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Challenges in Optimization with Complex PDE-Systems (hybrid meeting)

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ABSTRACT. The workshop concentrated on various aspects of optimization problems with systems of nonlinear partial differential equations (PDEs) or variational inequalities (VIs) as constraints. In particular, discussions around several keynote presentations in the areas of optimal control of nonlinear or non-smooth systems, optimization problems with functional and discrete or switching variables leading to mixed integer nonlinear PDE constrained optimization, shape and topology optimization, feedback control and stabilization, multi-criteria problems and multiple optimization problems with equilibrium constraints as well as versions of these problems under uncertainty or stochastic influences, and the respectively associated numerical analysis as well as design and analysis of solution algorithms were promoted. Moreover, aspects of optimal control of data-driven PDE constraints (e.g. related to machine learning) were addressed.

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Introduction by the Organizers

Nonlinear optimization problems with partial differential equation or variational inequality constraints play an ever increasing role in the applied sciences and confront mathematical research with major new challenges. This is even more the case if additional features such as data-driven model components or data uncertainty become relevant. As a result, besides new mathematical models, novel analytical as well as numerical tools need to be developed. Correspondingly, motivated by

optimization problems for nonlinear partial differential equation (PDE) systems which are related to practical applications, the aims of workshop were to gather a group of international experts working at the forefront of research in the field, to foster in-depth-discussions crystallizing around a number of keynote presentations as well as discussion groups on focal topics that emerged during the workshop, and to establish an (international) exchange forum for problems, techniques and solutions, both analytically as well as numerically.

Following the above motivation, the workshop consisted of 13 keynote presentations which were complemented by 17 short communications. Based on the various discussions following some of these presentations, on Wednesday evening of the workshop week a discussion forum on future topics and trends was scheduled. The latter focused in particular on the importance of machine-learning and data-driven techniques in optimization and control with PDEs, uncertainty of various constituents entering the problems under investigation, and major novel application fields resulting in nonlinear and possibly non-smooth coupled systems.

In general, the scientific activity of the workshop developed around keynote topics with associated keynote presentations, short communications, and the organization of discussion groups on emerging focal points. Within this context, the following focus topics were discussed:

- **Control of non-smooth or nonlocal operators.** Nonsmooth PDEs often give rise to non-differentiable, but yet Hadamard differentiable control-to-state mappings. For their tractable representations tools from set-valued analysis need to be further advanced. Subsequently, this will yield sharp stationarity conditions for characterizing solutions and the ansatz for developing tailored numerical solution schemes. Concerning nonlinear and nonlocal PDE operators in the constraints fractional operators as well as nonlocal phase field models which may also involve nonsmooth potentials were studied.
- **Shape and topology optimization.** This is an important branch of optimal design subject to partial differential equations with many applications in engineering and recently also biomedical sciences. Specific topics of interest are related to an efficient representation of the shape derivative, the establishment of analytical tools for enabling a joint shape and topological derivative, higher-order shape analysis, and problems with non-smooth components, either in the cost term or through considering variational inequality (VI) type state systems. Also Riemannian manifold techniques based on work by Michor and Mumford have been studied recently in the community and appear very promising also from a computational perspective.

In the workshop we also discussed phase-field techniques which have recently become a popular alternative to the above mentioned shape sensitivity and manifold approaches. They allow for a combined shape and topology optimization at the expense of operating with a diffuse (rather than a sharp) interface, only. Technically, the phase field method contains

a parameter dependent approximation of the interface perimeter and, in the limit for vanishing parameter and under suitable assumption, the derivative of the reduced objective of an associated minimization problem can be related to the shape gradient. Correspondingly, analytical and numerical aspects were highlighted in several presentations, along with specific applications, e.g., resulting from fluid structure interactions in marine technologies.

- **Feedback control and stabilization.** Feedback stabilization and control are important topics including aeronautics and fluid flow, flow over surfaces, injection of polymer solutions, mass transport through porous walls. Some of the major research questions involve the type of feedback law (linear vs. nonlinear), the proper choice of Lyapunov functionals, and the treatment of Riccati equations. The envisaged problem class typically requires to develop suitable solution techniques for ultra-high dimensional Riccati equations upon discretization. Nonlinear feedback relies on the Hamilton-Jacobi-Bellman equation. Its practical realization is impeded by the curse of dimensionality. Recent advances for numerical realization based on tensor analysis or approximate nonlinear closed feedback by deep neural networks were addressed.
- **Uncertainty and stochasticity.** For several reasons (e.g. modeling material or manufacturing imperfections, uncertain measurements or, in market applications, uncertain demands) it is of interest to study problems with uncertain parameters giving rise to stochastic states, while even assuming deterministic controls. Currently, the transfer to coupled or non-smooth structures (such as VIs) needs to be accomplished and the efficient numerical treatment is still a considerable challenge.

The main difficulty in the context of optimal control of (genuinely) stochastic PDEs (SPDEs) consists in solving the adjoint problem, which is a system of backward stochastic PDEs. Inverting time in stochastic dynamics is not straightforward and results in the introduction of additional variables. Moreover, in many cases the classical variational theory for backward SPDEs cannot be applied directly due to the presence of coupling terms and of possibly nonlinear terms (such as potentials in phase separation approaches) present in the equations.

- **Data-driven PDE models.** Due to the availability of vast amounts of data it has recently become feasible to hybridize *ab initio* PDE models with data-driven components in order to, e.g., cover wide ranges of applicability of a model family. Very often tools from machine learning, e.g., relying on deep networks help to identify data-driven components. Despite several analytical questions, e.g., related to density considerations in approximation through neural networks generated maps, optimization theoretic aspects arise, e.g., related to the derivation of adjoint systems. This novel research area may decisively shape the future of the entire field.

- **Nash games with PDEs.** Not only in multi-criteria engineering design, but also in markets with transport (of, e.g., energy carriers when considering models for the energy turnaround) the involved agents (controls) may have conflicting objectives while accessing a common state system (with possible state constraints). The appropriate mathematical formulation leads to (generalized) Nash games with PDE constraints and possibly under uncertainty. While there is some literature on the subject in finite dimensions, this field is rather open when it comes to PDE constraints.
- **Numerical analysis and algorithm design / analysis.** As many of the aforementioned problem classes are either entirely new or have been studied from an analytical point of view only, the workshop also strives for advancing the development of proper discretization and numerical solution schemes. Exemplarily we mention that optimal control problems for VIs cannot be solved by techniques known for the iterative solution of optimal control problems for PDE-systems. This is related to the non-smooth character of the VI problem and the constraint degeneracy which prevents existence of Karush-Kuhn-Tucker-type multipliers. Another example relates to sparse controls which gives rise to questions concerning the discretization of measures and their efficient numerical treatment.

Workshop (hybrid meeting): Challenges in Optimization with Complex PDE-Systems

Table of Contents

Hélène Frankowska (joint with Qi Lü) <i>Second Order Necessary Conditions for Optimal Control Problems of Evolution Equations Involving Final Point Equality Constraints</i>	427
Fredi Tröltzsch (joint with M. Soledad Aronna) <i>First and Second Order Optimality Conditions for the Optimal Control of Fokker–Planck Equations</i>	430
Daniel Walter (joint with Karl Kunisch) <i>Optimal Feedback Stabilization via Deep Neural Network Approximation</i>	432
Jean-Pierre Raymond (joint with Mehdi Badra) <i>Semidiscrete Approximation and Error Estimates for Feedback Gains Stabilizing Parabolic Systems - Application to the Navier–Stokes Equations</i>	434
Drew P. Kouri (joint with Thomas M. Surowiec) <i>A Primal-Dual Algorithm for Large-Scale Risk Minimization</i>	435
Hannes Meinlschmidt (joint with Karl Kunisch) <i>Optimal Control of a Semilinear Critical Wave Equation</i>	438
Michael Hinze (joint with Harald Garcke, Christian Kahle, and Andrew Lam (with phasefield approach), Klaus Deckelnick and Philip Herbert (with $W^{1,\infty}$ –descent)) <i>Shape Optimization with Phase Fields and a $W^{1,\infty}$–Descent Approach</i>	441
Laurent Pfeiffer (joint with P. Jameson Graber and Alan Mullenix) <i>First-Order Mean Field Games of Controls</i>	444
Volker Schulz (joint with Daniel Luft) <i>On Pre-Shape Calculus</i>	446
Caroline Geiersbach (joint with Michael Hintermüller and Winnifried Wollner) <i>Optimality Conditions and Regularization for Convex Stochastic Optimization with Almost Sure State Constraints</i>	448
John Allen Burns (joint with James Cheung, Michael Demetriou, Nikolaos Gatsonis, Weiwei Hu, and Xin Tian) <i>Real Time Estimation of 3D Advection Diffusion Equations</i>	450

