

Physics-Based Stochastic Optimization

Theory and Methods

ICSP 2025 Tutorial

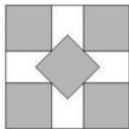
Caroline Geiersbach

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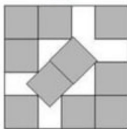
July 26, 2025

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how are you feeling today?**

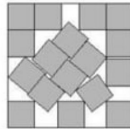
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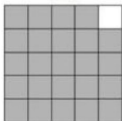
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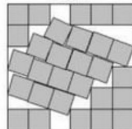
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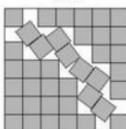
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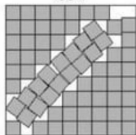
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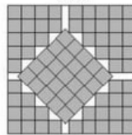
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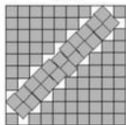
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Personal introduction

2010-2016	BSc., MSc., Technical University of Vienna
2016-2020	PhD, University of Vienna (Advisor: Georg Pflug)
2020-2024	Postdoc at Weierstrass Institute in Berlin (Group: Michael Hintermüller)
2024-2025	Tenure-track assistant professor, University of Hamburg
Fall 2025-	Full professor, Alpen-Adria University of Klagenfurt



Vienna Graduate School for Computational Optimization.

Today's agenda

- ➊ Introduction
 - Challenges and examples of applications in physics-based optimization.
- ➋ Foundations of stochastic optimization on Banach spaces
 - Basic definitions, most useful tools and results for optimization.
- ➌ Optimality conditions
 - Constraints on the first and second stage. Adjoint method.
- ➍ Case study
 - Analysis of example from PDE-constrained optimization under uncertainty.
- ➎ Stochastic approximation
 - Results in Hilbert spaces, handling of numerical error.

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2 Foundations of stochastic optimization on Banach spaces

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3 Optimality conditions

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4 Case study

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5 Stochastic approximation

- Results in Hilbert spaces, handling of numerical error.

Stochastic optimization

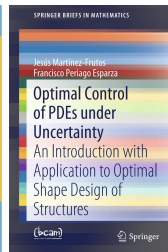
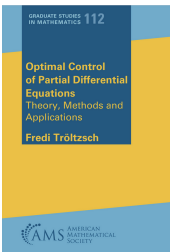
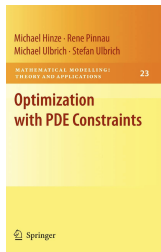
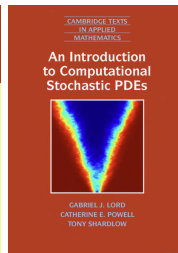
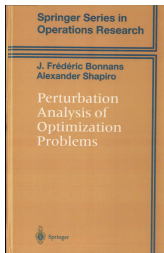
Abstract decision problem

Prototypical **decision problem** from stochastic optimization:

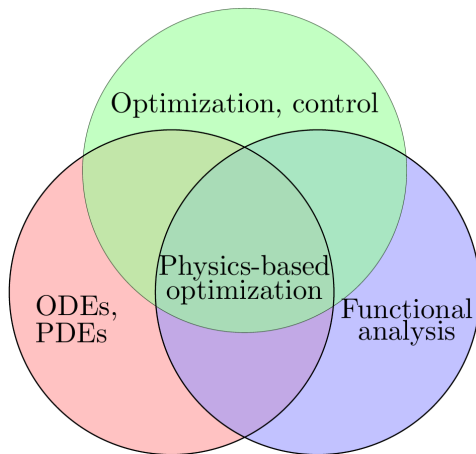
$$\min_{u \in U_{\text{ad}}} \mathbb{E}[J(u, \xi)] = \int_{\Omega} J(u, \xi(\omega)) \, d\mathbb{P}(\omega).$$

- A probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is assumed to be given.
- $U_{\text{ad}} \subset U$ is the *feasible set* of deterministic decisions with U **Banach space**.
- $\xi: \Omega \rightarrow \Xi \subset \mathbb{R}^m$ is the *random (i.e., measurable) vector with support Ξ* .
- $J: U \times \Xi \rightarrow \mathbb{R}$ is the parametrized objective function; the superposition $\mathcal{J}(u, \omega) := J(u, \xi(\omega))$ is the *random variable objective function*.

Literature



Physics-based optimization



Example optimal control problem

Boundary control problem for the 1D wave equation

Example

- An oscillating string is fixed at both ends of the interval $(0, \ell)$.
- The state y is the solution to the wave equation:

$$\begin{aligned} \text{state: } & y_{tt}(x, t) - c^2 y_{xx}(x, t) = 0 && \text{in } (0, \ell) \times (0, T), \\ \text{boundary conditions: } & y(0, t) = u_1(t), \quad y(\ell, t) = u_2(t) && \text{for } t \in (0, T), \\ \text{initial conditions: } & y(x, 0) = y_0(x), \quad y_t(x, 0) = y_1(x) && \text{for } x \in (0, \ell), \end{aligned}$$

where c is the wave speed.

- **Goal:** drive the string to rest at a given time T by controls u_1 and u_2 at $x = 0$ and $x = \ell$, respectively, i.e., to minimize the cost functional

$$\min_{(u, y) \in U \times Y} J(u, y) = \frac{1}{2} \|y\|_{L^2(0, T; (0, \ell))}^2 + \frac{1}{2} \|y(\cdot, T)\|_{L^2(0, \ell)}^2 + \frac{\mu}{2} \|u\|_{L^2(0, T)^2}^2$$

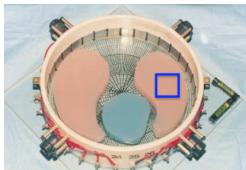
where $\mu > 0$ is a regularization parameter.

Simulation: <https://caroline.geiersbach.com/icsp/wave>.

(Credit: Felix Sauer, Weierstrass Institute)

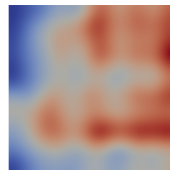
Uncertainty in physics-based optimization (1/2)

- **Material parameters** (conductivity, permittivity, elasticity)

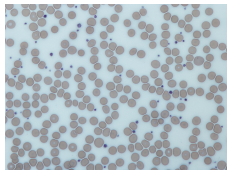


Left: Experimental setup.

Right: Simulation of admittivity (conductivity + permittivity) of tissue sample using Karhunen-Loève expansion.

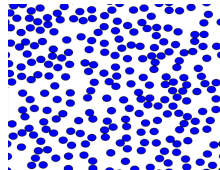


Left: Cheney et al. **Electrical impedance tomography** (1999).



Left: CC image showing blood smear with platelets (purple) and red blood cells (gray).

Right: Numerical simulation using randomly generated circles with periodic boundary.



Uncertainty in physics-based optimization (2/2)

● Boundary conditions (current density, forcing)

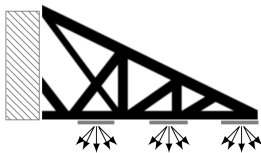
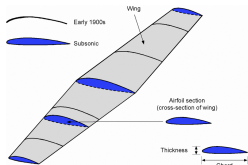


Figure showing cantilever attached to wall on left-hand side and subjected to different scenarios of forces on the lower boundary.

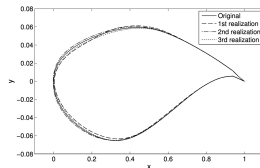
Conti et al. *Stochastic dominance constraints in elastic shape optimization* (2016).

● Manufacturing irregularities (random boundary)



Left: Graphic of airfoil.

Right: Simulation with randomly perturbed boundaries.



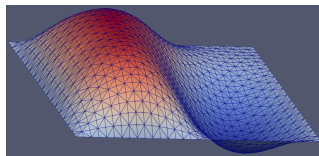
Left: CC; *Right:* Liu et al. *Quantification of airfoil geometry-induced aerodynamic uncertainties-comparison of approaches* (2017).

Application in control of stationary heat source under uncertainty

$$\begin{aligned} \min_{(u,y) \in U \times \mathcal{Y}} \quad & \frac{1}{2} \mathbb{E} [\|y - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2 \\ \text{s.t.} \quad & -\nabla \cdot (a(x, \omega) \nabla y(x, \omega)) = u(x), \text{ in } D \text{ a.s.}, \\ & y(x, \omega) = 0, \quad \text{in } \partial D \text{ a.s.} \end{aligned}$$

$y \dots$ random state (temperature),

$u \dots$ deterministic control (optimization variable).



Realization of temperature $y(\cdot, \omega)$ on domain D .

Interpretation as convex stochastic optimization problem:

- Definition of linear control-to-state map $S(u, \omega) = y(\cdot, \omega) \in Y$ using PDE theory.
- Objective $u \mapsto \frac{1}{2} \mathbb{E} [\|S(u, \cdot) - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2$ depends only on u .
- U, Y are **Banach spaces**.

a.s. = almost surely with respect to \mathbb{P} .

Variants of problem from previous slide

$$\begin{aligned}
 & \min_{(u,y) \in \mathcal{U}_{\text{ad}} \times \mathcal{Y}_{\text{ad}}} \frac{1}{2} \mathcal{R} [\|y - y_d\|_{\mathcal{U}}^2] + \frac{\mu}{2} \|u\|_{\mathcal{U}}^2 \\
 & \text{s.t. } -\nabla \cdot (a(x, \omega) \nabla y(x, \omega)) + y^3(x) = u(x), \text{ in } D \text{ a.s.,} \\
 & \quad \frac{\partial y}{\partial n}(x, \omega) = g(x, \omega), \text{ in } \partial D \text{ a.s.}
 \end{aligned}$$

Examples of popular variants in the literature:

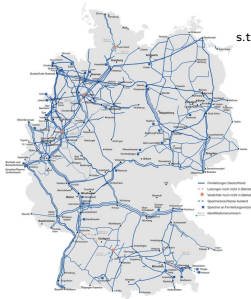
- **Additional constraints** (control or state constraints)
- **Risk measures** (e.g. AV@R)
- **Nonlinearities, other boundary conditions**

Application in gas markets

Subproblem of an N -player noncooperative game:

- Agent i makes decisions $u_i = (p_i^{\text{in}}, p_i^{\text{out}}, q_i^{\text{in}}, q_i^{\text{out}})$ on boundary nodes to minimize loss, while simultaneously satisfying operational constraints.
- System is driven by the collective decisions $u = (u_i)_{i=1}^N$ of all agents.
- Price π depends on decisions of all agents.

$$\max_{u_i \in U_{i,\text{ad}}} \mathbb{E} \left[\int_0^T \pi \left(t, q^{\text{out}}(t), \cdot \right) q_i^{\text{out}}(t) - c(t) q_i^{\text{in}}(t) dt \right] \quad [\text{Maximize profit}]$$



$$\text{s.t. } \left. \begin{aligned} \frac{\partial p_\omega}{\partial t} + \frac{c^2}{A} \frac{\partial q_\omega}{\partial x} &= 0, \\ \frac{\partial q_\omega}{\partial t} + A \frac{\partial p_\omega}{\partial x} &= -\frac{\lambda(\omega)c^2}{2dA} \frac{q_\omega |q_\omega|}{p_\omega} - \frac{Ag \sin \alpha}{c^2} p_\omega, \\ \text{boundary conditions depending on } (u_1, \dots, u_N), \end{aligned} \right\} \quad [\text{PDE describing gas transport}]$$

$$\left. \begin{aligned} \underline{p} &\leq p_\omega(t, x) \leq \bar{p}, \\ \underline{q} &\leq q_\omega(t, x) \leq \bar{q} \quad \text{in } [0, T] \times D \text{ a.s.} \end{aligned} \right\} \quad [\text{State constraints}]$$

Theoretical questions (1/2)

And potential difficulties in infinite dimensions

Problem

$$\min_{u \in U_{\text{ad}}} \mathbb{E}[J(u, \xi)] = \int_{\Omega} J(u, \xi(\omega)) \, d\mathbb{P}(\omega).$$

❶ Existence of solutions

Usual argument:

- Let j^* be optimal value (assumed to be attainable). Choose minimizing sequence (u^n) with $\lim_{n \rightarrow \infty} \mathbb{E}[J(u^n, \xi)] = j^*$
- Show (u^n) bounded \Rightarrow there exists a convergent subsequence (u^{n_k}) such that $u^{n_k} \rightarrow \bar{u}$.
↑ *only true in finite dimensions.*
- Use continuity to conclude that $\mathbb{E}[J(\bar{u}, \xi)] = \lim_{k \rightarrow \infty} \mathbb{E}[J(u^{n_k}, \xi)] = j^*$; feasibility of \bar{u} using closedness of U_{ad} .

❷ Uniqueness of solutions

With strict convexity (easily transferable to infinite dimensions).

Theoretical questions (2/2)

And potential difficulties in infinite dimensions

③ Optimality conditions (constrained problems)

Existence of Lagrange multipliers with (e.g. LI, Slater) constraint qualification.

(CQs generally not transferable to infinite dimensions; derivative needs generalization.)

④ Algorithms

Convergence of methods, e.g. using stochastic gradient:

$$u^{n+1} = u^n - t_n G(u^n, \xi^n), \quad G(u^n, \xi^n) \approx \nabla_u \mathbb{E}[G(u^n, \xi)].$$

(Generally no explicit formula for G ; need for discretization.)

Two-norm discrepancy (1/2)

- The two-norm discrepancy is a phenomenon in optimal control in infinite dimensions due to fact that **not all norms are equivalent**.¹
- Typical situation: **second-order derivative is coercive in weaker norm** than where it is (twice) continuously differentiable (\rightarrow next slide).
- Convergence of optimization algorithms in this setting need to handle this difficulty.

¹Casas, Tröltzsch. Second order analysis for optimal control problems: improving results expected from abstract theory (2012).
Ioffe. Necessary and sufficient conditions for a local minimum. 3: Second order conditions and augmented duality (1979).

