), \quad x \in D, \text{a.a. } \omega \in \Omega,$ $y(x,\omega) = 0.$ $x \in \partial D$, a.a. $\omega \in \Omega$. • Control deterministic \Rightarrow coupling $\int_{\Omega} \lambda(x, \omega) d\mathbb{P}(\omega) = \alpha u(x)$.

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Note on Finite Noise Assumption

- ▶ So far used $(\Omega, \mathcal{F}, \mathbb{P})$ complete probability space.
- Often consider a vector ξ : (Ω, F) → (Ξ, B_Ξ) of random variables. Ξ ⊂ ℝ^M is a nonempty set and B_Ξ is the Borel σ-algebra on Ξ.
- All our examples depended on finitely many random variables.
- Finite noise assumption needed for some methods, e.g., sparse grid discretization and quasi-Monte Carlo.
- Sometimes problem can be well-approximated by a finite noise problem, e.g., approximate diffusion coefficient

$$\kappa(x,\omega) = \exp\left(\sum_{m=1}^{\infty} b^{(m)}(x) \boldsymbol{\xi}^{(m)}(\omega)\right)$$
$$\approx \kappa_M(x, \boldsymbol{\xi}) = \exp\left(\sum_{m=1}^{M} b^{(m)}(x) \boldsymbol{\xi}^{(m)}\right).$$

Distribution (or law) of ξ on σ-algebra σ(ξ) = {ξ⁻¹(B) | B ∈ B_Ξ} is P^ξ = P ∘ ξ⁻¹.

► All previous results apply with $(\Omega, \mathcal{F}, \mathbb{P}) \to (\Xi, \mathcal{B}_{\Xi}, \mathbb{P}^{\xi}), \ \omega \to \xi.$

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Elliptic Model Problem - Discretization

Numerical solution requires discretization of the problem.

- Crucial component in solution process.
- Discretization of optimal control problem typically builds on discretization of underlying PDE.
- Good discretization scheme for underlying PDE is necessary but not sufficient for good discretization scheme of optimal control problem.

Elliptic Model Problem - Determinstic

Example, conforming Galerkin finite-element approximation:

 $\mathcal{U}_h = \operatorname{span}\{\psi_1, \dots, \psi_{n_u}\} \subset \mathcal{U}, \quad \mathcal{V}_h = \operatorname{span}\{\varphi_1, \dots, \varphi_{n_y}\} \subset \mathcal{V}.$

Approximate control and state by

$$u_h = \sum_{i=1}^{n_u} \mathbf{u}_i \psi_i, \quad y_h = \sum_{i=1}^{n_y} \mathbf{y}_i \varphi_i.$$

Replace weak form of state equation by

$$a(y_h, \varphi) + b(u_h, \varphi) = \ell(\varphi), \quad \forall \varphi \in \mathcal{V}_h.$$

This leads to

$$\mathbf{A}\mathbf{y} + \mathbf{B}\mathbf{u} = \mathbf{b},$$

with

$$\begin{aligned} \mathbf{A}_{ij} &= a(\varphi_j, \varphi_i), & i, j = 1, \dots n_y, \\ \mathbf{B}_{ij} &= b(\psi_j, \varphi_i), & i = 1, \dots n_y, j = 1, \dots n_u, \\ \mathbf{b}_i &= \ell(\varphi_i), & i = 1, \dots n_y. \end{aligned}$$

• Coercivity of a implies invertibility of $\mathbf{A} \in \mathbb{R}^{n_y \times n_y}$.

$$\mathbf{y}(\mathbf{u}) = \mathbf{A}^{-1}(\mathbf{b} - \mathbf{B}\mathbf{u}).$$

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Insert state and control approximation int objective to get

$$\frac{1}{2}\mathbf{y}^{\top}\mathbf{Q}\,\mathbf{y} + \mathbf{c}^{\top}\mathbf{y} + \frac{1}{2}\mathbf{u}^{\top}\mathbf{R}\,\mathbf{u}$$