Thomas M. Surowiec (joint with Sebastian Garreis and Michael Ulbrich) <i>An Interior Point Approach for a Class of Risk-Averse PDE-Constrained Optimization Problems with Coherent Risk Measures</i>	453
Behzad Azmi (joint with Dante Kalise and Karl Kunisch) <i>Optimal Feedback Law Recovery by Gradient-Augmented Sparse Polynomial Regression</i>	455
Stefan Ulbrich (joint with Anne-Therese Rauls) <i>Characterization of Generalized Derivatives for the Solution Operator of the Bilateral Obstacle Problem and a Posteriori Error Estimators for FE-Approximations of the Subgradient</i>	456
Amal Alphonse (joint with Michael Hintermüller and Carlos N. Rautenberg) <i>Directional Differentiability and Optimal Control for Elliptic Quasi-Variational Inequalities</i>	458
Michael Ulbrich (joint with Lukas Hertlein) <i>Inexact Bundle Methods for Nonconvex Nonsmooth Optimization in Hilbert Spaces</i>	460
Tobias Breiten (joint with Karl Kunisch) <i>Nonlinear Observer Design Based on Minimum Energy Estimation</i>	463
Enrique Zuazua (joint with Borjan Geshkovski) <i>Control and Deep Learning: Some Connections</i>	466
Pierluigi Colli (joint with Andrea Signori and Jürgen Sprekels) <i>Well-Posedness and Optimal Control of a Complex PDE-System Modelling Tumor Growth</i>	469
Christian Meyer (joint with Stephan Walther) <i>Optimal Control of Perfect Plasticity</i>	472
Sérgio S. Rodrigues <i>Semiglobal Oblique Projection Exponential Dynamical Observers for Nonautonomous Semilinear Parabolic-like Equations</i>	474
Boris Vexler (joint with Dmitriy Leykekhman and Daniel Walter) <i>Numerical Analysis of Sparse Initial Data Identification for Parabolic Problems</i>	477
Ira Neitzel (joint with Fabian Hoppe) <i>Optimal Control of Quasilinear Partial Differential Equations</i>	481
Konstantin Pieper (joint with Armenak Petrosyan) <i>Nonconvex Regularization in Spaces of Measures for Minimal Width Neural Networks</i>	483
Falk M. Hante (joint with Yan Brodskyi and Arno Seidel) <i>Sequential Action Control for Stabilization of PDE-Dynamical Systems</i> .	485
Arnaud Münch <i>Constructive Exact Controls for some Semilinear PDEs</i>	488

Irwin Yousept	
<i>Obstacle Problems in Electromagnetic Shielding</i>	491
Olivier Huber (joint with Martin Gugat, Jens Habermann, and Michael Hintermüller)	
<i>Constrained Exact Boundary Controllability for a System of Semilinear Hyperbolic PDEs</i>	494
Luca Scarpa (joint with Carlo Orrieri and Elisabetta Rocca)	
<i>Optimal Control of Stochastic Phase-Field Models for Tumor Growth</i> ..	497
Martin Brokate (joint with Pavel Krejčí)	
<i>A Variational Inequality for the Derivative of the Scalar Play Operator</i> .	500

Abstracts

Second Order Necessary Conditions for Optimal Control Problems of Evolution Equations Involving Final Point Equality Constraints

HÉLÈNE FRANKOWSKA

(joint work with Qi Lü)

Let $T > 0, \mathfrak{R}$ denote the set of all reals, H, H_2 be separable Hilbert spaces and $A : D(A) \rightarrow H$ an infinitesimal generator of a C_0 -semigroup on H . For a separable Banach space H_1 and a nonempty bounded closed subset $U \subset H_1$ put

$$\mathcal{U} = \{u : [0, T] \rightarrow U \mid u(\cdot) \text{ is Lebesgue measurable}\}.$$

Given $x_0 \in H$ and $f : [0, T] \times H \times H_1 \rightarrow H$, consider the control system:

$$(1) \quad x_t(t) = Ax(t) + f(t, x(t), u(t)), \quad t \in (0, T], \quad x(0) = x_0, \quad u \in \mathcal{U},$$

under the following final state constraints

$$(2) \quad g_j(x(T)) \leq 0, \quad j = 1, \dots, r, \quad h(x(T)) = 0,$$

where $g_j \in C(H; \mathfrak{R})$ for $j = 1, \dots, r, h \in C(H; H_2)$ and solutions $x(\cdot)$ of (1) are understood in the mild sense. Any trajectory-control pair (x, u) of (1) satisfying (2) is called an admissible pair.

Let $g_0 \in C(H; \mathfrak{R})$ be a given cost function. We state here a second order necessary optimality condition for the Mayer type optimal control problem:

$$(3) \quad \text{minimize } g_0(x(T))$$

over all admissible trajectories $x(\cdot)$. An admissible pair (\bar{x}, \bar{u}) is called a local minimizer of (3) if for some $\varepsilon > 0$, we have $g_0(x(T)) \geq g_0(\bar{x}(T))$ for each admissible trajectory-control pair (x, u) such that $\|u - \bar{u}\|_{L^1(0, T; H_1)} < \varepsilon$.

The Hamiltonian and the terminal Lagrange function are defined by

$$\mathcal{H}(t, x, u, p) = \langle p, f(t, x, u) \rangle_H, \quad l(x, \alpha, \beta) = \sum_{j=0}^r \alpha_j g_j(x) + \langle \beta, h(x) \rangle_{H_2},$$

where $p \in H, \alpha = (\alpha_0, \alpha_1, \dots, \alpha_r) \in \mathfrak{R}_+^{r+1}$ and $\beta \in H_2$. Set $K_j := \{x \in H \mid g_j(x) \leq 0\}$ for $j = 1, \dots, r$. Clearly, for every $x \in \partial K_j$, we have $g_j(x) = 0$.

Let (\bar{x}, \bar{u}) be a local minimizer of problem (3) and assume

(H1) For all $(x, u) \in H \times H_1, f(\cdot, x, u)$ is Lebesgue measurable, for all $(t, x) \in [0, T] \times H, f(t, x, \cdot)$ is continuous. The maps $f(t, \cdot, \cdot), g_j (j = 0, \dots, r)$ and h are twice continuously Fréchet differentiable for a.e. $t \in [0, T]$. Moreover,

$$\|f_x(t, x, u)\| + \|f_{xx}(t, x, u)\| + \|f_{xu}(t, x, u)\| + \|f_u(t, x, u)\| + \|f_{uu}(t, x, u)\| \leq C,$$

for all $(t, x, u) \in [0, T] \times H \times U$ and

$$\sum_{j=0}^r (\|g_{j,x}(x)\|_H + \|g_{j,xx}(x)\|) + \|h_x(x)\| + \|h_{xx}(x)\| \leq C, \quad \forall x \in H,$$

where $\|\cdot\|$ refers to operator norms in the corresponding spaces.

Then the first order necessary optimality condition is as follows: there exist $\alpha = (\alpha_0, \alpha_1, \dots, \alpha_r) \in \mathfrak{R}_+^{r+1}$ and $\beta \in H_2$, not vanishing simultaneously, satisfying

$$(4) \quad \alpha_j = 0 \quad \text{if} \quad j \notin I_g := \{j = 1, \dots, r \mid \bar{x}(T) \in \partial K_j\}$$

and such that for the (mild) solution $p \in C([0, T]; H)$ of

$$(5) \quad -p_t(t) = A^*p(t) + \mathcal{H}_x(t, \bar{x}(t), \bar{u}(t), p(t)), \quad t \in [0, T), \quad p(T) = l_x(\bar{x}(T), \alpha, \beta),$$

we have

$$(6) \quad \inf_{\kappa \in C_U(\bar{u}(t))} \mathcal{H}_u(t, \bar{x}(t), \bar{u}(t), p(t))(\kappa) \geq 0, \quad \text{for a.e. } t \in [0, T],$$

where \mathcal{H}_x and \mathcal{H}_u are the Fréchet derivatives of \mathcal{H} with respect to x and u , respectively and $C_U(\bar{u}(t))$ is the Clarke tangent cone to U at $\bar{u}(t)$. Put

$$\Lambda(\bar{x}, \bar{u}) = \{(\alpha, \beta, p) \in \mathfrak{R}_+^{r+1} \times H_2 \times C([0, T]; H) \mid (\alpha, \beta, p) \neq 0 \text{ and satisfies (4)–(6)}\}.$$

Denote by $T_U^b(\bar{u}(t))$ the adjacent tangent to U at $\bar{u}(t)$, see [1, Chapter 4], and consider two linearizations of control system (1) along (\bar{x}, \bar{u}) . The first one is

$$(7) \quad y_t = Ay + f_x[t]y + f_u[t]u(t), \quad u(t) \in T_U^b(\bar{u}(t)), \quad y(0) = 0, \quad u \in L^1(0, T; H_1),$$

where $f_x[t] = f_x(t, \bar{x}(t), \bar{u}(t))$ and $f_u[t] = f_u(t, \bar{x}(t), \bar{u}(t))$. The second one is

$$(8) \quad \tilde{y}_t(t) = A\tilde{y}(t) + f_x[t]\tilde{y}(t) + v(t), \quad v(t) \in \overline{\text{co}} f(t, \bar{x}(t), U) - f[t], \quad \tilde{y}(0) = 0,$$

where $v : [0, T] \rightarrow H_1$ is measurable and $f[t] = f(t, \bar{x}(t), \bar{u}(t))$.

The reachable set of (8) at time T is $R^L = \{\tilde{y}(T) \mid \tilde{y}(\cdot)$ is a trajectory of (8) $\}$. Clearly, R^L is convex. Put $\Xi = C([0, T]; H) \times L^2(0, T; H_1)$.

To express second order necessary conditions we introduce the set $\mathcal{C}(\bar{x}, \bar{u})$ of all *critical pairs* $(y, u) \in \Xi$ solving the linear system (7) such that

$$g_{0,x}(\bar{x}(T))(y(T)) \leq 0, \quad h_x(\bar{x}(T))(y(T)) = 0, \quad g_{j,x}(\bar{x}(T))(y(T)) \leq 0, \quad \forall j \in I_g,$$

and for some $\delta_0 > 0$, $c \in L^2(0, T; \mathfrak{R}_+)$ and for any $\delta \in [0, \delta_0]$ we have

$$\text{dist}(\bar{u}(t) + \delta u(t), U) \leq c(t)\delta^2 \quad \text{for a.e. } t \in [0, T].$$

The *critical set* $\mathcal{C}(\bar{x}, \bar{u})$ can be seen as the set of all the solutions to the strengthened linearized system (7) that satisfy the linearized final point constraints. It can be shown that for any $(y, u) \in \mathcal{C}(\bar{x}, \bar{u})$ we have $g_{0,x}(\bar{x}(T))(y(T)) = 0$ and, consequently, the word *critical* is inherited from the classical Calculus.