Two-norm discrepancy (2/2)

Example (2)

$$\min_{x \in L^2(0,1)} J(x) = \int_0^1 \sin(x(t)) \, dt.$$

Formally, $J''(\bar{x})v^2 = - \int_0^1 \sin(\bar{x}(t))v^2(t) \, dt = \|v\|_{L^2(0,1)}^2$ at global solution $\bar{x}(t) = -\frac{\pi}{2}$.

Other global solutions:

$$x_\varepsilon(t) = \begin{cases} -\frac{\pi}{2}, & \text{if } t \in [0, 1 - \varepsilon], \\ \frac{3\pi}{2}, & \text{if } t \in (1 - \varepsilon, 1] \end{cases} \quad \forall \varepsilon \in (0, 1).$$

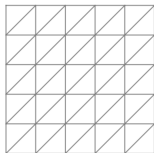
\Rightarrow infinitely many global solutions in L^2 -neighborhood of \bar{x} .

Problem: J is not C^2 in $L^2(0, 1)$ but rather $L^\infty(0, 1)$; but $J''(\bar{x})v^2 \geq c\|v\|_{L^\infty}^2$ not valid.

²Casas, Tröltzsch. Second order analysis for optimal control problems: improving results expected from abstract theory (2012).

Mesh dependence (1/2)

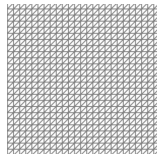
- In numerical simulations, infinite-dimensional problems without a closed-form solution need to be discretized.
- “Mesh independence” in methods refers to the property that convergence behavior should be invariant w.r.t. increasingly finer discretizations.



Two different meshes used in
finite element method.

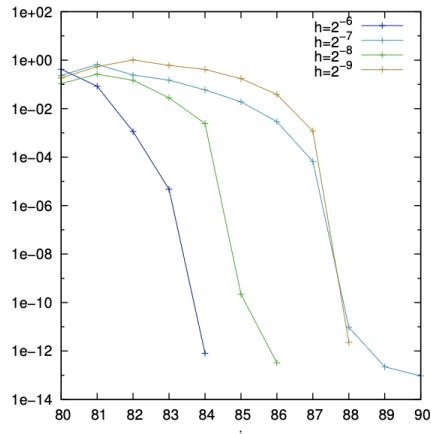
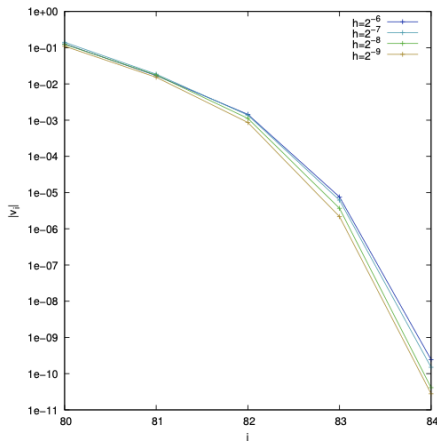
← coarse

fine →



- Mesh dependence can be observed, for example, if the inner product used for the discretized gradient is inconsistent with the correct inner product in the functional-analytic setting.

Mesh dependence (2/2)



Left: Residual as a function of iteration number with mesh independence; *Right:* with mesh dependence.

From C. Rupprecht. **Projection type methods in Banach space with application in topology optimization**, PhD thesis, 2016.

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Banach space

A (real) **Banach space** $(X, \|\cdot\|_X)$ is a complete normed space.

Example

- $L^p(D) = \{\text{Lebesgue-m.b. } u: D \rightarrow \mathbb{R} \mid \int_D |u(x)|^p dx < \infty\} / \sim, p \in [1, \infty), D \subset \mathbb{R}^d$.
- $L^p_\mu(\Omega) = \{\mathcal{F}\text{-m.b. } u: \Omega \rightarrow \mathbb{R} \mid \int_\Omega |u(\omega)|^p d\mu(\omega) < \infty\} / \sim, p \in [1, \infty), \text{ measure space } (\Omega, \mathcal{F}, \mu)$.
- $L^\infty_\mu(\Omega) = \{\mathcal{F}\text{-m.b. } u: \Omega \rightarrow \mathbb{R} \mid \text{esssup}_{\omega \in \Omega} |u(\omega)| < \infty\} / \sim$.
- $W^{k,p}(D) = \{u \in L^p(D) \mid \text{with weak derivatives}^3 D^\alpha u \in L^p(D) \text{ for } |\alpha| \leq k\}$.
- $\mathcal{C}(\bar{D}) = \{u: \bar{D} \rightarrow \mathbb{R} \mid u \text{ is continuous}\}$ with $\bar{D} \subset \mathbb{R}^d$ closed and bounded ($\|u\|_{\mathcal{C}(\bar{D})} := \sup_{x \in \bar{D}} |u(x)|$).
- Hilbert space $(H, (\cdot, \cdot)_H)$ with norm $\|u\|_H := \sqrt{(u, u)_H}$.
- Space $\mathcal{L}(X, Y)$ of all bounded linear operators from X to Y (Banach spaces).

³ $D^\alpha u := v \in L^1_{\text{loc}}(D)$ is the weak derivative of $u \in L^1_{\text{loc}}(D)$ if

$$\int_D v \varphi dx = (-1)^{|\alpha|} \int_D u D^\alpha \varphi dx \quad \text{for all } \varphi \in C_c^\infty(D).$$

Notions that carry over from finite dimensions

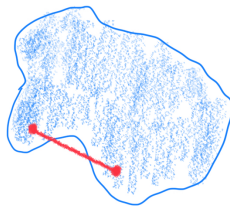
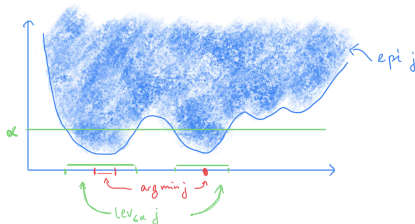
- Definitions of **epi** j , **lev** $_{\leq \alpha} j$, **argmin** j for $j: X \rightarrow \mathbb{R} \cup \{\infty\}$.

- $C \subset X$ is **convex** if $u, v \in C$ implies

$$\lambda u + (1 - \lambda)v \in C \quad (\forall \lambda \in [0, 1]).$$

- $j: X \rightarrow \mathbb{R} \cup \{\infty\}$ **μ -strongly convex** ($\mu > 0$) or **convex** ($\mu = 0$) on $C \subset X$ if

$$\mu \frac{\lambda(1 - \lambda)}{2} \|u - v\|^2 + j(\lambda u + (1 - \lambda)v) \leq \lambda j(u) + (1 - \lambda)j(v) \quad (\forall u, v \in C \text{ and } \lambda \in [0, 1]).$$



A nonconvex set.

Dual space

The topological **dual space** of Banach space X is defined by $X^* := \mathcal{L}(X, \mathbb{R})$ with norm

$$\|x^*\|_{X^*} := \sup_{\|x\|_X=1} \{x^*(x) =: \langle x^*, x \rangle_{X^*, X}\}.$$

Example (Dual space of L_μ^p)

$L_\mu^p(\Omega)^*$ can be identified with $L_\mu^q(\Omega)$ with $\frac{1}{p} + \frac{1}{q} = 1$, $p \in [1, \infty)$, via

$$\langle u^*, u \rangle_{(L_\mu^p)^*, L_\mu^p} := \int_{\Omega} u(\omega) v(\omega) \, d\mu(\omega), \quad u \in L_\mu^p, v \in L_\mu^q, u^* \in (L_\mu^p)^*.$$

Warning: $L_\mu^1(\Omega)$ is only a subspace of $L_\mu^\infty(\Omega)^*$!

Example (Bidual)

The topological bidual space is the dual of the dual space X^* ; i.e., it is defined by $X^{**} := \mathcal{L}(X^*, \mathbb{R})$. X can be identified with a closed subspace of X^{**} via

$$\langle x^{**}, x^* \rangle := \langle x^*, x \rangle \quad \forall x^* \in X^*.$$

Riesz representation theorem

Theorem (Riesz representation for Hilbert space H)

$H^* \cong H$, i.e., for every $u^* \in H^*$ there exists a unique $v \in H$ such that

$$\langle u^*, u \rangle_{H^*, H} = (v, u)_H \quad \forall u \in H, \quad \|u^*\|_{H^*} = \|v\|_H. \quad (1)$$

Conversely, for every $v \in H$, the linear functional u^* defined by (1) is in H^* .

Consequence: Hilbert spaces are reflexive. ⁴

⁴ A Banach space X is called **reflexive** if $X \ni x \mapsto \langle \cdot, x \rangle_{X^*, X} \in X^{**}$ is surjective, i.e.,

$$\forall x^{**} \in X^{**} \exists x \in X : \langle x^{**}, x^* \rangle_{X^{**}, X^*} = \langle x^*, x \rangle_{X^*, X} \quad \forall x^* \in X^*.$$

Derivatives, gradients

A function $F: O \subset X \rightarrow Y$ ($O \neq \emptyset$ open and X, Y Banach spaces) is **Gâteaux differentiable** if the limit

$$dF(x, h) = \lim_{t \rightarrow 0^+} \frac{F(x + th) - F(x)}{t} \in Y$$

exists for all $h \in X$ and $DF(x): X \ni h \mapsto dF(x, h) \in Y$ is bounded and linear, i.e., $DF(x) \in \mathcal{L}(X, Y)$.

It is **Fréchet differentiable** if it also holds that

$$\|F(x + h) - F(x) - DF(x)h\|_Y = o(\|h\|_X) \quad \text{for } \|h\|_X \rightarrow 0.$$

Special case for $j: X \rightarrow \mathbb{R}$, X Hilbert space: the **gradient** $\nabla j: X \rightarrow X$ is the Riesz representation of Dj , i.e.,

$$(\nabla j(x), v)_X = \langle Dj(x), v \rangle_{X^*, X} \quad \forall v \in X.$$

Separability

A Banach space X is **separable** if it contains a countable dense subset, meaning there exists $Y = \{x_i \in X \mid i \in \mathbb{N}\} \subset X$ such that

$$\forall x \in X \forall \varepsilon > 0 \exists y \in Y : \|x - y\|_X < \varepsilon.$$

Example

- $\mathcal{C}(\bar{D})$ with $\bar{D} \subset \mathbb{R}^d$ closed and bounded.
(Polynomials with rational coefficients are dense by Weierstraß's approximation theorem.)
- $L^p(D)$, $W^{k,p}(D)$, $p \in [1, \infty)$, $D \subset \mathbb{R}^d$.
- X is separable if X^* is; (norm)-closed subspaces of a separable X are separable.

Not separable: $L^\infty(D)$, $W^{k,\infty}(D)$!

Strong, weak, weak* topologies

Topologies of interest on Banach space $(X, \|\cdot\|)$ with $\langle \cdot, \cdot \rangle := \langle \cdot, \cdot \rangle_{X^*, X}$:

- **Strong topology** τ_S (generated on X by norm).
 x_n **strongly converges** to \bar{x} ($x_n \rightarrow \bar{x}$) if $\|x_n - \bar{x}\| \rightarrow 0$.
- **Weak topology** τ_W (coarsest one on X so $\langle x^*, \cdot \rangle: X \rightarrow \mathbb{R}$ continuous $\forall x^* \in X^*$).
 x_n **weakly converges** to \bar{x} ($x_n \rightharpoonup \bar{x}$) if $\langle x^*, x_n \rangle \rightarrow \langle x^*, \bar{x} \rangle \quad \forall x^* \in X^*$.
- **Weak* topology** τ_{W^*} (coarsest one on X^* so $\langle \cdot, x \rangle: X^* \rightarrow \mathbb{R}$ continuous $\forall x \in X$).
 x_n^* **weakly* converges** to \bar{x}^* ($x_n^* \rightharpoonup^* \bar{x}^*$) if $\langle x_n^*, x \rangle \rightarrow \langle \bar{x}^*, x \rangle \quad \forall x \in X$.

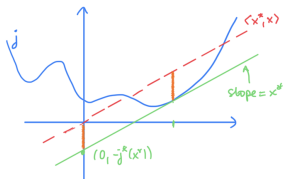
Hierarchy: $\tau_{W^*} \subset \tau_W \subset \tau_S$.

Closedness, lower semicontinuity, and compactness need to be qualified w.r.t. topology!

Notation: \overline{C}^τ ... closure of set C w.r.t. topology τ

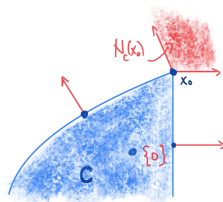
τ -lsc ... $x_n \rightarrow^\tau x$ implies $\liminf_{n \rightarrow \infty} j(x_n) \geq j(x)$.

Notions defined with respect to the dual pairing



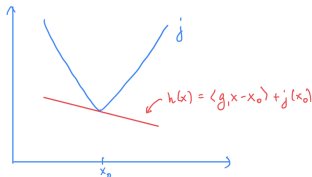
Convex conjugate:

$$j^*(x^*) := \sup_{x \in X} \{ \langle x^*, x \rangle - j(x) \}.$$



Normal cone:

$$N_C(x_0) := \{ y \in X^* \mid \langle y, x - x_0 \rangle \leq 0 \forall x \in C \}.$$



Subdifferential:

$$\partial j(x_0) := \{ g \in X^* \mid j(x) \geq j(x_0) + \langle g, x - x_0 \rangle \forall x \in X \}.$$

Compactness

Fact: closed and bounded sets are not compact in infinite dimensions.

Remedy: work with weaker topologies.

Theorem (Banach–Alaoglu)

Closed unit ball of X^ is weakly* compact.*

Corollary

*Closed unit ball of **reflexive** X is weakly compact.*

Topological minimization theorem

Theorem

Let (X, τ) be a topological space and assume $j: X \rightarrow \mathbb{R} \cup \{\infty\}$ is τ -lower semicontinuous and such that $\text{lev}_{\alpha} j$ is τ -compact. Then, $\inf_{x \in X} j(x) > -\infty$ and there exists some $\bar{x} \in X$ such that

$$j(\bar{x}) \leq j(x) \quad \forall x \in X.$$

Proof. See Theorem 3.2.2 ⁵.