 $\blacktriangleright \ \mathbf{Q} = \mathbf{Q}^\top \in \mathbb{R}^{n_y \times n_y}, \ \mathbf{R} = \mathbf{R}^\top \in \mathbb{R}^{n_u \times n_u}, \ \mathbf{c} \in \mathbb{R}^{n_y},$

$$\mathbf{Q}_{ij} = q(\varphi_i, \varphi_j), \ i, j = 1, \dots n_y, \quad \mathbf{R}_{ij} = r(\psi_i, \psi_j), \ i, j = 1, \dots n_u,$$

and $\mathbf{c}_i = c(\varphi_i)$, $i = 1, \dots n_y$.

- ► Assumptions on bilinear forms q and r imply that Q ∈ ℝ^{n_y×n_y} is symmetric positive semidefinite and R ∈ ℝ^{n_u×n_u} is symmetric positive definite.
- Discretization optimal control problem

$$\begin{split} \min_{\mathbf{u} \in \mathbb{R}^{n_u}} \; \frac{1}{2} \mathbf{u}^\top \big(\mathbf{B}^\top \mathbf{A}^{-\top} \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{B} + \mathbf{R} \big) \; \mathbf{u} - \big(\mathbf{B}^\top \mathbf{A}^{-\top} \big(\mathbf{c} + \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{b} \big) \big)^\top \mathbf{u} \\ &+ \frac{1}{2} \mathbf{b}^\top \mathbf{A}^{-\top} \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{b} + \mathbf{c}^\top \mathbf{A}^{-1} \mathbf{b}. \end{split}$$

Discretization optimal control problem

$$\begin{split} \min_{\mathbf{u} \in \mathbb{R}^{n_u}} \; & \frac{1}{2} \mathbf{u}^\top \big(\mathbf{B}^\top \mathbf{A}^{-\top} \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{B} + \mathbf{R} \big) \; \mathbf{u} - \big(\mathbf{B}^\top \mathbf{A}^{-\top} \big(\mathbf{c} + \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{b} \big) \big)^\top \mathbf{u} \\ & + \frac{1}{2} \mathbf{b}^\top \mathbf{A}^{-\top} \mathbf{Q} \, \mathbf{A}^{-1} \mathbf{b} + \mathbf{c}^\top \mathbf{A}^{-1} \mathbf{b}. \end{split}$$

• Has a unique solution $\mathbf{u} \in \mathbb{R}^{n_u}$.

ig> $\mathbf{u} \in \mathbb{R}^{n_u}$ solves Discretization optimal control problem if and only if

$$\left(\mathbf{B}^{\top}\mathbf{A}^{-\top}\mathbf{Q}\,\mathbf{A}^{-1}\mathbf{B}+\mathbf{R}\right)\,\mathbf{u}=\mathbf{B}^{\top}\mathbf{A}^{-\top}\big(\mathbf{c}+\mathbf{Q}\,\mathbf{A}^{-1}\mathbf{b}\big),$$

and if and only if there exists $\mathbf{y} \in \mathbb{R}^{n_y}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{n_y}$ such that

$$\begin{pmatrix} \mathbf{Q} & \mathbf{0} & \mathbf{A}^\top \\ \mathbf{0} & \mathbf{R} & \mathbf{B}^\top \\ \mathbf{A} & \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} -\mathbf{c} \\ \mathbf{0} \\ \mathbf{b} \end{pmatrix}$$

 Many solvers for such systems. See, e.g., [Benzi et al., 2005], [Borzì and Schulz, 2009], [Borzì and Schulz, 2012], [Pearson and Pestana, 2020], [Wathen, 2015].