For any $(\alpha, \beta, p) \in \Lambda(\bar{x}, \bar{u})$, $u \in \mathcal{U}$ and $t \in [0, T]$, define

$$\Upsilon(u(t), p(t)) = \inf \left\{ \mathcal{H}_u[t](v) \mid v \in T_U^{b(2)}(\bar{u}(t), u(t)) \right\},$$

where $\mathcal{H}_u[t] = \mathcal{H}_u(t, \bar{x}(t), \bar{u}(t), p(t))$, and, by convention, $\inf \emptyset = +\infty$.

With every $(y, u) \in \Xi$ we associate the second order quadratic form:

$$\begin{aligned} \Omega(y, u, \alpha, \beta, p) &:= l_{xx}(\bar{x}(T), \alpha, \beta)(y(T), y(T)) \\ &\quad + \int_0^T (\mathcal{H}_{xx}[t](y(t), y(t)) + 2\mathcal{H}_{xu}[t](y(t), u(t)) + \mathcal{H}_{uu}[t](u(t), u(t))) dt, \end{aligned}$$

where $\mathcal{H}_{xx}[t] = \mathcal{H}_{xx}(t, \bar{x}(t), \bar{u}(t), p(t))$ and $\mathcal{H}_{xu}[t]$, $\mathcal{H}_{uu}[t]$ are similarly defined.

Fix a trajectory-control pair $(y, u) \in \Xi$ of (7) and let $T_U^{b(2)}(\bar{u}(t), u(t))$ stands for the second order adjacent tangent to U at $(\bar{u}(t), u(t))$, see [1, Chapter 4]. Consider the following second order linearization of control system (1) along $(\bar{x}, \bar{u}), (y, u)$

$$(9) \quad \begin{cases} w_t(t) = Aw(t) + f_x[t]w(t) + f_u[t]v(t) + \frac{1}{2}[f_{xx}[t](y(t), y(t)) \\ \quad + 2f_{xu}[t](y(t), u(t)) + f_{uu}[t](u(t), u(t))], \\ w(0) = 0, v \in L^1(0, T; H_1), v(t) \in T_U^{b(2)}(\bar{u}(t), u(t)) \text{ a.e.,} \end{cases}$$

where $f_{xx}[t] = f_{xx}(t, \bar{x}(t), \bar{u}(t))$ and $f_{xu}[t], f_{uu}[t]$ are similarly defined. Denote by $R^{L(2)}$ the reachable set at time T of (9). It is well known that its closure, $\text{cl } R^{L(2)}$, is convex. Define the convex sets

$$\Theta = \left\{ \theta \in H \mid h_x(\bar{x}(T))\theta + \frac{1}{2}h_{xx}(\bar{x}(T))(y(T), y(T)) = 0 \right\},$$

$$\tilde{\Theta} = \left\{ \theta - \kappa \mid \theta \in \Theta, \kappa \in \text{cl}(R^{L(2)}) \right\}.$$

and assume that

(H2) There exists a closed subspace \tilde{H} of H such that $\tilde{\Theta} \subset \tilde{H}$ and $\text{int}_{\tilde{H}} \tilde{\Theta} \neq \emptyset$.

Theorem 1. Assume **(H1)** and let (\bar{x}, \bar{u}) be a local minimizer of (3) satisfying the two surjectivity assumptions: $h_x(\bar{x}(T))(H) = H_2$ and $0 \in \text{int } \text{cl } h_x(\bar{x}(T))(R^L)$. Let $(y, u) \in \mathcal{C}(\bar{x}, \bar{u})$ be such that **(H2)** holds and there exists a selection $v(t) \in T_U^{b(2)}(\bar{u}(t), u(t))$ for a.e. $t \in [0, T]$ such that $v \in L^2(0, T; H_1)$. Then for some $(\alpha, \beta, p) \in \Lambda(\bar{x}, \bar{u})$ such that $\alpha_j = 0$ whenever $g_{j,x}(\bar{x}(T))(y(T)) < 0$, the function $\Upsilon(u, p)$ is integrable and

$$\frac{1}{2}\Omega(y, u, \alpha, \beta, p) + \int_0^T \Upsilon(u(t), p(t))dt \geq 0.$$

The proof of this result is based on a metric inverse mapping theorem that implies a relevant second order variational inequality. Then a separation theorem is applied. Assumption **(H2)** is crucial to separate two convex sets in the infinite dimensional Hilbert space H . Details can be found in [2], where we also discuss how some assumptions can be relaxed using a regularizing effect of the semigroup and provide examples of application to a parabolic and a hyperbolic controlled PDEs. In the difference with the previous literature, we do not make reduction of the optimal control problem to an abstract mathematical programming one. Instead we linearize twice the control system and the constraints in the original state space. This allows us to work with merely measurable controls without any additional structure by the methods of variational analysis. Our approach yields also sufficient conditions for the normality of multipliers, that is for having $\alpha_0 > 0$.

Question of strengthening of the above second order condition to become sufficient for local minima is open.

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First and Second Order Optimality Conditions for the Optimal Control of Fokker–Planck Equations

FREDI TRÖLTZSCH

(joint work with M. Soledad Aronna)

We consider the optimal control of the Fokker-Planck equation with associated initial and boundary conditions

$$(1) \quad \begin{aligned} \partial_t \rho(x, t) - \nu \Delta \rho(x, t) - \operatorname{div}(\rho(x, t) B[u(t)](x)) &= 0 && \text{in } Q, \\ \rho(x, 0) &= \rho_0(x) && \text{in } \Omega, \\ (\nu \nabla \rho(x, t) + \rho(x, t) B[u(t)](x)) \cdot n(x) &= 0 && \text{on } \Sigma, \end{aligned}$$

where $\nu > 0$, $\rho_0 \in L^2(\Omega)$, $\Omega \subset \mathbb{R}^n$ is a bounded domain with Lipschitz boundary Γ , and we set $\Sigma := \Gamma \times (0, T)$, $Q := \Omega \times (0, T)$. The control is $u = (u_1, \dots, u_n) \in L^\infty(0, T; \mathbb{R}^n)$, and the function $B: \mathbb{R}^n \times \Omega \rightarrow \mathbb{R}^n$ is defined by

$$B[u](x) := c(x) + b(x) \otimes u,$$

with $c, b \in L^\infty(\Omega; \mathbb{R}^n)$ being fixed. In (1), the differential operators Δ and div act only with respect to the spatial coordinate x .

Given $\rho_Q \in L^2(Q)$, $\rho_\Omega \in L^2(\Omega)$, $\beta \geq 0$, $\gamma \geq 0$, $u_{\min} < u_{\max}$, $\alpha_Q \geq 0$, $\alpha_\Omega \geq 0$, we discuss the (slightly simplified compared with [1]) optimal control problem

$$\begin{aligned} \min J(\rho, u) := & \frac{\alpha_Q}{2} \int_0^T \|\rho(t) - \rho_Q(t)\|_{L^2(\Omega)}^2 dt + \frac{\alpha_\Omega}{2} \|\rho(T) - \rho_\Omega\|_{L^2(\Omega)}^2 \\ & + \frac{\gamma}{2} \|u\|_2^2 + \beta \sum_{i=1}^n \int_0^T u_i(t) dt, \end{aligned}$$

subject to the Fokker-Planck equation (1) and to the control constraints

$$u \in \mathcal{U}_{\text{ad}} := \{u \in L^\infty(0, T; \mathbb{R}^n) : u^{\min} \leq u(t) \leq u^{\max} \quad \text{a.e. in } [0, T]\}$$

with inequalities defined componentwise.

Slightly extending an existence and uniqueness result of [2], we have that for all $u \in L^2(0, T; \mathbb{R}^n)$ equation (1) has a unique solution $\rho \in W(0, T)$. By the implicit function theorem, we are able to show that the control-to-state mapping $G: L^2(0, T; \mathbb{R}^n) \rightarrow W(0, T)$, $G: u \mapsto \rho$ is of class C^∞ . This is due to the bilinear appearance of ρ and u and to the boundedness of b and c . The existence of at least one optimal control \bar{u} with associated state $\bar{\rho}$ is an easy consequence.

Since the reduced objective functional $F(u) = J(G(u), u)$ is of class C^∞ , too, the first-order necessary optimality condition $F'(\bar{u})(u - \bar{u}) \geq 0 \quad \forall u \in \mathcal{U}_{\text{ad}}$ follows

immediately. Here, the control u does not appear in an explicit form. Therefore, the adjoint equation

$$(2) \quad \begin{aligned} -\partial_t p - \nu \Delta p + B[u] \cdot \nabla p &= \alpha_Q(\rho - \rho_Q) && \text{in } Q, \\ p(T) &= \alpha_\Omega(\rho(T) - \rho_\Omega) && \text{in } \Omega, \\ \partial_n p &= 0 && \text{on } \Sigma \end{aligned}$$

is considered, where ρ is the solution of (1) associated with u .