⁵Attouch, Buttazzo, Michaille. **Variational Analysis in Sobolev and BV Spaces** (2014).

Choice of topology



Choice of topology requires **give-and-take**: if τ_1 is stronger than τ_2 , then

$$\overline{\text{lev}_\alpha j}^{\tau_1} \quad \tau_1\text{-compact} \quad \Rightarrow \quad \overline{\text{lev}_\alpha j}^{\tau_2} \quad \tau_2\text{-compact}$$

but

$$j \quad \tau_2\text{-lsc} \quad \Rightarrow \quad j \quad \tau_1\text{-lsc.}$$

Convexity, closedness, and lower semicontinuity

Proposition

(Strongly) **closed convex** subsets of X are weakly sequentially closed.

Corollary

Any **continuous convex** functional $j: X \rightarrow \mathbb{R}$ is weakly lower semicontinuous (lsc), i.e.,

$$x_n \rightharpoonup x \quad \Rightarrow \quad \liminf_{n \rightarrow \infty} j(x_n) \geq j(x).$$

Proof. Use j τ -lsc \Leftrightarrow epi j τ -closed \Leftrightarrow lev $_{\alpha}j$ τ -closed ($\alpha \in \mathbb{R}$).

Operators

A **compact operator** $A \in \mathcal{L}(X, Y)$ maps bounded sets to relatively bounded sets and has the property that

$$X \ni x_n \rightharpoonup x \quad \Rightarrow \quad Ax_n \rightarrow Ax \in Y \quad (\text{weak-to-strong continuity}).$$

Example (Compactness via Sobolev embedding theorem)

Let $D \subset \mathbb{R}^d$ open bounded with Lipschitz boundary ⁶.

- The embedding $\iota: W^{k_1, p_1}(D) \rightarrow W^{k_2, p_2}(D)$ is continuous and compact if

$$k_1 - \frac{d}{p_1} > k_2 - \frac{d}{p_2} \quad \text{and} \quad k_1 > k_2.$$

- The embedding $\iota: W^{k, p}(D) \rightarrow C^{\ell, \alpha}(\bar{D})$ is continuous and compact if

$$k - \frac{d}{p} > \ell + \alpha.$$

⁶meaning boundary can be represented as the graph of a Lipschitz continuous function.

Dual operator

Given an operator $A \in \mathcal{L}(X, Y)$, the **dual operator** $A^* \in \mathcal{L}(Y^*, X^*)$ is defined by

$$\langle A^*u, v \rangle_{X^*, X} = \langle u, Av \rangle_{Y^*, Y} \quad \forall u \in Y^*, \forall v \in X.$$

Theorem (Schauder)

$A \in \mathcal{L}(X, Y)$ is compact $\Leftrightarrow A^* \in \mathcal{L}(Y^*, X^*)$ is compact.

Now let's mix in some stochasticity....

From now on let $(\Omega, \mathcal{F}, \mathbb{P})$ denote a complete probability space.

How about **measurability** in ∞ -dimensions?

Vector-valued mappings

Banach space $(X, \|\cdot\|)$ with $\langle \cdot, \cdot \rangle := \langle \cdot, \cdot \rangle_{X^*, X}$.

A vector-valued mapping $x: \Omega \rightarrow X$ is said to be

- **strongly measurable**, if there exists a sequence of \mathbb{P} -simple functions $\{x_n\}$ such that $\|x_n - x\| \rightarrow 0$ a.s. (\mathbb{P} -a.e.)
- **weakly measurable**, if $\omega \mapsto \langle x^*, x(\omega) \rangle$ is measurable for all $x^* \in X^*$.

A mapping $x^*: \Omega \rightarrow X^*$ is said to be

- **weakly* measurable**, if $\omega \mapsto \langle x^*(\omega), x \rangle$ is measurable for all $x \in X$.

Theorem (Pettis measurability)

x strongly measurable $\Leftrightarrow x$ separably-valued and weakly measurable.

⁷ there exist $\chi_j \in X$, $F_j \in \mathcal{F}$ ($j = 1, \dots, N$) such that

$$x_n(\omega) = \sum_{j=1}^N \chi_j \mathbf{1}_{F_j}(\omega), \quad \omega \in \Omega.$$

Bochner space and its dual

The **Bochner space** $L_{\mathbb{P}}^p(\Omega, X)$ is the set of all (equivalence classes of) strongly measurable $x: \Omega \rightarrow X$ having finite norm given by

$$\|x\|_{L_{\mathbb{P}}^p(\Omega, X)} := \begin{cases} (\int_{\Omega} \|x(\omega)\|_X^p \, d\mathbb{P}(\omega))^{1/p}, & 1 \leq p < \infty, \\ \text{ess sup}_{\omega \in \Omega} \|x(\omega)\|_X, & p = \infty. \end{cases}$$

The limit of the integrals of \mathbb{P} -simple functions x_n gives the **Bochner integral**

$$\mathbb{E}[x] := \int_{\Omega} x(\omega) \, d\mathbb{P}(\omega) = \lim_{n \rightarrow \infty} \int_{\Omega} x_n(\omega) \, d\mathbb{P}(\omega) \in X.$$

Theorem

Suppose X is reflexive or X^ is separable. Then for all $1 \leq p < \infty$, we have the isometric isomorphism*

$$(L_{\mathbb{P}}^p(\Omega, X))^* = L_{\mathbb{P}}^q(\Omega, X^*), \quad \frac{1}{p} + \frac{1}{q} = 1.$$

Proof. See, e.g., Section 1.3 in ⁸

⁸Hytönen et al. **Analysis in Banach spaces** (2016).

Implicit measurability theorem

A helpful result for showing the **measurability of feasible points**:

Theorem (Filippov)

Let $F: X \times \Omega \rightarrow Y$ be a Carathéodory mapping, and suppose $C(\omega) \subset X$ and $D(\omega) \subset Y$ are closed sets that depend measurably on ω . Then the set

$$E = \{\omega \in \Omega \mid \exists x \in C(\omega) \text{ such that } F(x, \omega) \in D(\omega)\}$$

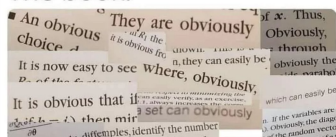
is measurable, and there exists a measurable function $x: E \rightarrow X$ such that

$$x(\omega) \in C(\omega) \quad \text{and} \quad F(x(\omega), \omega) \in D(\omega) \quad \forall \omega \in E.$$

Proof. See Section 8.1⁹ for the proof and other measurability properties.

Professor: "The answer can be found in the book"

The book:



⁹ Aubin, Frankowska. **Set-valued analysis** (1990).

Random linear operators

A random linear operator $A: \Omega \rightarrow \mathcal{L}(Y, W)$ is called **strongly measurable** if for all $y \in Y$, $\omega \mapsto A(\omega)y$ is strongly measurable.

Theorem (Hans¹⁰)

Let $A: \Omega \rightarrow \mathcal{L}(Y, W)$. Then

- $A(\omega)$ is invertible a.s. if and only if $\text{ran}(A^*(\omega)) = Y^*$ a.s.
- if $A(\omega)$ is invertible a.s., then $A^*(\omega)$ is invertible and $(A^*(\omega))^{-1} = (A^{-1}(\omega))^*$,
- if any of the operators $A(\omega)$, $A^{-1}(\omega)$, $A^*(\omega)$, $(A^{-1}(\omega))^*$ is strongly measurable, then they all are.

¹⁰Hans. Inverse and adjoint transforms of linear bounded random transforms (1957).

Derivative of expectation

Lemma

Let $J: X \times \Omega \rightarrow \mathbb{R}$. Suppose

- ❶ $j(v) = \mathbb{E}[J(v, \cdot)]$ is well-defined and finite-valued for all $v \in O \subset X$ (O open),
- ❷ $J_\omega := J(\cdot, \omega)$ is a.s. Fréchet differentiable at $x \in O$,
- ❸ there exists a positive random variable $C \in L^1_{\mathbb{P}}(\Omega)$ such that for all $v \in O$ and almost every $\omega \in \Omega$,

$$\|DJ_\omega(v)\|_{X^*} \leq C(\omega).$$

Then j is Fréchet differentiable at u and

$$Dj(x) = \mathbb{E}[DJ_\omega(x)].$$

Proof. See, e.g., Lemma C.3 in ¹¹.

¹¹G., Scarinci. **Stochastic proximal gradient methods for nonconvex problems in Hilbert spaces** (2021).

Today's agenda

- ➊ Introduction
 - Challenges and examples of applications in physics-based optimization.
- ➋ Foundations of stochastic optimization on Banach spaces
 - Basic definitions, most useful tools and results for optimization.
- ➌ **Optimality conditions**
 - **Constraints on the first and second stage. Adjoint method.**
- ➍ Case study
 - Analysis of example from PDE-constrained optimization under uncertainty.
- ➎ Stochastic approximation
 - Results in Hilbert spaces, handling of numerical error.

Two-stage problems

Two-stage (“recourse”) problem from stochastic programming (on Banach spaces U, Y):

$$\min_{u \in U_{\text{ad}}} J_1(u) + \mathbb{E} \left[\min_{y \in Y} J_2(u, y, \cdot) \right] \quad \text{s.t.} \quad y \in Y_{\text{ad}}(u, \omega) \quad \text{a.s.}$$

Sequence of events:



Interchangeability principle (for J_2 normal integrand ¹²):

$$\min_{y(\cdot) \in L^p_{\mathbb{P}}(\Omega, Y)} \mathbb{E}[J_2(u, y(\cdot), \cdot)] = \mathbb{E} \left[\min_{y \in Y} J_2(u, y, \cdot) \right].$$

¹² meaning $(\text{epi } J_2)(\omega) := \{(u, y, \alpha) \in U \times Y \times \mathbb{R} \mid J_2(u, y, \omega) \leq \alpha\}$ is closed-valued and measurable.

Recourse structures in stochastic programming

Definition (Recourse structures)

The problem

$$\min_{u \in U_{\text{ad}}} J_1(u) + \mathbb{E} \left[\min_{y \in Y} J_2(u, y, \cdot) \right] \quad \text{s.t.} \quad y \in Y_{\text{ad}}(u, \omega) \quad \text{a.s.}$$

is said to satisfy the assumption of

- **complete recourse**, if for every u there exists a feasible $y(\omega)$ \mathbb{P} -a.e. ω ;
- **relatively complete recourse**, if for every *feasible* u there exists a feasible $y(\omega)$ \mathbb{P} -a.e. ω .
- ... other notions (fixed, simple) not used here...

Relevance: special role in optimality conditions (two-stage problems).

Optimality conditions for constrained problem

Deterministic setting

Theorem

Let $U_{\text{ad}} \subset U$ be convex and j be Gâteaux differentiable on an open set covering U_{ad} . Then a necessary condition for $\bar{u} \in U_{\text{ad}}$ to be a solution to $\min_{u \in U_{\text{ad}}} j(u)$ is

$$dj(\bar{u})(v - \bar{u}) \geq 0 \quad \forall v \in U_{\text{ad}}. \quad (2)$$

In case j is convex, (2) is a sufficient condition for optimality of \bar{u} .

Proof. Necessity: For any $v \in U_{\text{ad}}$ and $\lambda \in (0, 1]$,

$$v(\lambda) = \bar{u} + \lambda(v - \bar{u}) \in U_{\text{ad}}.$$

Since \bar{u} is optimal, $j(v(\lambda)) \geq j(\bar{u})$, and also

$$\frac{1}{\lambda}(j(v(\lambda)) - j(\bar{u})) \geq 0.$$

Taking the limit as $\lambda \rightarrow 0$, we obtain (2).

Sufficiency: follows from $j(v) - j(\bar{u}) \geq dj(\bar{u})(v - \bar{u})$.

Problems with reducible objective

Framework for equality constraints

$$\begin{aligned} \min_{(u,y) \in U_{\text{ad}} \times L^p_{\mathbb{P}}(\Omega, Y)} \quad & J_1(u) + \mathbb{E}[J_2(u, y(\cdot), \cdot)] \\ \text{s.t.} \quad & e(u, y(\omega), \omega) = 0 \quad \text{a.s.} \end{aligned}$$

- Control problems are often modeled so that a **control-to-state** operator $S: U \times \Omega \rightarrow Y$ is well-defined (e.g., through PDE theory).
- Problem can be **reduced to single-stage** form

$$\min_{u \in U_{\text{ad}}} \{j(u) := J_1(u) + \mathbb{E}[J_2(u, S(u, \cdot), \cdot)]\}.$$

- For optimality conditions, we need $Dj(u)$ and therefore also the derivative $D_u S(u, \omega)$
 \rightsquigarrow apply implicit function theorem.

Notation: $J_{2,\omega}(u, y(\omega)) = J_2(u, y(\omega), \omega)$, $S_{\omega}(u) = S(u, \omega)$, $e_{\omega}(u, y(\omega)) = e(u, y(\omega), \omega)$.

Implicit function theorem

Theorem (IFT)

Let U, Y, Z be Banach spaces, $e: O \rightarrow Z$ (open $O \subset U \times Y$) continuously Fréchet differentiable, $(\bar{u}, \bar{y}) \in O$ such that $e(\bar{u}, \bar{y}) = 0$ and $D_y e(\bar{u}, \bar{y}) \in \mathcal{L}(Y, Z)$ has a bounded inverse.

Then there exists an open neighborhood $\mathcal{N}_U(\bar{u}) \times \mathcal{N}_Y(\bar{y}) \subset O$ of (\bar{u}, \bar{y}) and a unique continuous function $S: \mathcal{N}_U(\bar{u}) \rightarrow Y$ such that

- ❶ $S(\bar{u}) = \bar{y}$,
- ❷ For all $u \in \mathcal{N}_U(\bar{u})$, there exists exactly one $y \in \mathcal{N}_Y(\bar{y})$ with $e(u, y) = 0$, namely $y = S(u)$.