Basic Discretization Error

- ▶ Problem minimize_{$u \in \mathcal{U}$} $f(u) = \widetilde{f}(y(u), u)$.
- Approximate problem (e.g., discretization), $U_h \subset U$

minimize_{$$u_h \in \mathcal{U}_h$$} $f_h(u_h) = \tilde{f}_h(y_h(u_h), u_h).$

• u^* and u^*_h solutions. Taylor expansion

$$\nabla f(u^*) - \nabla f(u_h^*) = \nabla^2 f(u_h^* + t(u^* - u_h^*))(u^* - u_h^*).$$

(Local) convexity of f (true for quadratic model problem)

$$\begin{split} \langle \nabla f(u^*) - \nabla f(u_h^*), u^* - u_h^* \rangle_{\mathcal{U}} &= \langle \nabla^2 f\left(u_h^* + t(u^* - u_h^*)\right)(u^* - u_h^*), u^* - u_h^* \rangle_{\mathcal{U}} \\ &\geq \sigma \|u^* - u_h^*\|_{\mathcal{U}}^2. \end{split}$$

Hence

$$\sigma \|u^* - u_h^*\|_{\mathcal{U}} \le \|\underbrace{\nabla f(u^*)}_{=0} - \nabla f(u_h^*)\|_{\mathcal{U}} = \|\underbrace{\nabla f_h(u_h^*)}_{=0} - \nabla f(u_h^*)\|_{\mathcal{U}}.$$

 Error between solutions u*, u^{*}_h bounded by error in gradients at u^{*}_h.
 Not sufficient to approximate state y(u), i.e., function f(u). Must also approximate ∇f(u), i.e., the adjoint λ(u).

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In elliptic model problem, must interpret

$$\mathbf{A}^{\top} \boldsymbol{\lambda} + \mathbf{Q} \mathbf{y} = -\mathbf{c}$$

as discretization of adjoint equation

$$a(\varphi, \lambda) + q(y, \varphi) = -c(\varphi) \qquad \qquad \forall \varphi \in \mathcal{V},$$

▶ In conforming Galerkin disc., $\mathbf{A}^{\top} \boldsymbol{\lambda} + \mathbf{Q} \mathbf{y} = -\mathbf{c}$ is equivalent to

$$a(\varphi, \lambda_h) + q(y_h, \varphi) = -c(\varphi), \quad \forall \varphi \in \mathcal{V}_h,$$

where

$$\lambda_h = \sum_{i=1}^{n_y} \lambda_i \varphi_i \in \mathcal{V}_h.$$

Can prove discretization error result of the form

 $\begin{aligned} \|u^* - u_h^*\|_{L^2(D)} + h\|y(u^*) - y_h(u_h^*)\|_{H^1_0(D)} &\leq ch^2 \big(\|y(u^*)\|_{L^2(D)} + \|u^*\|_{L^2(D)}\big) \\ \text{[Hinze et al., 2009, Theorem 3.5]} \end{aligned}$

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Discretize-then-optimize = optimize-then-discretize



Not Always this Nice and Clean

- For stabilized finite element methods [Collis and Heinkenschloss, 2002], [Abraham et al., 2004], [Heinkenschloss and Leykekhman, 2010], [Quarteroni, 2009, §16.13], and
- several discontinuous Galerkin methods [Leykekhman, 2012] and [Leykekhman and Heinkenschloss, 2012].





SUPG Discretization of Advection Diffusion OCP

$$\min\frac{1}{2}\int_{\Omega}(y(x)-\widehat{y}(x))^2dx + \frac{\alpha}{2}\int_{\Omega}u^2(x)dx$$

subject to

$$\begin{aligned} -\epsilon \Delta y(x) + c(x) \cdot \nabla y(x) + r(x)y(x) &= f(x) + u(x), & x \in \Omega, \\ y(x) &= d(x), & x \in \Gamma_d, \\ \epsilon \frac{\partial}{\partial n} y(x) &= g(x), & x \in \Gamma_n, \end{aligned}$$

where $f,\widehat{y}\in L^{2}(\Omega)\text{, }\alpha>0\text{,}$

$$\begin{split} \epsilon &> 0, \quad c \in \left(W^{1,\infty}(\Omega)\right)^2, \quad r \in L^\infty(\Omega), \\ r(x) - \frac{1}{2} \nabla \cdot c(x) \geq r_0 > 0 \text{ a.e. in } \Omega, \quad n \cdot c(x) \geq 0 \text{ on } \Gamma_n. \end{split}$$

We are interested in the case $\epsilon \ll ||c(x)||$.