We can show that a unique weak solution $p \in W(0, T)$ exists provided that u belongs to $L^\infty(0, T; \mathbb{R}^n)$. For $u \in L^2(0, T; \mathbb{R}^n)$, we can only show a unique weak solution $p \in W_2^{1,0}(Q)$. If $\bar{u} \in \mathcal{U}_{\text{ad}}$ is an optimal solution with associated state $\bar{\rho}$, then the first-order necessary optimality condition can be formulated in the form

$$(3) \quad \int_0^T \bar{\Phi}(t) \cdot (u(t) - \bar{u}(t)) dt \geq 0 \quad \forall u \in \mathcal{U}_{\text{ad}},$$

where $\bar{\Phi}(t) = (\bar{\Phi}_1(t), \dots, \bar{\Phi}_n(t))^\top$, $\bar{\Phi}_i(t) := -\int_\Omega \bar{\rho}(t) b_i \frac{\partial \bar{p}(t)}{\partial x_i} dx + \gamma \bar{u}_i(t) + \beta$, $i = 1, \dots, n$, and the adjoint state \bar{p} is the solution of (2) associated with $\bar{\rho}$.

To set up second-order sufficient optimality conditions, we need higher regularity of \bar{p} , namely $\bar{p} \in C([0, T]; H^1(\Omega))$. To this end, we require the following conditions on the functions b and c in B , unless $\alpha_\Omega = 0$. These assumptions are adopted from [2].

Assumption (A) *The function b belongs to $W^{1,\infty}(\Omega; \mathbb{R}^n)$ and it holds*

$$(b(x) \otimes u) \cdot n(x) = 0 \quad \text{for all } u \in \mathbb{R}^n \text{ and a.a. } x \in \Gamma.$$

The function c has a potential $-V \in W^{2,\infty}(\Omega)$ so that $c = \nabla V$ or c belongs to $W^{1,\infty}(\Omega, \mathbb{R}^n)$ and satisfies the orthogonality relation $c(x) \cdot n(x) = 0$ a.e. on Γ . The initial and the desired distributions ρ_0 and ρ_Ω belong to $H^1(\Omega)$.

Under (A), we have that $\bar{p} \in C([0, T]; H^1(\Omega))$. To set up second-order sufficient optimality conditions, we invoke Thm. 2.2 of [3] and confirm the assumptions therein. Here, the higher regularity of \bar{p} is essential. In the result below, $C(\bar{u})$ denotes the critical cone, cf. [3], and $B_\varepsilon^2(\bar{u})$ is the closed ball of $L^2(0, T; \mathbb{R}^n)$ with radius ε centered at \bar{u} .

Theorem([1]) *Let \bar{u} satisfy, along with the associated state $\bar{\rho}$ and the adjoint state \bar{p} defined by (2), the necessary optimality condition (3) and*

$$F''(\bar{u})v^2 > 0 \quad \text{for all } v \in C(\bar{u}) \setminus \{0\}.$$

Assume that $\gamma > 0$. If $\alpha_\Omega = 0$ or (A) is satisfied, then there exist $\varepsilon > 0$ and $\delta > 0$ such that the quadratic growth condition

$$F(u) \geq J(\bar{u}) + \frac{\delta}{2} \|u - \bar{u}\|_2^2 \quad \text{for all } u \in \mathcal{U}_{\text{ad}} \cap B_\varepsilon^2(\bar{u})$$

holds. Therefore, \bar{u} is locally optimal in the sense of $L^2(0, T; \mathbb{R}^n)$.

With $z := G'(\bar{u})v$, the second-order derivative $F''(\bar{u})v^2$ is given by

$$F''(\bar{u})v^2 = \iint_Q \left[\alpha_Q z^2 - 2\nabla p \cdot (zb \otimes v) \right] dxdt + \gamma \|v\|_{L^2(0, T; \mathbb{R}^n)}^2 + \alpha_\Omega \int_\Omega z(T)^2 dx.$$

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Optimal Feedback Stabilization via Deep Neural Network Approximation

DANIEL WALTER

(joint work with Karl Kunisch)

In this talk we focus on stabilization problems of the form

$$(P_{\beta}^{y_0}) \quad \begin{cases} \inf_{u \in L^2(0, \infty; \mathbb{R}^m), y} \frac{1}{2} \int_0^{\infty} (|Qy(t)|^2 + \beta|u(t)|^2) dt \\ \text{s.t. } \dot{y} = f(y) + Bu, \quad y(0) = y_0, \end{cases}$$

where f describes the nonlinear dynamics, $B \in \mathbb{R}^{n \times m}$ is the control operator, $Q \in \mathbb{R}^{n \times n}$ is positive semi-definite, $\beta > 0$. The initial condition y_0 is contained in a given compact set $Y_0 \subset \mathbb{R}^n$. Our interest lies in optimal feedback controls i.e. control inputs that are constructed as a function of the state variable at every time point t . More in detail we are looking for an *optimal feedback law* $F^* : \mathbb{R}^n \rightarrow \mathbb{R}^m$ such that:

- For every $y_0 \in Y_0$ there is a solution y^* to

$$\dot{y} = f(y) + BF^*(y), \quad y(0) = y_0.$$

- For every $y_0 \in Y_0$, the pair $(y^*, F^*(y^*))$ is a minimizer to $(P_{\beta}^{y_0})$.

Constructing an optimal feedback F^* is closely related to the computation to the optimal value function $V(y_0) = \inf (P_{\beta}^{y_0})$ which satisfies a *Hamilton-Jacobi-Bellman equation*, a hyperbolic system whose dimension is that of the state space. Once available, the optimal control to $(P_{\beta}^{y_0})$ can be expressed in feedback form as $u^*(t) = -B^{\top} \nabla V(y^*(t))$. Following the HJB approach one is inevitably faced with the *curse of dimensionality*: If M degrees of freedom are used to discretize the HJB equation in each of the spatial directions, then this results in a discrete system with M^n degrees of freedom. Except for small dimensions n of the state equation this is unfeasible and alternatives must be sought. In this paper we propose to replace the control u in $(P_{\beta}^{y_0})$ by the closed loop expression $F_{\theta}^{\sigma}(y)$ where F_{θ}^{σ} denotes a deep neural network described by a finite dimensional parameter θ . Subsequently, a feedback law is determined from solving

$$(P_{Y_0}) \quad \begin{cases} \inf_{\theta} \frac{1}{2} \int_0^{\infty} (|Qy(t)|^2 + \beta|F_{\theta}^{\sigma}(y(t))|^2) dt \\ \text{s.t. } \dot{y} = f(y) + BF_{\theta}^{\sigma}(y), \quad y(0) = y_0, \end{cases}$$

It can be expected that the effectiveness of such a procedure depends on the location of the orbit $\mathcal{O} = \{y(t; y_0) : t \in (0, \infty)\}$ within the state space \mathbb{R}^n . To accommodate the case that \mathcal{O} does not ‘cover’ the state-space sufficiently well, we propose to look at the ensemble of orbits departing from the compact set Y_0 of initial conditions and reformulate the problem accordingly. For this purpose we introduce a probability measure μ on Y_0 describing a “training set” of initial conditions and replace (P_{Y_0}) by

$$(\mathcal{P}) \quad \begin{cases} \inf_{\theta} \frac{1}{2} \int_{Y_0} \int_0^{\infty} (|Qy(t; y_0)|^2 + \beta|F(y(t; y_0))|^2) dt d\mu \\ \text{s.t. } \dot{y}(y_0) = f(y(y_0)) + BF_{\theta}^{\sigma}(y(y_0)), \quad y(0) = y_0, \end{cases}$$

Here y is to be understood as an *ensemble* of state variables which assigns to every y_0 in the support of μ the solution of the closed loop state equation. Our work gives mathematical rigor to this formulation. This includes existence results for optimal neural network based feedback laws as well as the derivation of first order sufficient optimality conditions. Moreover we also address the convergence of feedback laws obtained as the networks get wider and deeper. Several numerical examples illustrate the practical applicability of our learning approach. These range from highly unstable low dimensional systems to extremely high dimensional examples stemming from the discretization of PDE systems. The approach itself is highly flexible in the sense that it directly allows to include control and/or state constraints into the problem as well as constraints on the feedback function itself, see e.g. [2].

In summary, on the one hand, the results presented in this talk show the great potential and success of learning feedback laws for the stabilization of unstable nonlinear systems. On the other hand, they also reveal open questions which stimulates further research. Amongst other things, this encompasses the development of fast and reliable solution methods as well as the extension of our approach to PDE systems.

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Semidiscrete Approximation and Error Estimates for Feedback Gains Stabilizing Parabolic Systems - Application to the Navier–Stokes Equations

JEAN-PIERRE RAYMOND

(joint work with Mehdi Badra)

We consider pairs (A, B) of operators, and approximate pairs (A_h, B_h) for $h > 0$, where $(A, \mathcal{D}(A))$ is the infinitesimal generator of an analytic semigroup on a Hilbert space Z and B is an unbounded control operator, and $(A_h, \mathcal{D}(A_h))$ is the infinitesimal generator of an analytic semigroup on a Hilbert space Z_h . But Z_h is not a subspace of Z . Thus we have to deal with nonconform approximations. Under some approximation assumptions satisfied by the pairs (A, B) and (A_h, B_h) , we prove that feedback laws stabilizing reduced order models for the system (A_h, B_h) , based on spectral projections, also stabilize the pair (A, B) .

We apply these results to the semidiscrete approximation, by a finite element method, of the linearized Navier-Stokes equations with a Dirichlet boundary control. In that case, feedback laws stabilizing reduced order models for the semidiscrete approximation of the linearized Navier-Stokes equations, also stabilizes the linearized Navier-Stokes equations, and locally the Navier-Stokes equations.

Convergence rates of semidiscrete approximations by finite element methods of feedback gains for parabolic equations and distributed controls have been obtained in [3]. These results have been extended to boundary controls in [5] and [4]. But in all these papers only conforming finite element methods are considered.