Moreover, $S: \mathcal{N}_U(\bar{u}) \rightarrow Y$ is continuously Fréchet differentiable with

$$DS(u) = -D_y e(u, S(u))^{-1} D_u e(u, S(u)).$$

If $e: O \rightarrow Z$ is m -times continuously Fréchet differentiable, then so is $S: \mathcal{N}_U(\bar{u}) \rightarrow Y$.

Adjoint method

Approach for computing derivative of $\hat{J}_\omega(u) := J_1(u) + J_{2,\omega}(u, S_\omega(u))$

- Chain rule + adjoint operator:

$$\begin{aligned}
 & \langle D\hat{J}_\omega(u), h \rangle_{U^*, U} \\
 &= \langle DJ_1(u), h \rangle_{U^*, U} + \langle D_u J_{2,\omega}(u, S_\omega(u)), h \rangle_{U^*, U} + \langle D_y J_{2,\omega}(u, S_\omega(u)), DS_\omega(u)h \rangle_{Y^*, Y} \\
 &= \langle DJ_1(u), h \rangle_{U^*, U} + \langle D_u J_{2,\omega}(u, S_\omega(u)), h \rangle_{U^*, U} + \langle (DS_\omega(u))^* D_y J_{2,\omega}(u, S_\omega(u)), h \rangle_{U^*, U}.
 \end{aligned}$$

- IFT in adjoint form: $(DS_\omega(u))^* = -(D_u e_\omega(u, S_\omega(u)))^* D_y e_\omega(u, S_\omega(u))^{-*}$.

$$\Rightarrow (DS_\omega(u))^* D_y J_{2,\omega}(u, S_\omega(u)) = -(D_u e_\omega(u, S_\omega(u)))^* \underbrace{D_y e_\omega(u, S_\omega(u))^{-*} D_y J_{2,\omega}(u, S_\omega(u))}_{=:-p_\omega}$$

- Derivative:

$$D\hat{J}_\omega(u) = DJ_1(u) + D_u J_{2,\omega}(u, S_\omega(u)) + D_u e_\omega(u, S_\omega(u))^* p_\omega,$$

where p_ω solves the adjoint equation

$$D_y e_\omega(u, S_\omega(u))^* p_\omega = -D_y J_{2,\omega}(u, S_\omega(u)).$$

Optimality conditions for reducible objective

Summary: necessary optimality conditions for $\bar{u} \in U_{\text{ad}}$ to be a solution to

$$\begin{aligned} \min_{(u,y) \in U_{\text{ad}} \times L^p_{\mathbb{P}}(\Omega, \mathcal{Y})} \quad & J_1(u) + \mathbb{E}[J_2(u, y(\cdot), \cdot)] \\ \text{s.t.} \quad & e(u, y(\omega), \omega) = 0 \quad \text{a.s.} \end{aligned}$$

given by

$$\langle DJ_1(\bar{u}) + \mathbb{E}[D_u J_{2,\omega}(\bar{u}, S_\omega(\bar{u})) + D_u e_\omega(\bar{u}, S_\omega(\bar{u}))^* \bar{p}_\omega], v - \bar{u} \rangle_{U^*, U} \geq 0 \quad \forall v \in U_{\text{ad}},$$

where \bar{p}_ω solves the adjoint equation

$$D_y e_\omega(\bar{u}, S_\omega(\bar{u}))^* p_\omega = -D_y J_{2,\omega}(\bar{u}, S_\omega(\bar{u})).$$

Note: “ $D\mathbb{E}[J_\omega] = \mathbb{E}[DJ_\omega]$ ” needs to be justified above.

Problems without reducible form

Historical development

PACIFIC JOURNAL OF MATHEMATICS
Vol. 42, No. 1, 1974

STOCHASTIC CONVEX PROGRAMMING: BASIC DUALITY

R. T. ROCKAFELLAR AND R. J.-B. WETS

A duality theory is developed for stochastic programs with convex objective and convex constraints. The problem consists in selecting $x_1 \in R^n$ and $x_2 \in \mathcal{L}^n(S, \Sigma, \sigma; R^n)$ so as to satisfy the constraints and minimize total expected cost, where σ is a probability measure and the constraints as well as the objective are functions of the random elements of the problem. Under the additional restriction that x_1 and $x_2(s)$ belong to compact subsets of R^n and R^n respectively, it is shown that the problem is equivalent to the more common dynamic formulation for stochastic programs with recourse, a basic duality theorem — of the type $\min = \sup$ — is proved and qualitative results on the existence of dual solutions are derived.

1. Introduction. In this paper we study a two-stage stochastic optimization problem associated with the following heuristic model. First, a vector x_1 in R^n is chosen subject to the constraints

$$(1.1) \quad x_1 \in C_1 \quad \text{and} \quad f_{i1}(x_1) \leq 0, \quad i = 1, \dots, m_1,$$

at a cost represented by the expression $f_{01}(x_1)$. Next an element s of S is "observed", where (S, Σ, σ) is a probability space. Finally, a vector $x_2(s)$ in R^n is chosen subject to the constraints

$$(1.2) \quad x_2(s) \in C_2 \quad \text{and} \quad f_{i2}(s, x_1, x_2(s)) \leq 0, \quad i = 1, \dots, m_2,$$

at a cost $f_{02}(s, x_1, x_2(s))$. The problem is to choose x_1 and the function $x_2(\cdot)$ so as to minimize the total expected cost

$$(1.3) \quad f_{01}(x_1) + \int_S f_{02}(s, x_1, x_2(s)) \sigma(ds).$$

This is a *stochastic programming problem with recourse*; the function $x_2(\cdot)$ specifies the recourse decision.

KKT conditions ¹³

- Choice of function space $L_P^\infty(\Omega, \mathbb{R}^n)$.
- Lagrange multipliers in $L_P^1(\Omega, \mathbb{R}^n)$ under **relatively complete recourse** condition, **constraint qualification**.

\rightsquigarrow convenient for algorithm building!

¹³

Rockafellar, Wets. Stochastic convex programming: Kuhn-Tucker conditions (1975), Stochastic convex programming: basic duality (1976), Stochastic convex programming: relatively complete recourse and induced feasibility (1976), Stochastic convex programming: singular multipliers and extended duality singular multipliers and duality (1976).

Problems without reducible form

Generalized Rockafellar/Wets framework ¹⁴

$$\begin{aligned} \min_{(u,y) \in U_{\text{ad}} \times L_{\mathbb{P}}^p(\Omega, Y)} \quad & \{\mathcal{J}(u, y) := J_1(u) + \mathbb{E}[J_2(u, y(\cdot), \cdot)]\} \\ \text{s.t.} \quad & e(u, y(\omega), \omega) = 0 \quad \text{a.s.}, \quad i(u, y(\omega), \omega) \leq_K 0 \quad \text{a.s.} \end{aligned}$$

Existence of Lagrange multipliers under **constraint qualification** (strict feasibility):

$$0 \in \text{int dom } v,$$

with value function of *perturbed problem*

$$\begin{aligned} v(\phi) &:= \inf_{(u,y) \in U \times L_{\mathbb{P}}^p(\Omega, Y)} \mathcal{J}(u, y) + \delta_{F_{\text{ad}, \phi}}(u, y), \\ \text{where } F_{\text{ad}, \phi} &:= \{(u, y) \in U_{\text{ad}} \times L_{\mathbb{P}}^p(\Omega, Y) \mid e(u, y(\omega), \omega) = \phi_e(\omega) \text{ a.s.}, \\ &\quad i(u, y(\omega), \omega) \leq_K \phi_i(\omega) \text{ a.s.}\}. \end{aligned}$$

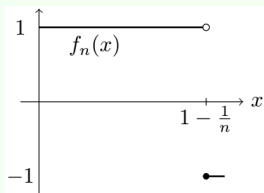
Notation: $k \leq_K 0 \Leftrightarrow -k \in K$.

¹⁴ G., Wollner. *Optimality conditions for almost sure state constraints* (2021). G., Hintermüller. *Moreau–Yosida regularization for almost sure state constraints* (2022). G., Henrion. *Optimality conditions with chance constraints* (2024).

Choice of function spaces depends on CQ

Fact: for $p \in [1, \infty)$, $K \subset L^p_{\mathbb{P}}(\Omega)$ has an empty interior unless Ω is finite dimensional.

Example ($L^2_+(0, 1) = \{f \in L^2(0, 1) \mid f \geq 0\}$ has empty interior ¹⁵)



For $\mathbb{P} = \text{Lebesgue measure}$; $\Omega = (0, 1)$:
 $f \equiv 1$ is not an interior point of $K = L^2_+(0, 1)$:
 for

$$f_n(x) = \begin{cases} 1, & [0, 1 - \frac{1}{n}) \\ -1, & [1 - \frac{1}{n}, 1] \end{cases},$$

we have $\|f_n - f\|_{L^2(0,1)} \rightarrow 0$ but $f_n \notin K$ for all n .
 $\Rightarrow f \notin \text{int } K$.

Consequence: CQ requires using function spaces with sets having nonempty interiors ($L^\infty_{\mathbb{P}}(\Omega, X)$, X sufficiently regular).

¹⁵Tröltzsch. Optimal control of partial differential equations (2009).

Yosida-Hewitt-type decomposition on $L_{\mathbb{P}}^{\infty}(\Omega, X)^*$

For X separable

Theorem ⁽¹⁶⁾

Every $v^* \in L_{\mathbb{P}}^{\infty}(\Omega, X)^*$ has a unique decomposition

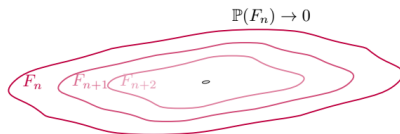
$$v^* = v + v^{\circ},$$

where v is absolutely continuous^{*} and v° is singular^{**} relative to \mathbb{P} .

(^{*}) \exists weakly^{*} measurable $x^* : \Omega \rightarrow X^*$ with $\|x^*(\cdot)\|_{X^*} \in L_{\mathbb{P}}^1(\Omega)$ s.t.

$$v(x) = \int_{\Omega} \langle x^*(\omega), x(\omega) \rangle_{X^*, X} d\mathbb{P}(\omega).$$

(^{**}) There exist $\{F_n\} \subset \mathcal{F}$ such that
 $\forall n : x|_{F_n} = 0 \Rightarrow \langle \lambda^{\circ}, x \rangle = 0.$



If X **separable and reflexive**, absolutely continuous functionals belong to $L_{\mathbb{P}}^1(\Omega, X^*)$.

¹⁶ Ioffe, Levin. Subdifferentials of convex functions (1972).
 Corrected proof in Levin. The Lebesgue decomposition for functionals on the vector-function space L_X^{∞} (1974).

Existence of Lagrange multipliers

Convex problems: conjugate duality à la Rockafellar and Wets:

- ① Show saddle points $\lambda^* := (\lambda_e^*, \lambda_i^*) \in (L_{\mathbb{P}}^p(\Omega, W))^* \times (L_{\mathbb{P}}^p(\Omega, R))^*$ of Lagrangian

$$\bar{L}(u, y, \lambda^*) = j(u, y) + \langle \lambda_e^*, e(u, y, \cdot) \rangle + \langle \lambda_i^*, i(u, y, \cdot) \rangle$$

exist (assumption: CQ + bounded feasible set or coercive j).

- ② Use Yosida–Hewitt decomposition

$$\lambda_e^* = \lambda_e^a + \lambda_e^o \in L_{\mathbb{P}}^\infty(\Omega, W)^*, \quad \lambda_i^* = \lambda_i^a + \lambda_i^o \in L_{\mathbb{P}}^\infty(\Omega, R)^*$$

and argue that singular multipliers λ_e^o, λ_i^o vanish (with **relatively complete recourse**).
Generally **not** satisfied by optimal control problems with state constraints!

Nonconvex problems: existence of Lagrange multipliers with ¹⁷

¹⁷ Zowe, Kurcyusz. Regularity and stability for the mathematical programming problem in Banach spaces (1979).

Problem with purely singular multipliers

Example ⁽¹⁸⁾

Problem:

$$\min_{u \geq 0} -u \quad \text{s.t.} \quad G(u, \omega) := u - \omega \leq 0 \text{ in } \Omega := [1, 2]. \quad (3)$$

- Solution $u^* = 1$.
- Optimality conditions:

$$\langle \lambda^*, \mathbf{1}(\cdot) \rangle = -1, \quad G(u^*, \omega) \leq 0 \text{ in } \Omega, \quad \lambda^* \in \mathcal{K}^-, \quad \langle \lambda^*, G(u^*, \cdot) \rangle = 0.$$

- $F_n := (1, 1 + 1/n)$ so that $\mathbb{P}(F_n) \rightarrow 0$ as $n \rightarrow \infty$ for Lebesgue measure \mathbb{P} .
- Since $G(u^*, \cdot) < -1/n$ on $\Omega \setminus F_n$, we have $B_{1/n}(G(u^*, \cdot)) \subset L_-^\infty(\Omega)$.
- $y \in L^\infty(\Omega)$ with $y = 0$ on F_n , ρ_n small enough so that $\rho_n y \in B_{1/n}(G(u^*, \cdot))$.
- Due to complementarity conditions, we have

$$\begin{aligned} \langle \lambda^*, G(u^*, \cdot) \pm \rho_n y \rangle &= \pm \rho_n \langle \lambda^*, y \rangle \leq 0 \quad \Rightarrow \langle \lambda^*, y \rangle = 0 \quad \forall y : y = 0 \text{ on } F_n \\ &\Rightarrow \lambda^* = \lambda^\circ \neq 0 \quad (\langle \lambda^*, \mathbf{1}(\cdot) \rangle = -1). \end{aligned}$$

Notation: $\mathbf{1}(\omega) = 1$ for all $\omega \in \Omega$, $\mathcal{K}^- = \{k^* \in L^\infty(\Omega)^* \mid \langle k^*, k \rangle \leq 0 \forall k \in L_-^\infty(\Omega)\}$.

¹⁸Bonnans. *Convex and stochastic optimization* (2019).