Galerkin/Least Squares (GaLS) Stabilized FEM for Oseen

$$\min \frac{1}{2} \int_{\Omega_{\rm obs}} |\boldsymbol{\nabla} \times \mathbf{u}|^2 d\Omega + \frac{\alpha}{2} \int_{\Gamma_c} |\mathbf{g}|^2 d\Gamma_c,$$

subject to

$$\begin{split} (\mathbf{a}\cdot\boldsymbol{\nabla})\mathbf{u} - \boldsymbol{\nabla}\cdot[-p\mathbf{I} + \boldsymbol{\mu}(\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\mathbf{u}^T)] &= 0 \quad \text{in} \quad \Omega, \\ \mathbf{\nabla}\cdot\mathbf{u} &= 0 \quad \text{in} \quad \Omega, \end{split}$$

$$\begin{split} \mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_c, \quad \mathbf{u} = \mathbf{u}_{\text{in}} \quad \text{on } \Gamma_{\text{in}}, \quad \mathbf{u} = \mathbf{0} \quad \text{on } \partial \Omega \backslash (\Gamma_c \cup \Gamma_{\text{in}} \cup \Gamma_{\text{out}}), \\ \mathbf{n} \cdot [-p\mathbf{I} + \mu (\boldsymbol{\nabla} \mathbf{u} + \boldsymbol{\nabla} \mathbf{u}^T)] = \mathbf{0} \quad \text{on } \Gamma_{\text{out}}. \end{split}$$



Note change of notation: \mathbf{u}, p (velocities, pressure) states, \mathbf{g} control. Replace Dirichlet boundary condition $\mathbf{u} = \mathbf{g}$ on Γ_c by

$$\mathbf{n} \cdot [-p\mathbf{I} + \mu (\boldsymbol{\nabla} \mathbf{u} + \boldsymbol{\nabla} \mathbf{u}^T)] + 10^5 \mathbf{u} = 10^5 \mathbf{g} \text{ on } \Gamma_c.$$

[Hou and Ravindran, 1998]



Optimal controls obtained using DO and OD, coarse discretization, $\alpha = 10^{-5}$.



Optimal controls obtained using DO and OD, fine discretization, $\alpha = 10^{-5}$.



Uncontrolled flow



Controlled flow

$$\mu = 5 * 10^{-4}, \ \alpha = 10^{-5}$$

Elliptic Model Problem - Uncertainties in PDE

Need to also apply discretization in random variables.

- Many more variations that for deterministic problem.
- Discretize-then-optimize (e.g., sample average approximation (SAA)) vs. optimize-then-discretize (e.g., stochastic approximation).
- ▶ Will focus on sample average approximation (SAA).

Sample Average Approximation (SAA)

For a given control $u \in \mathcal{U}$, the objective function involves expectation of

$$F = \mathcal{J} \circ S : \mathcal{U} \to L^{1}_{\mathbb{P}^{\xi}}(\Xi),$$
$$u \mapsto [F(u)](\cdot) = \frac{1}{2}q(y(u; \cdot), y(u; \cdot), \cdot) + c(y(u; \cdot), \cdot), \cdot)$$

where $y(u;\xi)$ solves state equation at sample ξ .

Monte Carlo, quasi-Monte Carlo, multilevel/mult-fidelity Monte Carlo, and sparse-grid methods approximate

$$\mathbb{E}[F(u)] = \int_{\Xi} [F(u)](\xi) \, \mathrm{d}\mathbb{P}^{\xi}(\xi)$$

$$\approx \sum_{i=1}^{N} \zeta_{i} [F_{h_{i}}(u)](\xi_{i})$$

$$:= \sum_{i=1}^{N} \zeta_{i} \left(\frac{1}{2}q(y_{h_{i}}(u;\xi_{i}), y_{h_{i}}(u;\xi_{i}), \xi_{i}) + c(y_{h_{i}}(u;\xi_{i}), \xi_{i})\right),$$

where $\zeta_i \in \mathbb{R}$ and $y_{h_i}(u;\xi_i)$ is an approximation of state at $\xi = \xi_i$.