Here, because of the divergence condition in the Oseen system, it is natural to consider nonconforming finite element methods. In [1], we extend the results of [3], [5], and [4] to nonconforming finite element methods both in the case of either a distributed control or a boundary control.

In [2], to stabilize the Oseen system, we study feedback laws constructed by stabilizing unstable invariant subsets of the Oseen system. We prove convergence rates in that case too, which are better than those in [1] where we do not use reduced order models based on spectral projections.

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A Primal-Dual Algorithm for Large-Scale Risk Minimization

DREW P. KOURI

(joint work with Thomas M. Surowiec)

Many practical applications require the optimization of partial differential equations (PDEs) with uncertain inputs such as unknown problem data, random operating conditions, and unverifiable modeling assumptions. In this work, we formulate these problems as stochastic optimization problems and seek to minimize a measure of risk associated with a given system output. For many popular risk models, the resulting risk-averse objective function is not differentiable, significantly complicating the numerical solution of the optimization problem. Unfortunately, methods for nonsmooth optimization are limited by slow (i.e., sublinear) convergence rates and therefore are often intractable for problems in which the objective function and its derivatives are expensive to evaluate. To address this challenge, we introduce a primal-dual algorithm for solving large-scale nonsmooth risk-averse optimization problems. At each iteration of the algorithm, we approximately solve a smooth optimization problem using, e.g., a rapidly-converging Newton-type method.

Let Z be a reflexive Banach space and let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, where Ω denotes the set of outcomes, $\mathcal{F} \subseteq 2^\Omega$ is a σ -algebra of events, and $\mathbb{P} : \mathcal{F} \rightarrow [0, 1]$ is a probability measure. We consider optimization problems with the form

$$(1) \quad \min_{z \in Z_{\text{ad}}} \mathcal{R}(F(z)) + \wp(z)$$

where $Z_{\text{ad}} \subseteq Z$ is a nonempty, closed and convex set of admissible optimization variables, $F : Z \rightarrow L^2(\Omega, \mathcal{F}, \mathbb{P})$ is a random loss function, $\wp : Z \rightarrow \mathbb{R}$ is a deterministic loss functional, and $\mathcal{R} : L^2(\Omega, \mathcal{F}, \mathbb{P}) \rightarrow \mathbb{R}$ is a risk functional. We make the following basic assumptions on the risk functional: \mathcal{R} is convex, positively homogeneous and satisfies the monotonicity condition

$$\forall X, X' \in L^2(\Omega, \mathcal{F}, \mathbb{P}) \quad \text{with} \quad X \leq X' \quad \text{a.s.} \quad \implies \quad \mathcal{R}(X) \leq \mathcal{R}(X').$$

Under these assumptions, the Fenchel-Moreau Theorem [2] ensures that

$$(2) \quad \mathcal{R}(X) = \sup_{\theta \in \mathfrak{A}} \mathbb{E}[\theta X] \quad \text{where} \quad \mathfrak{A} := \partial \mathcal{R}(0) \subseteq \{ \theta \in L^2(\Omega, \mathcal{F}, \mathbb{P}) \mid \theta \geq 0 \text{ a.s.} \}.$$

Here, $\mathbb{E}[Y]$ denotes the expected value of the random variable Y and $\partial \mathcal{R}(0)$ denotes the convex subdifferential of \mathcal{R} at 0. Substituting (2) into the optimization problem (1) results in the min-max problem

$$(3) \quad \min_{z \in Z_{\text{ad}}} \sup_{\theta \in \mathfrak{A}} \{ \ell(z, \theta) := \mathbb{E}[\theta F(z)] + \wp(z) \}.$$

The functional $\ell(z, \theta)$ in (3) resembles the Lagrangian functional from nonlinear programming. With this as motivation, we define the augmented Lagrangian functional as

$$(4) \quad L(z, \lambda, r) := \max_{\theta \in \mathfrak{A}} \left\{ \ell(z, \theta) - \frac{1}{2r} \mathbb{E}[(\lambda - \theta)^2] \right\}$$

for $z \in Z$, $\lambda \in L^2(\Omega, \mathcal{F}, \mathbb{P})$ and $r > 0$. Applying results from convex and variational analysis, one can show that $L(z, \lambda, r)$ is continuously Fréchet differentiable with respect to z and λ as long as φ and F are. In this case, the partial derivative of $L(z, \lambda, r)$ with respect to z is given by

$$L'_z(z, \lambda, r) = \varphi'(z) + \mathbb{E}[\mathbf{P}_{\mathfrak{A}}(rF(z) + \lambda)F'(z)],$$

where $\mathbf{P}_{\mathfrak{A}}$ denotes the metric projection onto the convex set \mathfrak{A} [1, 3]. Based on these properties of L , we define the primal-dual risk minimization algorithm as the following generalization of the classical method of multipliers.

Algorithm 1 Primal-Dual Risk Minimization

Initialize: Given $z_0 \in Z_{\text{ad}}$, $r_0 > 0$ and $\lambda_0 \in \mathfrak{A}$.

While(“Not Converged”)

- (1) Compute $z_{k+1} \in Z_{\text{ad}}$ that approximately minimizes $L(\cdot, \lambda_k, r_k)$.
- (2) Set $\lambda_{k+1} = \mathbf{P}_{\mathfrak{A}}(r_k F(z_{k+1}) + \lambda_k)$.
- (3) Update r_{k+1} .

End While

If the iterates z_{k+1} of Algorithm 1 are ϵ_k -minimizers of $L(\cdot, \lambda_k, r_k)$, i.e.,

$$L(z_{k+1}, \lambda_k, r_k) - \inf_{z \in Z_{\text{ad}}} L(z, \lambda_k, r_k) \leq \epsilon_k$$

for $\epsilon_k \geq 0$, then any weak accumulation point of $\{z_k\}$ is an ϵ -minimizer of (1) [4, Thm. 1] with ϵ given by

$$\epsilon = \frac{K^2}{r^*} + \epsilon^*,$$

where $K \geq 0$ is the Lipschitz modulus of \mathcal{R} at 0, $r^* > 0$ is the limit of $\{r_k\}$ (possibly $+\infty$) and $\epsilon^* \geq 0$ is the limit of $\{\epsilon_k\}$ (possibly 0). If $\{\epsilon_k\}$ satisfies the additional conditions

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

then the entire sequence of dual variables $\{\lambda_k\}$ converges to a maximizer of the dual problem

$$(5) \quad \max_{\theta \in \mathfrak{A}} v(\theta) \quad \text{where} \quad v(\theta) := \inf_{z \in Z_{\text{ad}}} \ell(z, \theta)$$

[4, Thm. 2]. This result exploits the relationship between Algorithm 1 and the proximal point method [5] applied to solve the dual problem. Aside from convex problems, we typically cannot ensure that z_{k+1} is an ϵ_k -minimizer. Consequently, these results are of little practical use for general PDE-constrained optimization problems. For nonconvex problems, we often can only ensure that the iterates z_{k+1} are ϵ_k -stationary points of $L(\cdot, \lambda_k, r_k)$. That is, if φ and F are continuously Fréchet differentiable, then

$$\langle \varphi'(z_{k+1}) + \mathbb{E}[\lambda_{k+1} F'(z_{k+1})], z - z_{k+1} \rangle_{Z^*, Z} \geq -\epsilon_k \|z - z_{k+1}\|_Z \quad \forall z \in Z_{\text{ad}}.$$

Under additional assumptions on the continuity of φ' and F' , we can prove that if z_{k+1} are ϵ_k -stationary points with $\epsilon_k \rightarrow 0$ and $r_k \rightarrow +\infty$, then any weak accumulation point of $\{z_k\}$ is a stationary point of (1) [4, Thm. 3].

To demonstrate the primal-dual risk minimization algorithm, we apply Algorithm 1 to two convex (`elliptic 1d/2d`) and one nonconvex (`burgers`) PDE-constrained optimization problems. We investigate the numerical performance for five common risk measures: mean plus semi-deviation (`MPSD`), mean plus semi-deviation from a target (`MPSDFT`), a convex combination of the expectation and the conditional value-at-risk (`CVAR`), the second-order higher moment coherent risk measure (`HMCR`), and the buffered probability (`bPOE`). In Table 1, we compare Algorithm 1 with the nonsmooth, nonconvex bundle method described in [6].

example	risk	PD Algorithm				Bundle		Speed Up
		iter	nfval	ngrad	subiter	iter	neval	
elliptic 1d	MPSD	7	14	14	7	31	208	14.86x
	MPSDFT	7	11	11	4	24	206	18.73x
	CVAR	7	23	23	16	39	88	3.83x
	HMCR	6	16	15	10	40	104	6.50x
	BPOE	11	49	36	38	---	---	---
elliptic 2d	MPSD	5	10	10	5	---	---	---
	MPSDFT	6	13	13	7	---	---	---
	CVAR	9	35	30	26	---	---	---
	HMCR	7	25	23	18	---	---	---
	BPOE	9	72	41	63	---	---	---
burgers	MPSD	12	31	26	19	51	176	5.68x
	MPSDFT	9	17	17	8	53	123	7.24x
	CVAR	8	46	44	38	69	197	4.28x
	HMCR	8	79	73	71	84	182	2.17x
	BPOE	9	52	42	43	---	---	---

TABLE 1. Numerical comparison of the primal-dual risk minimization algorithm with a nonsmooth, nonconvex bundle method.