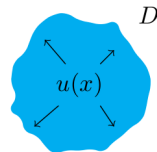
Today's agenda

- ➊ Introduction
 - Challenges and examples of applications in physics-based optimization.
- ➋ Foundations of stochastic optimization on Banach spaces
 - Basic definitions, most useful tools and results for optimization.
- ➌ Optimality conditions
 - Constraints on the first and second stage. Adjoint method.
- ➍ **Case study**
 - **Analysis of example from PDE-constrained optimization under uncertainty.**
- ➎ Stochastic approximation
 - Results in Hilbert spaces, handling of numerical error.

Case study

Optimal control of stationary heat source under uncertainty

$$\begin{aligned}
 & \min_{(u,y) \in U_{\text{ad}} \times \mathcal{Y}} \frac{1}{2} \mathbb{E} [\|y - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2 \\
 & \text{s.t. } -\nabla \cdot (a(x, \omega) \nabla y(x, \omega)) = u(x) + f(x, \omega), \quad x \in D \quad \text{a.s.}, \\
 & \quad \quad y(x, \omega) = 0, \quad x \in \partial D \quad \text{a.s.}
 \end{aligned}
 \tag{P}$$



Theoretical questions:

- Solvability of random PDE
- Solvability of optimization problem
- Optimality conditions

Notation: $\nabla \cdot (a(x, \omega) \nabla y(x, \omega)) = \sum_{i=1}^d \frac{\partial}{\partial x_i} \left(a(x, \omega) \frac{\partial y(x, \omega)}{\partial x_i} \right)$

Case study

Solution to the random PDE

Lemma

Suppose $D \subset \mathbb{R}^d$ is open and bounded with Lipschitz boundary, $u, f(\cdot, \omega) \in U := L^2(D)$, and $0 < a_{\min} < a(x, \omega) < a_{\max} < \infty \forall x \in D$. Then **there exists a unique weak solution** $y(\cdot, \omega) \in H_0^1(D)$ to PDE in (P) that satisfies

$$\int_D a(x, \omega) \nabla y(x, \omega) \cdot \nabla v(x) \, dx = \int_D (u(x) + f(x, \omega)) v(x) \, dx \quad \forall v \in H_0^1(D).$$

Moreover, there exists $C_1 > 0$ such that

$$\|y(\cdot, \omega)\|_{H^1(D)} \leq C_1 (\|u\|_{L^2(D)} + \|f(\cdot, \omega)\|_{L^2(D)}). \quad (4)$$

Moreover, if $a \in L_{\mathbb{P}}^{\infty}(\Omega, L^{\infty}(D))$, $f \in L_{\mathbb{P}}^p(\Omega, L^2(D))$, then $y \in \mathcal{Y} := L_{\mathbb{P}}^p(\Omega, H_0^1(D))$.

Proof. Existence/uniqueness by Lax–Milgram lemma. Strong measurability by Filippov's theorem.

Notation: $H_0^1(D) := \overline{C_c^{\infty}(D)}^{\|\cdot\|_{H^1(D)}}$ and $H^1(D) = W^{1,2}(D)$.

Case study

Definition of control-to-state operator

Lemma justifies writing PDE as operator equation in $H^{-1}(D) := (H_0^1(D))^*$:

$$\mathbf{A}(\omega)\mathbf{y}(\omega) = \mathbf{B}(\mathbf{u} + \mathbf{f}(\omega))$$

with

$$\begin{aligned} A(\omega): H_0^1(D) &\rightarrow H^{-1}(D) & A(\omega)y &:= -\nabla \cdot (a(\cdot, \omega) \nabla y), \\ B: L^2(D) &\rightarrow H^{-1}(D) & & \text{(compact) embedding.} \end{aligned}$$

(Parametrized) **control-to-state map**

$$S: \underbrace{U}_{:=L^2(D)} \times \Omega \rightarrow \underbrace{Y}_{:=H_0^1(D)}, \quad (u, \omega) \mapsto A^{-1}(\omega)B(u + f(\omega)).$$

Linear and continuous in u by (4)!

Case study

Existence of solution

Reduced formulation of problem (P):

$$\min_{(u,y) \in U_{\text{ad}} \times \mathcal{Y}} \left\{ \frac{1}{2} \mathbb{E} [\|y - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2 \right\} \longrightarrow \min_{u \in U_{\text{ad}}} \frac{1}{2} \mathbb{E} [\|S(u, \cdot) - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2.$$

s.t. $A(\omega)y(\omega) = B(u + f(\omega))$

Proposition

Suppose $y_d \in L^2(D)$, $f \in L^2_{\mathbb{P}}(\Omega, L^2(D))$, and $\emptyset \neq U_{\text{ad}} \subset L^2(D)$ is closed and convex. Then if U_{ad} is bounded or $\mu > 0$, there exists a solution to problem (P).

Case study

Existence of solution

Proof.

- $j(u) := \frac{1}{2} \mathbb{E} [\|S(u, \cdot) - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2$ bounded below $\Rightarrow j^* = \inf_{u \in U_{\text{ad}}} j(u)$ exists.
- Take minimizing sequence $\{u_n\} \subset U_{\text{ad}}$ with $j(u_n) \rightarrow j^*$ (bounded by assumption).
- $L^2(D)$ is reflexive, so there exists $\{u_{n_k}\}$ and $\bar{u} \in U_{\text{ad}}$ such that $u_{n_k} \rightharpoonup u^*$.
- j continuous since $u \mapsto \frac{1}{2} \|S(u, \omega) - y_d\|_U^2 + \frac{\mu}{2} \|u\|_U^2$ continuous a.s. and $S(u, \cdot) \in L^2_{\mathbb{F}}(\Omega, H^1_0(D))$.
- j is weakly lsc since it is continuous* and convex $\Rightarrow u^*$ solves problem (P).

Case study

Optimality conditions (1/2)

Necessary and sufficient conditions in an optimum \bar{u} :

$$\langle Dj(\bar{u}), v - \bar{u} \rangle_{U^*, U} \geq 0 \quad \forall v \in U_{\text{ad}}.$$

Computation using $D_u S(u, \omega) = D_u A^{-1}(\omega) B(u + f(\omega)) = A^{-1}(\omega) B$:

$$\begin{aligned} \langle Dj(\bar{u}), v \rangle_{U^*, U} &= \left\langle D_u \left(\frac{1}{2} \mathbb{E} [\|S(\bar{u}, \cdot) - y_d\|_U^2] + \frac{\mu}{2} \|\bar{u}\|_U^2 \right), v \right\rangle_{U^*, U} \\ &= \int_{\Omega} \left\langle D_u \left(\frac{1}{2} \|S(\bar{u}, \omega) - y_d\|_U^2 \right), v \right\rangle_{U^*, U} d\mathbb{P}(\omega) + \left\langle D_u \frac{\mu}{2} \|\bar{u}\|_U^2, v \right\rangle_{U^*, U} \\ &= \int_{\Omega} \langle S(\bar{u}, \omega) - y_d, D_u S(\bar{u}, \omega) v \rangle_{U^*, U} d\mathbb{P}(\omega) + \langle \mu \bar{u}, v \rangle_{U^*, U} \\ &= \int_{\Omega} \langle D_u S(\bar{u}, \omega)^* (S(\bar{u}, \omega) - y_d), v \rangle_{U^*, U} d\mathbb{P}(\omega) + \langle \mu \bar{u}, v \rangle_{U^*, U} \\ &= \int_{\Omega} \langle B^* \underbrace{A^{-*}(\omega)(S(\bar{u}, \omega) - y_d)}_{=: \bar{p}(\omega)}, v \rangle_{U^*, U} d\mathbb{P}(\omega) + \langle \mu \bar{u}, v \rangle_{U^*, U}. \end{aligned}$$

\rightsquigarrow **Introduction of adjoint variable $\bar{p}(\omega)$ allows for numerical computation.**

Case study

Optimality conditions (2/2)

Resulting optimality conditions:

$$\begin{aligned}\langle \mathbb{E}[B^* \bar{p}(\cdot)] + \mu \bar{u}, v - \bar{u} \rangle_{U^*, U} &\geq 0 \quad \forall v \in U_{\text{ad}}, \\ A^*(\omega) \bar{p}(\omega) &= \bar{y}(\omega) - y_d \quad \text{a.s.} \\ A(\omega) \bar{y}(\omega) &= B(\bar{u} - f(\omega)) \quad \text{a.s.}\end{aligned}$$

Or more explicitly:

$$\begin{aligned}\langle \mathbb{E}[B^* \bar{p}(\cdot)] + \mu \bar{u}, v - \bar{u} \rangle_{U^*, U} &\geq 0 \quad \forall v \in U_{\text{ad}}, \\ -\nabla \cdot (a(x, \omega) \nabla \bar{p}(x, \omega)) &= \bar{y}(x, \omega) - y_d(x) \text{ on } D \times \Omega, & \bar{p}(x, \omega) &= 0 \text{ on } \partial D \times \Omega, \\ -\nabla \cdot (a(x, \omega) \nabla \bar{y}(x, \omega)) &= \bar{u}(x) - f(x, \omega) \text{ on } D \times \Omega, & \bar{y}(x, \omega) &= 0 \text{ on } \partial D \times \Omega.\end{aligned}$$

Gradient $\nabla j(\bar{u}) = \mathbb{E}[\bar{p}] + \mu \bar{u} \in L^2(D)$ (application of Riesz representation theorem).

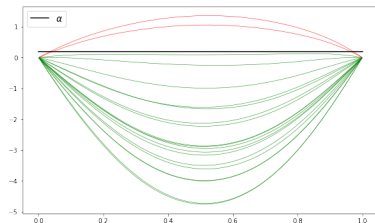
The model problem with almost sure state constraints (irreducible)

$$\begin{aligned}
 \min_{(u,y) \in U_{\text{ad}} \times \mathcal{Y}} \quad & \frac{1}{2} \mathbb{E} [\|y - y_d\|_U^2] + \frac{\mu}{2} \|u\|_U^2 \\
 \text{s.t.} \quad & -\nabla \cdot (a(x, \omega) \nabla y(x, \omega)) = u(x) + f(x, \omega), \quad x \in D \quad \text{a.s.}, \\
 & y(x, \omega) = 0, \quad x \in \partial D \quad \text{a.s.}, \\
 & \mathbf{y(x, \omega) \leq \alpha} \quad x \in D \quad \text{a.s.}
 \end{aligned} \tag{P_s}$$

- Problem (P_s) fits the framework of a two-stage decision problem.
- More forgiving model: **chance-constrained** setting

$$\mathbb{P}(y(x, \omega) \leq \alpha \quad \forall x \in D) \geq p, \quad p \in (0, 1).$$

- Theoretical challenges (optimality conditions) and numerical methods currently unsatisfactory.



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Solution of stochastic optimization problems

Strategies for solving stochastic optimization problem

$$\min_{u \in U} \left\{ j(u) = \mathbb{E}[J(u, \xi)] := \int_{\Omega} J(u, \xi(\omega)) \, d\mathbb{P}(\omega) \right\} :$$

- For small stochastic dimension: quadrature/other discretization for the integral.
- Sample average approximation (SAA): take one-time sample $\{\hat{\xi}^1, \dots, \hat{\xi}^m\}$ and solve

$$\min_{u \in U} \frac{1}{m} \sum_{i=1}^m J(u, \hat{\xi}^i)$$

using, e.g., deterministic optimization method.

- “Stochastic approximation” (SA): dynamically sample while optimizing, e.g., with stochastic gradient method (SG)

$$u^{n+1} := u^n - t_n G(u^n, \xi^n), \quad G(u^n, \xi^n) \approx \nabla j(u^n).$$

Inspiration for SA: up-and-down method

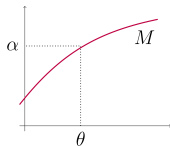
Dixon and Mood's “up-and-down” method ¹⁹ for finding the root of a function, demonstrated on an application where the critical height for explosives to detonate is determined experimentally:

RECORD OF A SAMPLE OF SIXTY TESTS				
Normalized Height				Number of x's o's
2.0	x			1
1.7	x x x		x x x	10
1.4		o x o x	x x x x o o x o x x x o x x x o x x o x x o x	18 9
1.1		o	x o o o o o o	2 18
0.8			o	2

FIGURE 1

¹⁹Dixon and Mood. A method for obtaining and analyzing sensitivity data (1948).

Stochastic approximation (origins)



- Stochastic version by Robbins & Monro ²⁰ for computing the (unique) root of an equation $M(u) = \alpha$, for a monotone function $M(u) = \int_{-\infty}^{\infty} y \, dH(y|u)$.

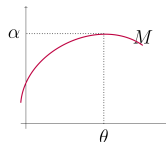
- Iterations of the form

$$u^{n+1} = u^n - t_n(y^n - \alpha),$$

$y^n \dots$ random variable with CDF $H(y|u^n)$.

- Kiefer & Wolfowitz ²¹ procedure for maximizing a regression function M using central-difference approximations:

$$u^{n+1} = u^n - t_n \frac{y^{2n-1} - y^{2n}}{c_n}.$$



Convergence in L^2 and in probability with proper choice of t_n , c_n .

²⁰ Robbins, Monro. **A stochastic approximation method** (1951).

²¹ Kiefer, Wolfowitz. **Stochastic estimation of the maximum of a regression function** (1952).

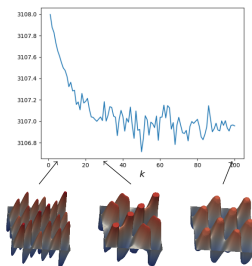
SA in function spaces

Literature:

- Goldstein. **Minimizing noisy functionals in Hilbert space: an extension of the Kiefer–Wolfowitz procedure** (1988).
- Yin and Zhu. **On H -valued Robbins–Monro processes** (1990).
- Culioli and Cohen. **Decomposition/coordination algorithms in stochastic optimization** (1990).
- Barty, Roy, and Strugarek. **Hilbert-valued perturbed subgradient algorithms** (2007).
- Bittar, Carpentier, Chancelier. **The stochastic auxiliary problem principle in Banach spaces: measurability and convergence** (2022).