Algebraic Form

▶ Algebraic representation of $y_{h_i}(u_h; \xi_i)$ at control $u_h \in U_h$ given by

$$\mathbf{y}_i(\mathbf{u}) = \mathbf{A}_i^{-1}(\mathbf{b}_i - \mathbf{B}_i \mathbf{u}),$$

Algebraic representation of SAA is

$$\begin{split} &\sum_{i=1}^{N} \zeta_{i} \Big(\frac{1}{2} \mathbf{u}^{\top} \mathbf{B}_{i}^{\top} \mathbf{A}_{i}^{-\top} \mathbf{Q}_{i} \mathbf{A}_{i}^{-1} \mathbf{B}_{i} \mathbf{u} - \big(\mathbf{B}_{i}^{\top} \mathbf{A}_{i}^{-\top} \big(\mathbf{c}_{i} + \mathbf{Q}_{i} \mathbf{A}_{i}^{-1} \mathbf{b}_{i} \big) \big)^{\top} \mathbf{u} \Big) \\ &+ \sum_{i=1}^{N} \zeta_{i} \Big(\frac{1}{2} \mathbf{b}_{i}^{\top} \mathbf{A}_{i}^{-\top} \mathbf{Q}_{i} \mathbf{A}_{i}^{-1} \mathbf{b}_{i} + \mathbf{c}_{i}^{\top} \mathbf{A}_{i}^{-1} \mathbf{b}_{i} \Big). \end{split}$$

• Weights ζ_i

- ▶ Monte Carlo and quasi-Monte Carlo set $\zeta_i = 1/N$
- Multilevel/mult-fidelity Monte Carlo, and sparse-grid methods generate negative and positive weights!
 - \Rightarrow potential loss of convexity.

Optimality Conditions

- $\mathbf{A}_i \in \mathbb{R}^{n_{y,i} \times n_{y,i}}$, i = 1, ..., N, invertible, $\mathbf{R} \in \mathbb{R}^{n_u \times n_u}$ symmetric positive definite, $\mathbf{R} + \sum_{i=1}^N \zeta_i \mathbf{B}_i^\top \mathbf{A}_i^{-\top} \mathbf{Q}_i \mathbf{A}_i^{-1} \mathbf{B}_i$ be symmetric positive definite.
- SAA discretization has unique solution $\mathbf{u} \in \mathbb{R}^{n_u}$.
- $\mathbf{u} \in \mathbb{R}^{n_u}$ solves SAA discretization if and only if

$$\left(\sum_{i=1}^{N}\zeta_{i}\mathbf{B}_{i}^{\top}\mathbf{A}_{i}^{-\top}\mathbf{Q}_{i}\mathbf{A}_{i}^{-1}\mathbf{B}_{i}+\mathbf{R}\right)\mathbf{u}=\sum_{i=1}^{N}\zeta_{i}\mathbf{B}_{i}^{\top}\mathbf{A}_{i}^{-\top}(\mathbf{c}_{i}+\mathbf{Q}_{i}\mathbf{A}_{i}^{-1}\mathbf{b}_{i}),$$

and if and only if there exist

$$ec{\mathbf{y}} = egin{pmatrix} \mathbf{y}_1 \ ec{\mathbf{y}}_N \ \mathbf{y}_N \end{pmatrix}, \quad ec{oldsymbol{\lambda}} = egin{pmatrix} oldsymbol{\lambda}_1 \ ec{ec{\mathbf{y}}}_N \ \mathbf{\lambda}_N \end{pmatrix},$$

such that

$$egin{pmatrix} ec{\mathbf{Q}} & \mathbf{0} & ec{\mathbf{A}}^{ op} \ \mathbf{0} & \mathbf{R} & ec{\mathbf{B}}^{ op} \ ec{\mathbf{A}} & ec{\mathbf{B}} & \mathbf{0} \end{pmatrix} egin{pmatrix} ec{\mathbf{y}} \ ec{\mathbf{y}} \ ec{\mathbf{u}} \ ec{\mathbf{A}} & ec{\mathbf{c}} & ec{\mathbf{0}} \ ec{\mathbf{b}} \end{pmatrix},$$