We see that Algorithm 1 requires between 2 and 18 times fewer function and gradient evaluations than the bundle method. In Table 2, we compare Algorithm 1 with epi-regularization [3]. For consistency, we update the epi-regularization parameter in a similar fashion to r_k . In particular, the `epireg` algorithm in Table 2 is simply Algorithm 1 with λ_k set to zero for all k , which is analogous to a quadratic penalty method. Again, we see that Algorithm 1 outperforms the epi-regularization approach. For a thorough discussion of these results see [4].

example	algo	iter	nfval	ngrad	nhess	subiter
elliptic 1d	pdrisk	7	23	23	90	16
	epireg	8	33	29	99	25
elliptic 2d	pdrisk	9	35	30	138	26
	epireg	10	80	45	296	70
burgers	pdrisk	8	46	44	128	38
	epireg	8	72	63	182	64

TABLE 2. Numerical comparison of the primal-dual risk minimization algorithm with epi-regularization.

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Optimal Control of a Semilinear Critical Wave Equation

HANNES MEINLSCHMIDT

(joint work with Karl Kunisch)

This talk is based on [1]. We consider the optimal control problem

$$\begin{array}{ll}
 \min_{y,u} & \ell(y, u) \\
 \text{(OCP)} & \text{s.t.} \quad \begin{cases} u \in \mathcal{U}_{\text{ad}}, \\ y \text{ is the solution to (CWE)}, \end{cases}
 \end{array}$$

where the underlying partial differential equation is the H^1 -critical defocusing wave equation on a bounded domain $\Omega \subset \mathbb{R}^3$ with smooth boundary over a finite interval $(0, T)$, complemented with homogeneous Dirichlet boundary conditions and with distributed control, in the prototype form

$$(CWE) \quad \begin{cases} \partial_t^2 y - \Delta y + y^5 = u & \text{in } (0, T) \times \Omega, \\ y = 0 & \text{on } (0, T) \times \partial\Omega, \\ (y(0), \partial_t y(0)) = (y_0, y_1) & \text{in } \Omega. \end{cases}$$

We suppose that $(y_0, y_1) \in \mathcal{E} := H_0^1(\Omega) \times L^2(\Omega)$ which is the natural energy space, and that $u \in L^1(0, T; L^2(\Omega))$. The particular feature of this critical wave equation is that, as the nomenclature suggests, its power nonlinearity is exactly the extreme case for which one has unconditional well-posedness and eventually globally-in-time existence. The performance index ℓ for (CWE) is chosen to be

$$\begin{aligned} \ell(y, u) := & \frac{1}{2} \|y(T) - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|\partial_t y(T)\|_{H^{-1}(\Omega)}^2 + \frac{\gamma}{4} \|y\|_{L^4(0, T; L^{12}(\Omega))}^4 \\ & + \beta_1 \|u\|_{L^1(0, T; L^2(\Omega))} + \frac{\beta_2}{2} \|u\|_{L^2(0, T; L^2(\Omega))}^2 \end{aligned}$$

for $y_d \in L^2(\Omega)$. The objective in (OCP) is thus to find a control $u \in \mathcal{U}_{ad}$ such that the associated solution to (CWE) $y(T)$ at time T matches a given profile y_d as well as possible in the L^2 -sense while simultaneously minimizing the (scaled) velocity $\partial_t y(T)$ at time T . While the $L^2(0, T; L^2(\Omega))$ term in ℓ describes a quadratic control cost, the $L^1(0, T; L^2(\Omega))$ term is known to be sparsity enhancing. We also consider an $L^4(0, T; L^{12}(\Omega))$ regularization for the state y which is used in the proof of existence of a globally optimal solution for (OCP). The constraint set \mathcal{U}_{ad} is of the form

$$\mathcal{U}_{ad} := \left\{ v : (0, T) \rightarrow L^2(\Omega) : \|v(t)\|_{L^2(\Omega)} \leq \omega(t) \text{ f.a.a. } t \in (0, T) \right\}$$

for a measurable function ω which is nonnegative almost everywhere on $(0, T)$, so spatially integrated pointwise-in-time constraints of Trust-Region type. To the best of our knowledge, this kind of constraint has not been investigated yet in an evolution equation setting.

Basing on recent papers by wave equation experts ([2, 3]), we show that for every control $u \in L^1(0, T; L^2(\Omega))$, there exists a unique (mild) solution y for which $(y, \partial_t y) \in C([0, T]; \mathcal{E})$ and $y \in L^5(0, T; L^{10}(\Omega))$. The additional integrability for y is exactly such that $y^5 \in L^1(0, T; L^2(\Omega))$. Together with Strichartz estimates as in [3], this regularity is an important ingredient in local wellposedness for (CWE). Global-in-time existence is proven by localizing the wave equation to backwards light cones; then a nontrivial L^6 -nonconcentration property for y allows to bootstrap boundedness in $L^5(0, T; L^{10}(\Omega))$ on these light cones, from which a continuation argument yields global-in-time existence. We consider this the first main result of our work.

We moreover obtain existence of globally optimal solutions to (OCP). Since mild solutions are also weak ones, the proof follows the standard reasoning from the calculus of variations; however, as mentioned above, due to the critical power

nonlinearity, we can only show that the limit state is unique if we admit the state regularization in the objective, i.e., if $\gamma > 0$ in ℓ .

Finally, we also consider optimality conditions. For first order necessary ones, we combine smoothness of the control-to-state mapping $u \mapsto y$ with the theory established in [4] for $j(u) := \|u\|_{L^1(0,T;L^2(\Omega))}$ —which is nonsmooth—to obtain a bounded Lagrange multiplier $\bar{\mu}$ associated to the constraint given by \mathcal{U}_{ad} for every locally optimal control $\bar{u} \in \mathcal{U}_{\text{ad}}$.

The second main result(s) are then second-order optimality conditions of both necessary and sufficient type. Here, we deal with both nonsmoothness of j and with the nonzero curvature of the Trust-Region type constraint given by \mathcal{U}_{ad} . For the second-order necessary conditions, this necessitates to carefully combine Taylor expansion for j (away from nonsmoothness points) with a nonlinear path of controls $\mathcal{U}_{\text{ad}} \ni u_\rho \rightarrow \bar{u}$. From there, we obtain sufficient conditions in the sense that if $\ell_r''(\bar{u})(v, v) > 0$ for all $v \neq 0$ from the critical cone, then the *strong* quadratic growth property

$$\ell(\bar{y}, \bar{u}) + \frac{\eta}{2} \|u - \bar{u}\|_{L^2(0,T;L^2(\Omega))}^2 \leq \ell(y, u) \text{ for all } u \in \mathcal{U}_{\text{ad}}, \|u - \bar{u}\|_{L^2(0,T;L^2(\Omega))} < \varepsilon$$

holds true for appropriate $\eta, \varepsilon > 0$. We point out that we need the fully quadratic control regularization, i.e., $\beta_2 > 0$ in ℓ here; the case $\beta_2 = 0$ is an open problem. The strong form of the quadratic growth property then allows to derive stability estimates for (OCP) for controls satisfying the second-order sufficient condition.

Possible extensions of this work would concern the case of homogeneous Neumann boundary conditions instead of Dirichlet ones, based on [5], and moreover, much more involved, the case of boundary control instead of distributed one.

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Shape Optimization with Phase Fields and a $W^{1,\infty}$ -Descent Approach

MICHAEL HINZE

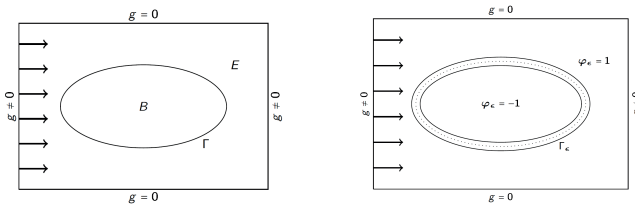
(joint work with Harald Garcke, Christian Kahle, and Andrew Lam (with phasefield approach), Klaus Deckelnick and Philip Herbert (with $W^{1,\infty}$ -descent))

We sketch two approaches for PDE constrained shape optimization of domains. In the first approach we consider a phasefield method for fluid mechanic shape optimization, where the shape of the sought domain is approximated by the zero level set of a phasefield function. This turns the shape optimization problem into a PDE constrained optimization problem where the phasefield enters as control in the coefficients of the PDE. The second approach uses the method of mappings, where we propose a new minimization approach using steepest descent in the $W^{1,\infty}$ -topology. The numerical example indicates that minimization in the $W^{1,\infty}$ -topology seems to be superior over the classical minimization in Hilbert spaces, in particular when the optimal shape has sharp corners.

Diffuse interface approach. Let $\Omega \subset \mathbb{R}^n$ denote an open bounded hold-all domain with Lipschitz-boundary. We assume an incompressible fluid inside $E \subset \Omega$ and a non-permeable obstacle $B = \Omega \setminus E$. The velocity field u together with the pressure field p satisfy the Navier–Stokes equations in E with prescribed boundary data $g \in H^{1/2}(\partial\Omega)$ and volume force $f \in L^2(\Omega)$. Moreover, $u = 0$ on ∂B . We identify $E \subset \Omega$ with $\varphi := 2\chi_E - 1 \in BV(\Omega, \{\pm 1\})$. Then for any $\varphi \in BV(\Omega, \{\pm 1\})$ the set $E^\varphi := \{\varphi = 1\}$ is the corresponding Caccioppoli set describing the fluid region. The shape optimization problem for those vector fields u and controls φ then reads

$$(P) \quad \min_{\{u, \varphi\}} J(u, p, \varphi) = \int_{\Omega} h_b(u, p, \varphi) dx + \int_{\Omega} h_{\Gamma}(u, p, \nu_{\varphi}) d|D\varphi| + \frac{\gamma}{2} |D\varphi|(\Omega).$$

Here, ν_{φ} is the *outer normal* on $\Gamma := \Omega \cap \partial E^\varphi$, and $\frac{\gamma}{2} |D\varphi|(\Omega) = \gamma \int_{\Gamma} ds$ is the perimeter regularization, where $D\varphi$ denotes the distributional derivative of φ and represents a finite Radon measure concentrated on Γ with $|D\varphi|$ its total variation. The functions $h_b(u, p, \varphi)$ and $h_{\Gamma}(u, p, \nu_{\varphi})$ contain mathematical expressions of the physical quantities to be minimized, like drag, lift, hydrodynamic force, and/or total potential power of the flow. The minimization problem (P) also may be accompanied by further integral constraints on the state variables.