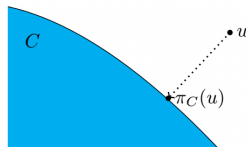
For PDE-constrained optimization under uncertainty:

- Martin, Nobile, (Krumscheid, Tsilifis) (2018, 2019, 2021)
- G. (Pflug, Scarinci, Wollner) (2019, 2020, 2021, 2023)
- Kouri, Surowiec, Staudigl (2023)
- Other recent contributions...



The projection operator

For $C \subset U$, the **projection operator** is defined by the point-to-set mapping $\pi_C: U \rightrightarrows C$, $u \mapsto \pi_C(u) = \operatorname{argmin}_{v \in C} \|u - v\|$.



Projection generally set-valued.

Lemma

If $C \neq \emptyset$ is closed and convex, then (1) $\pi_C: U \rightarrow C$ (single-valued).
 (2) π_C is non-expansive, i.e., $\|\pi_C(u) - \pi_C(v)\| \leq \|u - v\|$ for all u, v .

Proof. Bauschke & Combette, Section 3.2.

Problem structures

The structure of the objective function plays a huge role in convergence proofs of iterative methods.

- **Finite sum:** $\min_{u \in U_{\text{ad}}} \frac{1}{m} \sum_{i=1}^m J_i(u)$
 \rightsquigarrow Special benefit of finite-sum structure: regular sampling of full gradient possible.
- **General (finite or infinite sum):** $\min_{u \in U_{\text{ad}}} \mathbb{E}[J(u, \xi)]$.
- **Strongly convex, convex, quasiconvex**
- **Lipschitz gradient**
- ...

(Strong) convexity for smooth objectives

Lemma

If $j: U \rightarrow \mathbb{R}$ is μ -strongly convex and differentiable, then

$$j(u) - j(v) \geq (\nabla j(v), u - v) + \frac{\mu}{2} \|u - v\|^2 \quad \forall u, v \in U. \quad (5)$$

In the convex and differentiable case, (5) holds with $\mu = 0$.

Proof. Convex case: we have

$$\begin{aligned} j(\lambda u + (1 - \lambda)v) &\leq \lambda j(u) + (1 - \lambda)j(v) \\ \Leftrightarrow \frac{j(v + \lambda(u - v)) - j(v)}{\lambda} &\leq j(u) - j(v). \end{aligned}$$

Taking limit as $\lambda \rightarrow 0$, we obtain $(\nabla j(v), u - v) \leq j(u) - j(v)$.

Strongly convex case: first prove that j is strongly convex iff there exists a convex h such that $j(u) = h(u) + \frac{\mu}{2} \|u\|^2$. Then, proceed as above.

Uniqueness of minimizers in strongly convex case

Lemma

If j is μ -strongly convex and $U_{\text{ad}} \neq \emptyset$ is closed and convex, then

$$\min_{u \in U_{\text{ad}}} j(u)$$

has a unique solution.

Proof. (**for differentiable j**): optimality of $\bar{u} \in U_{\text{ad}}$ gives $(\nabla j(\bar{u}), v - \bar{u}) \geq 0$ for all $v \in U_{\text{ad}}$. Then for two optima \bar{u}_1, \bar{u}_2 , we have

$$0 = j(\bar{u}_1) - j(\bar{u}_2) \geq \frac{\mu}{2} \|\bar{u}_1 - \bar{u}_2\|^2.$$

L -smooth functions

A function $j: U \rightarrow \mathbb{R}$ is called **L -smooth** ($L > 0$) if it is differentiable and the gradient $\nabla j: U \rightarrow U$ is L -Lipschitz, i.e.,

$$\|\nabla j(u) - \nabla j(v)\| \leq L\|u - v\| \quad \forall u, v \in U.$$

The set of L -smooth functions is denoted by $\mathcal{C}_L^{1,1}(U)$.

Lemma

If $j \in \mathcal{C}_L^{1,1}(U)$, then

$$j(u) \leq j(v) + (\nabla j(v), u - v) + \frac{L}{2}\|u - v\|^2 \quad \forall u, v \in U. \quad (6)$$

Proof. By the fundamental theorem of calculus,

$$\begin{aligned} j(u) &= j(v) + \int_0^1 (\nabla j(v + t(u - v)), u - v) \, dt \\ &= j(v) + (\nabla j(v), u - v) + \int_0^1 (\nabla j(v + t(u - v)) - \nabla j(v), u - v) \, dt. \end{aligned}$$

Use Cauchy–Schwarz combined with Lipschitz condition and integrate.

L -smoothness and convexity

Lemma

If $j: U \rightarrow \mathbb{R}$ is convex and L -smooth, then it is also **cocoercive**, i.e.,

$$\frac{1}{L} \|\nabla j(u) - \nabla j(v)\|^2 \leq (\nabla j(v) - \nabla j(u), v - u). \quad (7)$$

Proof. Using convexity and L -smoothness,

$$j(u) - j(v) \pm j(z) \leq (\nabla j(u), u - z) + (\nabla j(v), z - v) + \frac{L}{2} \|z - v\|^2. \quad (\star)$$

Minimizing right-hand side w.r.t. z , we get $z = v - \frac{1}{L}(\nabla j(v) - \nabla j(u))$. Substituting z into (\star) , we can verify

$$j(u) - j(v) \leq (\nabla j(u), u - v) - \frac{1}{2L} \|\nabla j(v) - \nabla j(u)\|^2. \quad (\star\star)$$

Claim follows by applying $(\star\star)$ twice (exchanging roles of u and v).

Projected stochastic gradient (PSG) method

PSG method for solving $\min_{u \in U_{\text{ad}}} \{j(u) := \mathbb{E}[J(u, \xi)]\}$:

$$u^{n+1} = \pi_{U_{\text{ad}}} \left(u^n - t_n G(u^n, \xi^n) \right), \quad G(u^n, \xi^n) \approx \nabla j(u^n)$$

Notes:

- Robbins–Monro step-sizes:

$$t_n \geq 0, \quad \sum_{n=1}^{\infty} t_n = \infty, \quad \sum_{n=1}^{\infty} t_n^2 < \infty.$$

$\rightsquigarrow j(u^{n+1}) > j(u^n)$ possible: technically not a descent method!

- ξ^n is randomly chosen and independent of previous realization ξ^1, \dots, ξ^{n-1} .

With bias (“quasigradient”):

$$G(u^n, \xi^n) = \nabla j(u^n) + \underbrace{r^n}_{\text{bias}} + \underbrace{w^n}_{\text{mean 0}}$$

(∞ -dimensional case: discretization needed).

Example

- Single realization: $\nabla_u J(u^n, \xi^n)$
- Minibatch: $\frac{1}{m_n} \sum_{i=1}^{m_n} \nabla_u J(u^n, \xi^{n,i})$
- Minibatch/single with additive bias: $\frac{1}{m_n} \sum_{i=1}^{m_n} \nabla_u J(u^n, \xi^{n,i}) + r^n$

Types of probabilistic convergence

Feature: the i.i.d. sequence $\xi^n \sim \mathbb{P}$, $n \in \mathbb{N}$, induces a discrete stochastic process $\{u^n\} \rightarrow$ probabilistic convergence statements.

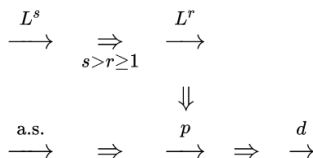


Figure: Relationship between convergence in L^p , almost sure (a.s.), probability (p), and distribution (d).

Typical for SA: proofs of L^2 convergence and almost sure convergence.

- **Convex case:** convergence of $\{u^n\}$ to set of minimizers, convergence of $\{j(u^n)\}$.
- **Nonconvex case:** convergence of stationarity measure, convergence of $\{j(u^n)\}$.

Nonconvergence with constant step-sizes

Example

Let $J(u, \xi) := (u + \xi)^2 \Rightarrow \nabla_u J(u, \xi) = 2(u + \xi)$ and $\xi = \pm 1$ (with equal probability). The minimizer of

$$\mathbb{E}[J(u, \xi)] = \frac{1}{2}((u + 1)^2 + (u - 1)^2)$$

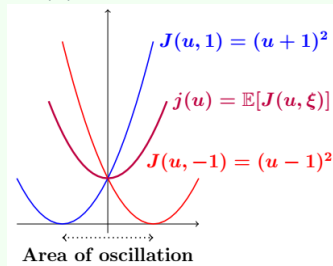
is $\bar{u} = 0$.

Suppose $t_n = \alpha > 0$ is constant.

We prove: $|u^n| < \varepsilon \Rightarrow |u^{n+1}| > \varepsilon$ for $\varepsilon < \frac{\alpha}{1-\alpha}$.

$$\begin{aligned} \text{Case } \xi = -1: \quad u^{n+1} &= u^n - \alpha \nabla_u J(u^n, -1) \\ &\geq -\varepsilon(1 - 2\alpha) + 2\alpha > \varepsilon. \end{aligned}$$

Case $\xi = 1$: Analogous argument. Thus $u^n \not\rightarrow 0$.



- Example explains why Armijo backtracking fails; variance from stochastic gradient needs to be damped! Two basic strategies: increase batch sizes and/or use decreasing step-sizes.

Python script: <https://nbviewer.org/url/caroline.geiersbach.com/PSGD.ipynb>

Assumptions for convergence

- ❶ **Constraint set:** $U_{\text{ad}} \neq \emptyset$ is closed and convex.
- ❷ **Convexity, smoothness, boundedness of expectation.**
- ❸ **Measurability:** $\{u^n\}$ and $\{r^n\}$ are \mathcal{F}_n -measurable. ²²
- ❹ **Bias decays fast enough:** $\sum_{n=1}^{\infty} t_n \|r^n\|_{L_{\mathbb{P}}^{\infty}(\Omega)} < \infty$ and $\sup_n \|r^n\|_{L_{\mathbb{P}}^{\infty}(\Omega)} < \infty$ are satisfied.
- ❺ **Growth condition:** There exist $M_1, M_2 \geq 0$ such that $\mathbb{E}[\|G(u, \xi)\|^2] \leq M_1 + M_2 \|u\|^2$ for all $u \in U_{\text{ad}}$.

²²Measurability can be argued if G and j are continuous and U is separable.

Almost sure convergence for convex problems

Theorem (Convergence for convex j)

Under assumptions,

- 1 $\{j(u^n)\}$ *converges a.s. to the minimum*,
- 2 $\{u^n\}$ *weakly converges a.s. to some minimizer*,
- 3 Strongly convex case: $\{u^n\}$ *converges strongly a.s. to the unique minimizer*.

u^n converges “weakly a.s.” to \bar{u} if $\mathbb{P}(\{\omega \in \Omega \mid \lim_{n \rightarrow \infty} \langle v, u^n \rangle = \langle v, \bar{u} \rangle \quad \forall v \in U\}) = 1$.

Notes about proof technique

The **natural filtration** is denoted by $\mathcal{F}_n = \sigma(\{\xi^1, \dots, \xi^{n-1}\})$, $n \in \mathbb{N}$.²³ The *conditional expectation* $\mathbb{E}[u|\mathcal{F}_n]$ of a random vector u is a random vector such that

$$\int_A \mathbb{E}[u|\mathcal{F}_n](\omega) \, d\mathbb{P}(\omega) = \int_A u(\omega) \, d\mathbb{P}(\omega) \quad \forall A \in \mathcal{F}_n.$$

Thus, if u is \mathcal{F}_n -measurable, we have $\mathbb{E}[u|\mathcal{F}_n] = u$ a.s. Also, since $\Omega \in \mathcal{F}_n$, $\mathbb{E}[\mathbb{E}[u|\mathcal{F}_n]] = \mathbb{E}[u]$ (law of total expectation).

Lemma (Robbins–Siegmund)²⁴

Suppose $\{\mathcal{F}_n\}$ is an increasing sequence of σ -algebras and v_n, a_n, b_n, c_n are \mathcal{F}_n -measurable nonnegative random variables. If

$$\mathbb{E}[v_{n+1}|\mathcal{F}_n] \leq v_n(1 + a_n) + b_n - c_n, \quad \sum_{n=1}^{\infty} a_n < \infty, \quad \sum_{n=1}^{\infty} b_n < \infty,$$

then $\{v_n\}$ converges and $\sum_{n=1}^{\infty} c_n < \infty$ a.s.

²³ $\sigma(\{\xi^1, \dots, \xi^n\})$ is the smallest σ -algebra such that ξ^i is measurable for all i .

²⁴ Robbins, Siegmund. A convergence theorem for non negative almost supermartingales and some applications (1971).

Efficiency estimates - strongly convex case

Rules for bias and step-sizes for μ -strongly convex objective:

$$\|r^n\|_{L_{\mathbb{F}}^{\infty}(\Omega)} \leq \frac{\kappa}{n + \nu}, \quad t_n = \frac{\theta}{n + \nu},$$

where $\theta > 1/(2\mu)$, and $\nu \geq 2\theta\kappa/(2\mu\theta - 1) - 1$, and $\kappa > 0$.

Efficiency estimates:

$$\mathbb{E}[\|u^n - \bar{u}\|] \leq \sqrt{\frac{\rho}{n + \nu}}, \quad \text{where } \rho = \rho(\nu, \mu, \theta, \|u^1 - \bar{u}\|, \kappa, M_1, M_2).$$

If additionally $j \in C_L^{1,1}$ and $\nabla j(\bar{u}) = 0$, then

$$\mathbb{E}[j(u^n) - j(\bar{u})] \leq \frac{L\rho}{2(n + \nu)}.$$

\rightsquigarrow Same order of convergence as for bounded U_{ad} , unbiased case!