where

KKT conditions

$$\begin{pmatrix} \vec{\mathbf{Q}} & \mathbf{0} & \vec{\mathbf{A}}^\top \\ \mathbf{0} & \mathbf{R} & \vec{\mathbf{B}}^\top \\ \vec{\mathbf{A}} & \vec{\mathbf{B}} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \vec{\mathbf{y}} \\ \mathbf{u} \\ \vec{\lambda} \end{pmatrix} = \begin{pmatrix} -\vec{\mathbf{c}} \\ \mathbf{0} \\ \vec{\mathbf{b}} \end{pmatrix},$$

where

$$\vec{\mathbf{A}} = \begin{pmatrix} \zeta_1 \mathbf{A}_1 & & \\ & \ddots & \\ & & \zeta_N \mathbf{A}_N \end{pmatrix}, \ \vec{\mathbf{Q}} = \begin{pmatrix} \zeta_1 \mathbf{Q}_1 & & \\ & \ddots & \\ & & & \zeta_N \mathbf{Q}_N \end{pmatrix}, \ \vec{\mathbf{B}} = \begin{pmatrix} \zeta_1 \mathbf{B}_1 \\ \vdots \\ \zeta_N \mathbf{B}_N \end{pmatrix}$$

and

$$\vec{\mathbf{b}} = \left(\zeta_1 \mathbf{b}_1^\top, \dots, \zeta_N \mathbf{b}_N^\top\right)^\top, \quad \vec{\mathbf{c}} = \left(\zeta_1 \mathbf{c}_1^\top, \dots, \zeta_N \mathbf{c}_N^\top\right)^\top.$$

Note coupling

$$\mathbf{R}\mathbf{u} + \vec{\mathbf{B}}^{\top}\vec{\lambda} = \mathbf{R}\mathbf{u} + \sum_{i=1}^{N}\zeta_i\mathbf{B}_i\lambda_i = \mathbf{0}.$$

 Requires modification of standard KKT iterative solvers. See, e.g., [Kouri and Ridzal, 2018, Section 5.2] and [Nobile and Vanzan, 2023], [Ciaramella et al., 2024].

Matthias Heinkenschloss

April 17, 2025

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Discretization Error Analyses

- Monte Carlo, quasi-Monte Carlo, multilevel/mult-fidelity Monte Carlo generate random samples
 - \Rightarrow Need to measure error in expectation or probability.
- Multilevel/mult-fidelity Monte Carlo and sparse-grid methods generate negative and positive weights!
 Need to assume convexity of SAA problems. Numerical observation indicates that this is often true for sparse-grid methods (once sparse-grid is sufficiently fine) [Kouri, 2012], [Kouri, 2014], but no proof (yet).
- Recent error estimates for Monte Carlo and Galerkin FEM of elliptic linear-quadratic optimal control problems by [Milz, 2023a, Milz, 2023b, Milz, 2023c], [Milz and Ulbrich, 2024], and [Römisch and Surowiec, 2024].

Discretization Error Analyses (cont.)

Error estimate for Monte Carlo and Galerkin FEM (piecewise constant controls, piecewise linear states) discretization of elliptic linear-quadratic optimal control problems [Milz, 2023b]:

$$\mathbb{E}\left[\|u_{h,N} - u\|_{L^2(D)}^2\right] \le c_1 h^2 + c_2/N$$

For each $\delta \in (0, 1)$, with a probability $1 - \delta$,

$$||u_{h,N} - u||_{L^2(D)} \le \tilde{c}_1 h + \tilde{c}_2 \sqrt{2\ln(2/\delta)/N},$$

▶ Note sample size N typically limiting, not FEM mesh size h, i.e., $h < 1/\sqrt{N}$.

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