BV–approach (left) and phasefield relaxation (right)

Since this minimization problem may lack well-posedness and is formulated within a complicated mathematical framework, we relax the sharp interface formulation

through introducing a phasefield approximation φ_ϵ of φ combined with a Darcy-flow relaxation of the fluid flow and substitute all quantities related to φ in (P) by according expressions with φ_ϵ . This leads to a mathematical setting where $\varphi_\epsilon \in H^1(\Omega) \cap L^\infty(\Omega)$, $|\varphi_\epsilon| \leq 1$ and $E_\epsilon = \{x \in \Omega \mid \varphi_\epsilon(x) = 1\}$, $B_\epsilon = \{x \in \Omega \mid \varphi_\epsilon(x) = -1\}$, and $\Gamma_\epsilon = \{x \in \Omega \mid |\varphi_\epsilon(x)| < 1\}$ (diffuse interface) denote the relaxed counterparts of E, B and Γ , respectively. An important ingredient is the relaxation of the perimeter regularization in (P) by the Ginzburg–Landau energy associated to φ_ϵ , which is known to be Γ -convergent to a multiple of the perimeter [5], i.e.

$$G(\varphi_\epsilon) := \int_\Omega \frac{\epsilon}{2} |\nabla \varphi_\epsilon|^2 + \frac{1}{\epsilon} W(\varphi_\epsilon) dx \xrightarrow{\epsilon \rightarrow 0} c_0 \int_\Gamma ds$$

holds with some $c_0 > 0$ only depending on the free energy W . This free energy could be chosen as logarithmic, double well, or double obstacle potential. The final step consists in approximating the fluid equation by a porous medium approach [2]. This is performed by introducing the interpolation function $\alpha_\epsilon(\varphi_\epsilon) = \bar{\alpha}_\epsilon \frac{1-\varphi_\epsilon}{2}$ with $\bar{\alpha}_\epsilon \xrightarrow{\epsilon \rightarrow 0} \infty$. The final optimization problem then is of the form

$$(P) \quad \min_{(u, \varphi_\epsilon)} J(u, p, \varphi_\epsilon) := \int_\Omega h_b(u, p, \varphi_\epsilon) dx + \int_\Omega \frac{1}{2} h_\Gamma(u, p, \nabla \varphi_\epsilon) dx \\ + \frac{\gamma}{c_0} \int_\Omega \frac{\epsilon}{2} |\nabla \varphi_\epsilon|^2 + \frac{1}{\epsilon} W(\varphi_\epsilon) dx + \int_\Omega \frac{1}{2} \alpha_\epsilon(\varphi_\epsilon) |u|^2 dx$$

subject to

$$(NS) \quad \begin{aligned} \alpha_\epsilon(\varphi_\epsilon) u + (u \nabla) u - \mu \Delta u + \nabla p &= 0 && \text{in } \Omega, \\ -\operatorname{div} u &= 0 && \text{in } \Omega, \\ u &= g && \text{on } \partial\Omega, \end{aligned}$$

complemented with additional constraints on the state u and/or the control φ_ϵ . For $\varphi_\epsilon = -1$ the term $\alpha_\epsilon(\varphi_\epsilon)u$ dominates in the momentum equation, which corresponds to Darcy flow. The last term in the cost functional is added to further enforce $u = 0$ on the obstacle for $\epsilon \rightarrow 0$. Problem (P) is a constrained control-in-the-coefficient problem, for which one can prove e.g. existence of solutions and establish first order necessary optimality conditions, see [3], where also a couple of numerical examples can be found.

Shape optimization with $W^{1,\infty}$ descent. Let $\Omega \subset \mathbb{R}^n$ be a bounded and open Lipschitz domain. Let

$$\Omega_V := \Omega + V(\Omega), \text{ where } V \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n),$$

so that for $\|V\|_{1,\infty} < 1$ the transformed domain Ω_V is Lipschitz. Let J denote a shape differentiable shape functional with $DJ(\Omega)[\cdot]$ denoting its differential at Ω . Our idea now consists in using $W^{1,\infty}$ -steepest descent directions V^* of J in a shape optimization algorithm. Those directions are characterized as solutions to the minimization problem

$$(\Delta_\infty) \quad V^* = \underset{\{V \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n), \|V\|_{1,\infty} \leq 1\}}{\operatorname{arg\,min}} \quad DJ(\Omega)[V].$$

Known practical approaches use Hilbert space methods, i.e. seek fields V^* determined by

$$a(V^*, W) = DJ(\Omega)[W] \text{ for all } W \in H^1(\mathbb{R}^n)^n,$$

where $a(\cdot, \cdot)$ denotes an appropriate inner product on $H^1(\mathbb{R}^n)$, see [1] for an extensive discussion. A mathematical framework for the solution of minimization problems of type (Δ_∞) is provided in e.g. [4].

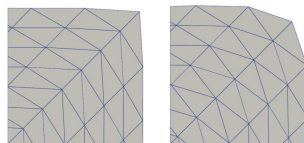
Numerical example for a model problem: Set $F(x_1, x_2) = 0$ and $z(x_1, x_2) = |x_1 + x_2| + |x_1 - x_2|$. Let $0 < c_0 < 1$ denote a given constant. For $f \in W^{1,\infty}(\mathbb{S}^1)$ let Ω_f denote the domain enclosed by the curve $\partial\Omega_f := \{y \in \mathbb{R}^2 : y = xf(x), x \in \mathbb{S}^1\}$. We consider the shape optimization problem of finding a function $f^* \in W := \{f \in W^{1,\infty}(\mathbb{S}^1) : \int_{\mathbb{S}^1} \tilde{f}^2 = \pi, \tilde{f} \geq c_0\}$ which solves

$$f^* = \arg \min_{f \in W} \mathcal{J}(f) := \frac{1}{2} \int_{\Omega_f} |u_f - z|^2 dx,$$

and where $u_f \in H_0^1(\Omega_f)$ is the solution to

$$\int_{\Omega_f} \nabla u \cdot \nabla v = \langle F|_{\Omega_f}, v \rangle \quad \forall v \in H_0^1(\Omega_f).$$

Since in the present example $u_f \equiv 0$ for all $f \in W$ and z is constant on the boundary of the square $\Omega_{f^*} := \left(-\frac{\sqrt{\pi}}{2}, \frac{\sqrt{\pi}}{2}\right)^2$ with center $0 \in \mathbb{R}^2$, it can be shown that $\langle J'(f^*), g \rangle = 0$ for all $g \in W^{1,\infty}(\mathbb{S}^1)$ satisfying $\int_{\mathbb{S}^1} f^* g do_w = 0$, so that Ω_{f^*} is a minimizer. We solve this minimization problem with the steepest descent algorithm initialized with Ω_f the unit circle corresponding to $f = 1$. We employ the Armijo step size rule with slope factor 10^{-5} and use 10^{-8} as lower bound for the Armijo step size. After 185 iterations, the Lipschitz method terminated, while the H^1 -method was stopped after the maximum of 250 iterations. The picture on the right shows a zoom on the right upper corners of the respective triangulated final domains. As one can clearly see the Lipschitz method yields significantly better pronounced corners.



Lipschitz (left) versus H^1 -descent

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First-Order Mean Field Games of Controls

LAURENT PFEIFFER

(joint work with P. Jameson Graber and Alan Mullenix)

INTRODUCTION

Mean field game (MFG) theory aims at describing Nash equilibria involving a large number of agents, all optimizing their own dynamical system. Mathematically, MFGs take the form of a coupled system of PDEs, the Fokker-Planck and the Hamilton-Jacobi-Bellman equations. It has been known, since the early developments of the theory by P.L. Lions and J.M. Lasry in 2006, that the coupled system coincides with the optimality system associated with two convex PDE-optimization problems in duality (under appropriate assumptions). Later this observation allowed P. Cardaliaguet and co-authors to obtain existence results for MFGs with congestion when the diffusion is degenerate in [1]. We follow this methodology in [2] in order to prove the existence of a solution of a mean field game involving some interaction term via the controls of the agents.

THE MFG SYSTEM AND ITS INTERPRETATION

We give in this extended abstract a very rough overview of that methodology. A (slightly) simplified version of the mean field game that we have considered is the following:

$$(1) \quad \left\{ \begin{array}{ll} (i) & -\partial_t u + H(Du(x, t) + P(t)) = f(m(x, t)), \quad (x, t) \in Q, \\ (ii) & \partial_t m + \nabla \cdot (vm) = 0 \quad (x, t) \in Q, \\ (iii) & P(t) = \Psi\left(\int_{\mathbb{T}^d} v(x, t)m(x, t)dx\right) \quad t \in [0, T], \\ (iv) & v(x, t) = -DH(Du(x, t) + P(t)) \quad (x, t) \in Q, \\ (v) & m(x, 0) = m_0(x), \quad u(x, T) = u_T(x), \quad x \in \mathbb{T}^d. \end{array} \right.$$

Here $Q := \mathbb{T}^d \times [0, T]$. The maps $H: \mathbb{R}^d \rightarrow \mathbb{R}$, $f: \mathbb{R}_+ \rightarrow \mathbb{R}$, $\Psi: \mathbb{R}^d \rightarrow \mathbb{R}^d$, $m_0: \mathbb{T}^d \rightarrow \mathbb{R}$, and $u_T: \mathbb{T}^d \rightarrow \mathbb{R}$ are given. The unknown variables are $u: Q \rightarrow \mathbb{R}$, $m: Q \rightarrow \mathbb{R}$, $v: Q \rightarrow \mathbb{R}^d$, $P: [0, T] \rightarrow \mathbb{R}^d$.