Poor convergence in convex case

Example (25)

- **Poor choice of step size:** Consider $j(u) = \frac{1}{10}u^2$, $U_{\text{ad}} = [-1, 1]$, $G(u, \xi) = \nabla j(u)$. Suppose that we choose $\theta = 1$ (here we have $\mu = \frac{1}{5}$). Then,

$$\begin{aligned} u^n &= \prod_{s=1}^{n-1} \left(1 - \frac{1}{5s}\right) = \exp \left\{ - \sum_{s=1}^{n-1} \ln \left(1 + \frac{1}{5s-1}\right) \right\} > \exp \left\{ - \sum_{s=1}^{n-1} \frac{1}{5s-1} \right\} \\ &> \exp \left\{ - \left(0.25 + \int_1^{n-1} \frac{1}{5t-1} dt \right) \right\} > 0.8n^{-1/5}. \end{aligned}$$

At iterate $n = 10^9$, the iterated solution is greater than 0.015 (the solution is $\bar{u} = 0$).

- **Convex (not strongly convex) case:** Consider $j(u) = u^4$, $U_{\text{ad}} = [-1, 1]$, $G(u, \xi) = \nabla j(u)$, $t_n = \frac{\theta}{n}$, $0 < u_1 \leq \frac{1}{6\sqrt{\theta}}$. Then,

$$u^n \geq \frac{u^1}{\sqrt{1 + 32\theta(u^1)^2(1 + \ln(n+1))}}.$$

Remedy: iterate averaging ²⁶

²⁵ Nemirovski, Juditsky, Lan, Shapiro. **Robust stochastic approximation approach to stochastic programming** (2009).

²⁶ Polyak and Juditsky. **Acceleration of stochastic approximation by averaging** (1992).

Efficiency estimates with iterate averaging

Iterate averaging: run PSG with larger steps; compute the **running average** of the iterates:

$$\tilde{u}_i^N = \sum_{n=i}^N \gamma_n u^n, \quad \gamma_n := t_n / \left(\sum_{\ell=i}^N t_\ell \right).$$

Rules for bias and step-sizes (U_{ad} bounded):

$$\sum_{n=i}^N \frac{\|r^n\|_{L_{\mathbb{P}}^\infty(\Omega)}}{\sqrt{n}} \propto 1, \quad t_n = \frac{\theta D_{\text{ad}}}{\sqrt{Mn}}, \quad \theta > 0, D_{\text{ad}} := \max_{u \in U_{\text{ad}}} \|u^1 - u\|, \text{ and } M = M_1.$$

Efficiency estimate for $i = \lceil \alpha N \rceil$ for some $\alpha \in (0, 1)$:

$$\mathbb{E}[j(\tilde{u}_i^N) - j(u)] \leq \frac{\rho}{\sqrt{N}} \quad \rho = \rho(\theta, M, D_{\text{ad}}, \|r^n\|_{L_{\mathbb{P}}^\infty(\Omega)}).$$

Note: for unbounded U_{ad} , possible to show that convergence is nearly $\mathcal{O}(1/\sqrt{N})$.

Finite element method (FEM) in 2D

Weak formulation of model problem:

Find $y = y(\xi) \in V := H_0^1(D)$ such that

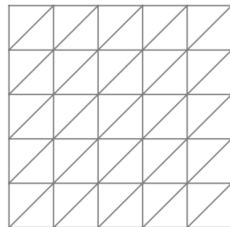
$$\int_D a(x, \xi) \nabla y(x) \cdot \nabla v(x) \, dx = \int_D u(x) v(x) \, dx \quad \forall v \in V.$$

Finite element approximation:

- Triangulate D into elements $\mathcal{T}_h = \{T_i\}$.
- Choose basis $\{\psi_j\} \subset V_h \subset V$.
- Stiffness matrix:

$$A_{k\ell} = \sum_{T \in \mathcal{T}_h} \int_T \sum_{i,j} a_{ij} \partial_i \psi_k \partial_j \psi_\ell \, dx.$$

- Load vector: $l_i = \int_D u \psi_i \, dx$.
- Solve: $AY = l$.



Triangulation \mathcal{T}_h showing triangles $(T_i)_{i=1, \dots, 50}$ defined by edges and nodes.

Discretization

State/adjoint equations - piecewise linear finite elements:

$$Y_h := \{v \in H^1(D) \mid v|_T \in \mathcal{P}_1(T) \text{ for all } T \in \mathcal{T}_h\},$$
$$Y_h^0 := Y_h \cap H_0^1(D).$$

Controls - discretization using piecewise constant finite elements:

$$U_h := \{u \in L^2(D) \mid v|_T \in \mathcal{P}_0(T) \text{ for all } T \in \mathcal{T}_h\}, \quad U_{\text{ad},h} = U_h \cap U_{\text{ad}}.$$

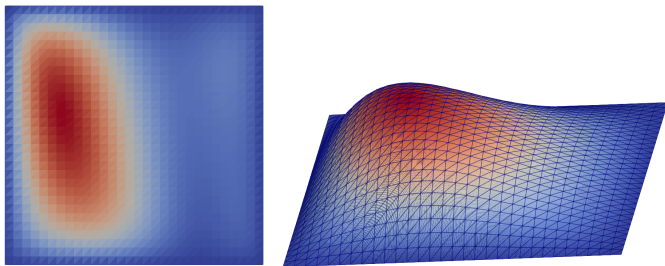


Figure: Example $u_h \in U_{\text{ad},h}$ (left) and $y_h \in Y_h^0$ (right).

Discretization of problem and stochastic gradient

The (spatially) discretized version of the model problem:

$$\begin{aligned} \min_{u \in U_{ad,h}} \quad & \frac{1}{2} \mathbb{E} \left[\|y_h - y_d\|_{L^2(D)}^2 \right] + \frac{\mu}{2} \|u_h\|_{L^2(D)}^2 \\ \text{s.t.} \quad & \int_D l_h a(\xi) \nabla y \cdot \nabla v \, dx = \langle u_h, v_h \rangle_{L^2(D)} \quad \forall v_h \in Y_h^0. \end{aligned} \tag{P'_h}$$

$l_h \dots$ interpolation into element wise constant or linear finite elements.

Stochastic gradient with bias (numerical error):

$$\nabla_u J_h(u_h, \xi) = \mu u_h + P_h p_h(\xi),$$

where $p_h(\xi) \in Y_h^0$ solves the PDE

$$\int_D l_h a(\xi) \nabla p_h(\xi) \cdot \nabla v_h \, dx = (y_h(\xi) - y_d, v_h)_{L^2(D)} \quad \forall v_h \in Y_h^0.$$

$P_h: U \rightarrow U_h \dots$ L^2 -projection, defined for $v \in L^2(D)$ by $P_h(v) \Big|_T = \frac{1}{|T|} \int_T v \, dx$.

Error in stochastic gradient

Error in the stochastic gradient can be split as follows:

$$\nabla j(u_h) = \underbrace{\mu u_h^n + P_h p_h^n(\xi^n)}_{=:\nabla_u J_h(u_h^n, \xi^n)} + \underbrace{\mathbb{E}[p^n(\xi)] - p^n(\xi^n)}_{=:w^n} + \underbrace{p^n(\xi^n) - P_h p_h^n(\xi^n)}_{=:r^n}$$

Sketch of estimate for $K_n = \|p^n(\xi) - P_h p_h^n(\xi)\|_{L_p^\infty(\Xi, U)}$, $U = L^2(D)$:

$$\begin{aligned} \|p^n(\xi) - P_h p_h^n(\xi)\|_U &\leq \|P_h p_h^n(\xi) - P_h p^n(\xi)\|_U + \|p^n(\xi) - P_h p^n(\xi)\|_U \\ &\leq \|p_h^n(\xi) - p^n(\xi)\|_U + ch \|\nabla p^n(\xi)\|_U \quad (\text{Projection + Error for } P_h) \\ &\leq \|p_h^n(\xi) - p^n(\xi)\|_U + ch (\|y_d\|_U + \|u_h\|_U) \quad (\text{Stability of } p(\xi) \text{ and } y(\xi)) \\ &\leq ch^{\min(2s, t)} (\|y_d\|_U + \|u_h\|_U) + ch (\|y_d\|_U + \|u_h\|_U) \quad (\text{Aubin-Nitsche trick }^{27}) \end{aligned}$$

\Rightarrow **Bound for bias:** $K_n \leq ch^{\min(2s, t, 1)}$.

²⁷ For $a(\xi) \in C^t(\bar{D})$, $\exists s_0 \in (0, t]$: for any $0 \leq s < s_0$, any $u \in H^{s_0-1}(D)$, it holds that $\|y(\xi)\|_{H^{1+s}(D)} \leq C_s \|u\|_{H^{s-1}(D)}$.

Mesh refinement rule

For the **strongly convex** case, we get with the requirement that $K_n \leq \frac{K}{n+\nu}$ the rule

$$t_n = \frac{\theta}{n+\nu}, \quad h_n \leq \left(\frac{c}{n+\nu} \right)^{1/\min(2s,t,1)}. \quad (8)$$

For the **convex** case, we get with the requirement $\sum_{n=i}^N \frac{K_n}{\sqrt{n}} \propto 1$ the rule

$$t_n = \frac{\theta D_{\text{ad}}}{\sqrt{Mn}}, \quad h_n \leq \left(\frac{c}{\sqrt{n} + \sqrt{n-1}} \right)^{1/\min(2s,t,1)}. \quad (9)$$

PSG with mesh refinement for (P'_h)

Initialization: Select $h_1 > 0$, $u_h^1 \in U_{\text{ad},h}$

for $n = 1, 2, \dots$ **do**

if $h = h_n$ **is too large per (8) or (9)** **then**

Refine mesh \mathcal{T}_{h_n} **until** $h = h_n$ **is small enough.**

end if

 Given new sample ξ^n , calculate (y_h^n, p_h^n) by solving corresponding state, adjoint equations.

$u_h^{n+1} := \pi_{U_{\text{ad},h}}(u_h^n - t_n(\lambda u_h^n + P_h p_h^n)).$

end for

Obtained solutions

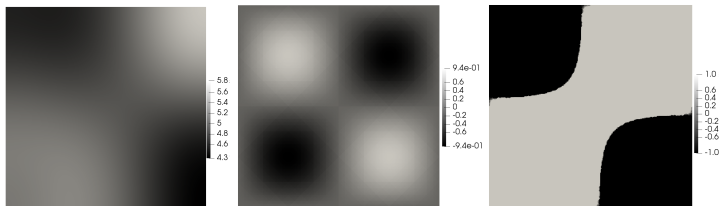


Figure: “Smooth field” (left) with control in strongly convex setting (middle) and convex setting (right).

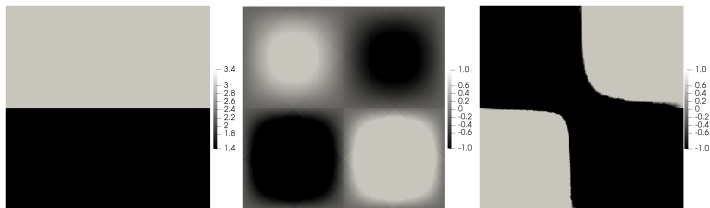


Figure: “Piecewise constant field” (left) with control in strongly convex setting (middle) and convex setting (right).

Convergence behavior: strongly convex case

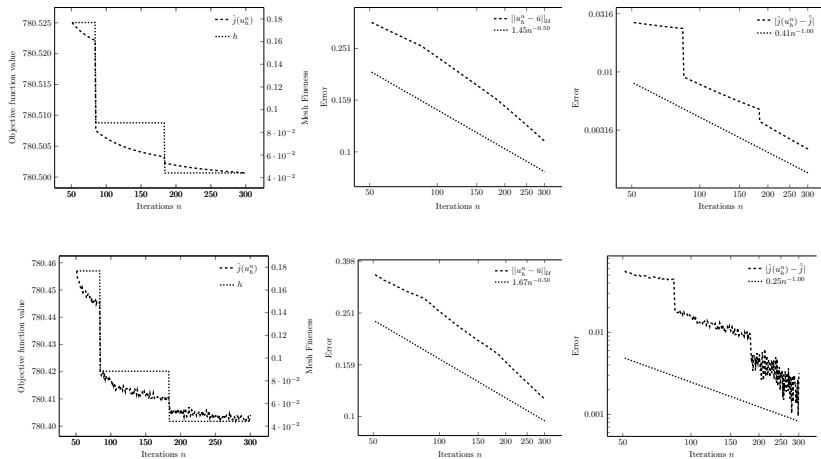


Figure: Smooth random field (top row) and piecewise constant random field (bottom row).

Convergence behavior: convex case

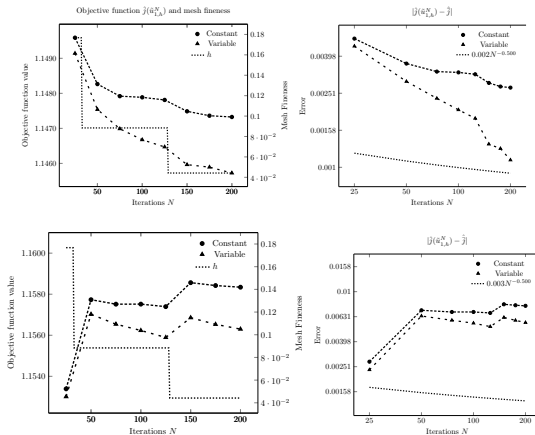


Figure: Smooth random field (top row) and piecewise constant random field (bottom row).

→ Reduced convergence rate for piecewise constant a !

Convergence behavior: convex case

.... Expected convergence rate can be achieved by choosing a more aggressive mesh refinement strategy. Here, we chose $\min(2s, t, 1) = 0.5$.

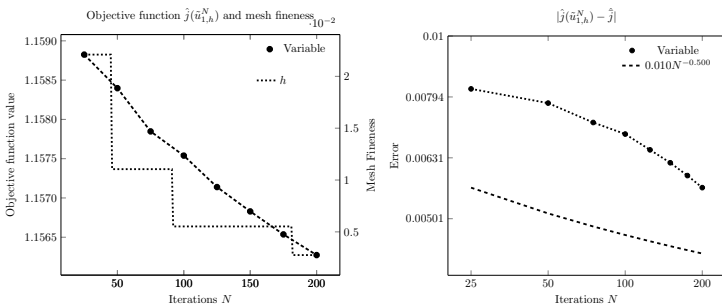
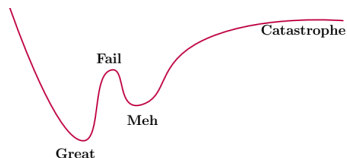


Figure: Piecewise constant random field using variable step-size rule.

Nonconvex objective

Motivation: in many applications, j is nonconvex (e.g., if $u \mapsto S(u, \omega)$ is nonlinear). What can be said about convergence of SA for nonconvex problems?



Without convexity, one can only expect to converge to stationary points.

\leadsto Need to ensure iterates $\{u^n\}$ are bounded along with some smoothness assumption on ∇j .

Minimal assumption: objective has L -Lipschitz gradients, so that we have inequality

$$j(u) \leq j(v) + \langle \nabla j(v), u - v \rangle + \frac{L}{2} \|u - v\|^2 \quad \forall u, v \in U. \quad (10)$$

Assumptions for convergence

SG method for solving unconstrained $\min_{u \in U} \{j(u) := \mathbb{E}[J(u, \xi)]\}$:

$$u^{n+1} = u^n - t_n G(u^n, \xi^n), \quad \text{with RM rule: } t_n \geq 0, \quad \sum_{n=1}^{\infty} t_n = \infty, \quad \sum_{n=1}^{\infty} t_n^2 < \infty.$$

Assumptions - SG with bias: $G(u^n, \xi^n) = \nabla j(u^n) + r^n + w^n$

- **Iterates are bounded** ²⁸.
- $j \in C_L^{1,1}$ is bounded below.
- **Measurability**: $\{u^n\}$ and $\{r^n\}$ are \mathcal{F}_n -measurable.
- **Bias decays fast enough**: $r^n = \mathbb{E}[G(u^n, \xi^n) | \mathcal{F}_n] - \nabla j(u^n)$ is \mathcal{F}_n -measurable for all n and $\sum_{n=1}^{\infty} t_n \|r^n\|_{L_{\mathbb{P}}^{\infty}(\Omega)} < \infty$ and $\sup_n \|r^n\|_{L_{\mathbb{P}}^{\infty}(\Omega)} < \infty$ are satisfied.
- **Growth condition**: There exists a function $M: U \rightarrow [0, \infty)$, that is bounded on bounded sets, such that $\mathbb{E}[\|G(u, \xi)\|^2] \leq M(u)$.

²⁸ Boundedness of iterates can be shown under additional growth conditions on the gradient.

Almost sure convergence result

Theorem (Convergence for $j \in C_L^{1,1}$)

- ❶ The sequence $\{j(u^n)\}$ **converges a.s.** & **$\liminf_{n \rightarrow \infty} \|\nabla j(u^n)\| = 0$ a.s.**
- ❷ If $F(u) := \|\nabla j(u)\|^2$ satisfies $F \in C_{L_F}^{1,1}(U)$, then **$\lim_{n \rightarrow \infty} \nabla j(u^n) = 0$ a.s.**

Note: No convergence statement for iterates.

Proof of first claim

Since $j \in C_L^{1,1}$ and $g^n = \nabla j(u^n) + r^n + w^n$,

$$j(u^{n+1}) \stackrel{(10)}{\leq} j(u^n) - t_n(\nabla j(u^n), g^n) + \frac{Lt_n^2}{2} \|g^n\|^2$$

Monotonicity of

$$\stackrel{\mathbb{E}[\cdot|\mathcal{F}_n]}{\implies} \mathbb{E}[j(u^{n+1})|\mathcal{F}_n] \leq j(u^n) - t_n(\nabla j(u^n), \overbrace{\mathbb{E}[g^n|\mathcal{F}_n]}^{=\nabla j(u^n)+r_n}) + \frac{Lt_n^2}{2} \mathbb{E}[\|g^n\|^2|\mathcal{F}_n].$$

Apply Robbins–Siegmund lemma.

Proof of second claim

Since $F \in C_{L_F}^{1,1}$,

$$\begin{aligned}
 |\mathbb{E}[\underbrace{F(u^{n+1})}_{=:v_{n+1}} - F(u^n) | \mathcal{F}_n]| &\leq \left| -t_n(\nabla F(u^n), \mathbb{E}[g^n | \mathcal{F}_n]) + \frac{L_F t_n^2}{2} \mathbb{E}[\|g^n\|^2 | \mathcal{F}_n] \right| \\
 &\leq | -t_n(2(\nabla^2 j(u^n))^* \nabla j(u^n), \nabla j(u^n) + r^n) | + \frac{L_F M(u^n) t_n^2}{2} \\
 &\leq 2L t_n \|\nabla j(u^n)\|^2 + 2LM_1 t_n \|r^n\|_{L_P^\infty(\Omega)} + \frac{L_F M(u^n) t_n^2}{2}.
 \end{aligned}$$

Result follows with following theorem.

Lemma (Quasimartingale convergence theorem)

Suppose $\{\mathcal{F}_n\}$ is an increasing sequence of σ -algebras and v_n is a \mathcal{F}_n -measurable random variable. If

$$\sup_n \mathbb{E}[\max\{0, -v\}] < \infty \quad \text{and} \quad \sum_{n=1}^{\infty} \mathbb{E}[\mathbb{E}[v_{n+1} - v_n | \mathcal{F}_n]] < \infty,$$

then $\{v_n\}$ converges a.s. to a \mathbb{P} -integrable random variable v_∞ .

Convergence rates?

In the nonconvex case, it's possible to show that if t_n is decreasing and

$$\sum_{j=1}^{\infty} \frac{t_j}{\sum_{k=1}^j t_k} = \infty \quad ^{29} \text{ then, almost surely,}$$

$$\min_{t=1,\dots,n} \|\nabla j(u^t)\|^2 = o\left(\frac{1}{\sum_{j=1}^n t_j}\right).$$

Poor scaling of the step size in the nonconvex setting \rightarrow convergence may be very slow...



Figure: Heat death of the universe?

Scaling of

$$t_n = \theta/n^s$$

obtained by intuition and offline tuning.

²⁹ Satisfied for e.g. $t_n = \theta/n^s$ with $\theta > 0$ and $s \in (0.5, 1]$.

Model problem

Optimal control of semilinear elliptic equation under uncertainty

$$\begin{aligned}
 \min_{u \in L^2(D)} \quad & \frac{1}{2} \mathbb{E}[\|y(\xi) - y_d\|_{L^2(D)}^2] + \frac{\mu}{2} \|u\|_{L^2(D)}^2 \\
 \text{s.t.} \quad & -\nabla \cdot (a(x, \xi) \nabla y(x)) + y(x) + \mathbf{y}^5(\mathbf{x}) = u(x), \quad x \in D \quad \text{a.s.}, \\
 & \frac{\partial y}{\partial n} = 0, \quad x \in \partial D \quad \text{a.s.}
 \end{aligned}$$

- **Nonlinear** control-to-state map $u \mapsto S(u, \omega)$.
- Good performance with step size $t_n = \theta/n$ with $\theta = 2/\mu$ informed by strongly convex objective.

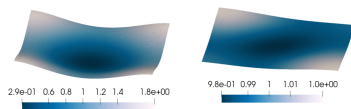


Figure: Computed optimal control (left) and state (right) for $\mu = 1$.

Convergence behavior

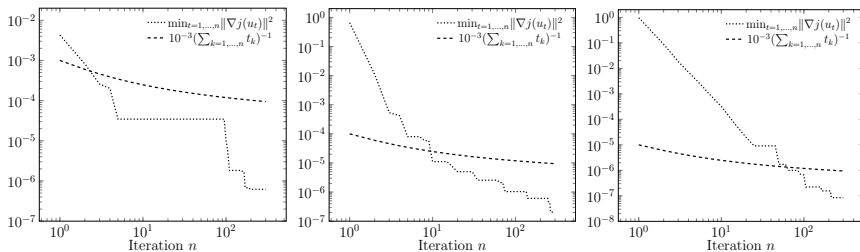


Figure: Convergence for $\mu = 1$ (left), $\mu = 0.1$ (middle), $\mu = 0.01$ (right).

Performance outperforms theory \rightsquigarrow nonconvexity is rather harmless for this problem.

Evidence of mesh independence

Idea: run algorithm on different meshes and compare # of iterations needed until the (estimated!) residual \hat{r}_N reaches a tolerance tol .

Hope: # of iterations stays stable \rightarrow *independent* of the discretization.

h	# triangles	objective function \hat{r}_N	# iterations N until $\hat{r}_N \leq \text{tol}$
$7.1e^{-2}$	800	$4.160e^{-2}$	191
$4.7e^{-2}$	1800	$4.157e^{-2}$	295
$3.5e^{-2}$	3200	$4.157e^{-2}$	233
$2.8e^{-2}$	5000	$4.156e^{-2}$	257
$2.4e^{-2}$	7200	$4.156e^{-2}$	271
$2.0e^{-2}$	9800	$4.155e^{-2}$	251

Mesh independence test for SA + FEM method showing evidence of mesh independence.

Example for numerics - with state constraints

Modification of problem (P) to include state constraint “ $y(\cdot, \xi) \leq \alpha$ ”: Moreau–Yosida regularized problem is

$$\begin{aligned} \min_{u \in U_{\text{ad}}} \quad & \frac{1}{2} \mathbb{E}[\|y - y_d\|_{L^2(D)}^2] + \frac{\mu}{2} \|u\|_{L^2(D)}^2 + \frac{\gamma}{2} \mathbb{E}[\|\max(0, y - \alpha)\|_{L^2(D)}^2] \\ \text{s.t.} \quad & -\nabla \cdot (a(x, \xi) \nabla y(x, \xi)) = u(x), \quad \text{on } D \times \Xi, \\ & y(x, \xi) = 0, \quad \text{on } \partial D \times \Xi. \end{aligned}$$

With $J(u, \xi) = \frac{1}{2} \|y - y_d\|_{L^2(D)}^2 + \frac{\mu}{2} \|u\|_{L^2(D)}^2 + \frac{\gamma}{2} \|\max(0, y - \alpha)\|_{L^2(D)}^2$, stochastic gradient can be computed by:

$$\begin{aligned} D_u J(u, \xi)[h] &= \langle y - y_d, A^{-1}(\xi)h \rangle + \langle \mu u, h \rangle + \langle \gamma \max(0, y - \alpha), A^{-1}(\xi)h \rangle \\ &= \underbrace{\langle A^{-*}(\xi)(y - y_d) + \gamma \max(0, y - \alpha), h \rangle}_{=: p(\xi)} + \langle \mu u, h \rangle. \\ &\quad \underbrace{\hspace{10em}}_{=: G^\gamma(u, \xi)} \end{aligned}$$

Path-following PSG method

Initialization: Select γ_1 , $h_1 > 0$, $u_h^1 \in U_{\text{ad},h}$.

for $m = 1, 2, \dots$ **do**

$u_h^{m_n} \leftarrow$ Run PSG with mesh refinement with gradient $G_h^{\gamma_m}(u_h^n, \xi^n)$ for m_n steps.

Increase γ_m , choose $h = h_1$, project u_h^{n+1} onto mesh h_1 .

end for

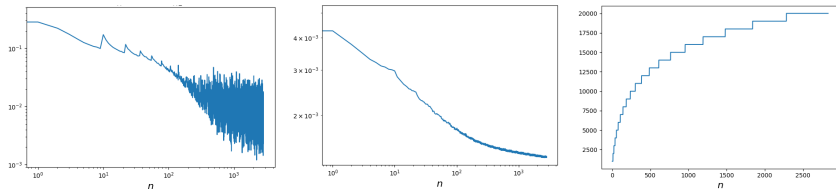


Figure: Plot of stationarity measure $\|G^{\gamma_n}(u^n, \xi^n)\|_{L^2}^2$ (left); infeasibility measure $\|\max(0, y^n - \alpha)\|_{L^2}^2$ (middle); sequence of γ_n (right).

Notes:

- U_{ad} chosen large enough so that $\|G^{\gamma_n}(u^n, \xi^n)\|_{L^2(D)}^2$ is a stationarity measure.
- Variance reduction (increased batch sizes) may improve performance for larger γ_n .

Main takeaways

- Introduction to stochastic optimization on Banach spaces.
- Optimality conditions in reducible form and challenges in irreducible form.
- Case study from PDE-constrained optimization under uncertainty.
- Results in Hilbert-valued stochastic approximation
 - It is possible to show almost sure convergence in Hilbert spaces even with (decreasing) numerical error, unbounded U_{ad} , and/or nonconvex functions.
- SA applicable to more involved problems (nonconvexity, nonsmoothness) but further development is needed!

~> Many open questions for further research: optimality conditions, models with risk measures, higher-order and accelerated methods, line search methods for nonconvex problems, more robust methods for state constraints, convergence of SA for nonconvex problems in Banach spaces . . .

References

For technical details behind theory/numerics in this lecture, see:

- SA - convex setting
 - G., Pflug. **PSGM for convex constrained probs. in Hilbert spaces**. SIOPT (2019).
 - G., Wollner. **SGM with mesh refinement**. SISC (2020).
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- Optimality conditions for probabilistic state constraints
 - G., Wollner. **Optimality conditions for almost sure state constraints**. SIOPT (2021).
 - G., Hintermüller. **Moreau–Yosida regularization for almost sure state constraints**. ESAIM: COCV (2022).
 - G., Henrion. **Optimality conditions with chance constraints**. Math. Oper. Res. (2024).

Other recommended reading:

- Heinkenschloss and Kouri. **Optimization problems governed by systems of PDEs with uncertainties** (2025).
- Kouri and Surowiec. **Existence and optimality conditions for risk-averse PDE-constrained optimization** (2018).
- Shapiro, Dentcheva, and Ruszczyński. **Lectures on stochastic programming: modeling and theory**. (2009).
- Bottou, Curtis, and Nocedal. **Optimization methods for large-scale machine learning** (2018).

Cartoon images in this lecture were generated using ChatGPT.