The heuristic interpretation of the above system is the following. Each agent controls the following dynamical system in \mathbb{T}^d :

$$dX_t = \alpha_t dt.$$

The associated cost (to be minimized) is given by

$$\int_0^T \left(H^*(-\alpha_t) + \langle P(t), \alpha_t \rangle + f(m(x, t)) \right) dt + u_T(X_T).$$

At optimality, the control α is in feedback form, i.e.

$$\alpha_t = v(X_t, t) = -DH(Du(X_t, t) + P(t)),$$

where u denotes the associated value function. Its evolution is given by the Hamilton-Jacobi-Bellman equation (equation (i)). The variable m denotes the

distribution of all agents with respect to their state variable. Its evolution is given by the Fokker-Planck equation (ii). On top of the interaction induced by the congestion term, we have an interaction through the variable P , defined in equation (iii) as the average value of the control variable. This interaction is classical in Cournot equilibrium models.

The basic structural assumptions are the following:

- the Hamiltonian H is convex,
- the congestion function f is increasing,
- the price function Ψ is the gradient of some convex function Φ .

The analysis requires additional growth assumptions on f , H , Ψ and regularity assumptions on m_0 and u_T which we do not detail, see [2, Section 1.2].

After performing the Benamou-Brenier change of variables $w = mv$, we obtain the system:

$$(2) \quad \begin{cases} (i) & -\partial_t u + H(Du(x, t) + P(t)) = 0 & (x, t) \in Q, \\ (ii) & \partial_t m + \nabla \cdot w = 0 & (x, t) \in Q, \\ (iii) & P(t) = \Psi\left(\int_{\mathbb{T}^d} w(x, t) dx\right) & t \in [0, T], \\ (iv) & w(x, t) = -DH(Du(x, t) + P(t))m(x, t) & (x, t) \in Q, \\ (v) & m(x, 0) = m_0(x), \quad u(x, T) = u_T(x), & x \in \mathbb{T}^d. \end{cases}$$

THE TWO PROBLEMS IN DUALITY

We define

$$F(m) = \int_0^m f(\theta) d\theta$$

if $m \geq 0$ and $F(m) = +\infty$ otherwise. Note that F is convex.

Formally, the coupled system (2) is the optimality system associated with two problems in duality. The first one is an optimal control problem of the Hamilton-Jacobi-Bellman equation:

$$(3) \quad \begin{aligned} & \inf_{(u, P, \gamma)} - \int_{\mathbb{T}^d} u(x, 0) m_0(x) dx + \int_0^T \Phi^*(P(t)) dt + \iint_Q F^*(\gamma(x, t)) dx dt, \\ \text{subject to: } & \begin{cases} -\partial_t u + H(Du(x, t) + P(t)) = \gamma, \\ u(x, T) = u_T(x). \end{cases} \end{aligned}$$

The second one is an optimal control problem of the Fokker-Planck equation:

$$(4) \quad \begin{aligned} & \inf_{(m, w)} \iint_Q \left(H^* \left(-\frac{w(x, t)}{m(x, t)} \right) m(x, t) + F(m(x, t)) \right) dx dt \\ & \quad + \int_0^T \Phi \left(\int_{\mathbb{T}^d} w(x, t) dx \right) dx dt + \int_{\mathbb{T}^d} u_T(x) m(x, T) dx, \\ \text{subject to: } & \begin{cases} \partial_t m + \nabla \cdot w = 0, \\ m(x, 0) = m_0(x). \end{cases} \end{aligned}$$

The main steps of analysis are the following.

- We formulate Problem (3) in spaces of (sufficiently) smooth functions, so that the HJB equation can be understood in the classical sense.
- We prove that Problem (4) is the dual problem to (3). By the Fenchel-Rockafellar duality theorem, it possesses a solution, which is shown in Lemma 2.1 to lie in some L^p -space, thanks to the growth assumption on H and F . The Fokker-Planck equation is understood in the weak sense.
- It is unclear whether Problem (3) has a solution. One can instead prove the existence of a solution to a relaxed variant in some L^p space, see Proposition 3.10. The relaxed problem is obtained by requiring that u is (only) a weak subsolution to the HJB equation. The existence is obtained with the direct method of the calculus of variations. Again, the growth assumptions on the data functions play an important role to bound the minimizing sequence.
- Using the solution to problem (4) and the solution to the relaxed variant of (3), we construct a quadruplet (u, m, P, v) which is shown to be a solution in a relaxed sense to the MFG system (1). See Theorem 4.3.

SOME OPEN ISSUES

Some classical issues from MFG theory are still open for problems of the form (1). They concern in particular: (i) the asymptotic behavior when $T \rightarrow \infty$, (ii) the numerical resolution in the second-order case, (iii) the convergence of the fictitious play method, which would indicate that such equilibria are likely to arise.

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On Pre-Shape Calculus

VOLKER SCHULZ

(joint work with Daniel Luft)

Studies in shape optimization are motivated by a wide variety of applications in practice. Current examples of application projects involving the author are the determination of shapes for gas turbine blades aiming at robustness with respect to low cycle fatigue (BMBF project GIVEN with partners Trier University, University of Wuppertal, DLR, Siemens AG, 2018-2021) or shape optimization for mitigating coastal erosion (DFG-SPP 1962 project with partners Trier University and University Cheikh Anta Diop of Dakar, 2019-2022). The handling of the computational mesh is of special importance in all applications. During geometry changes, this mesh has to be carried along, which often leads to problems in the

solution of partial differential equations on the changed meshes. In the publication [2] it was shown, how by mesh deformations, which are based on the solution of the elasticity equation, a shape-Hessian approximation of Steklov-Poincaré type and an efficient and practicable mesh fitting in normal direction can be accomplished at the same time.

However, almost all shape optimization studies, like [2], focus on geometry changes in normal directions, which is quite natural since according to [3] shape optimization can be interpreted as optimization on the manifold of shapes, where shapes are considered as equivalence classes of embeddings that are invariant under (tangential) reparametrizations. Nevertheless, all mesh deformations have tangential effects on the surface mesh, which are thus systematically overlooked and not controlled. Often, deformations form regions on the shape where tangential stretching or compression occurs. In these regions, one would actually like to move surface mesh points during optimization in such a way that the mesh quality of the deformed mesh does not suffer. So far, no methods are available for this purpose. The publication [1], which treats this problem for the first time and is the basis of this talk, goes one step behind [3] and opens the notion of a shape for the explicit consideration of the parameterization of the shape and thus implicitly also for the control of the surface mesh. The notion of pre-shape, which goes back to [4], is used here as a shape concept motivating a pre-shape calculus based on it, which includes the classical shape calculus as a special case. On the one hand, this leads to an exciting new mathematical calculus with sophisticated theoretical results. On the other hand, from a numerical point of view, degradation of the tangential mesh quality, which is otherwise observed during shape optimization, is prevented. This effect is supported by preliminary numerical examples. Further research may involve the choice of proper shape cost functionals taking into account meshes, detailed analysis of the interplay between a pure shape functional and a mesh oriented functional and details on the numerical implementation in a practical environment.

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Optimality Conditions and Regularization for Convex Stochastic Optimization with Almost Sure State Constraints

CAROLINE GEIERSBACH

(joint work with Michael Hintermüller and Winnifried Wollner)

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. Consider a risk-neutral stochastic optimization problem of the form

$$(P') \quad \begin{aligned} & \underset{(x_1, x_2) \in L^2(D) \times L^\infty(\Omega, X_2)}{\text{minimize}} && \int_{\Omega} \int_D (x_2(s, \omega) - y_D(s))^2 \, ds \, d\mathbb{P}(\omega) + \alpha \int_D x_1(s) \, ds \\ & \text{s.t.} \quad \begin{cases} -\nabla \cdot (a(s, \omega) \nabla x_2(s, \omega)) = x_1(s) + g(s, \omega) & \text{on } D \times \Omega \text{ a.e. a.s.,} \\ x_2(s, \omega) = 0 & \text{on } \partial D \times \Omega \text{ a.e. a.s.,} \\ x_2(s, \omega) \leq \psi(s, \omega) & \text{on } D \times \Omega \text{ a.e. a.s.,} \end{cases} \end{aligned}$$

where $y_D \in L^2(D)$, $\alpha > 0$, and $\psi \in L^\infty(\Omega, X_2)$. This PDE-constrained problem with uncertainty and “almost sure”-type constraints on the state is new. One can, however, understand this problem in the setting of two-stage stochastic optimization, where x_1 is the first stage and x_2 is the second stage. Such problems are well-understood, thanks to a series of papers by Rockafellar and Wets [2, 3, 4, 5]. In these works, they consider second-stage variables belonging to the space $L^\infty(\Omega, \mathbb{R}^n)$. In [1], we revisit these papers to handle problems like (P'). It turns out that in spite of the analytical difficulties, one can develop rich duality theory if the problem is convex. We work with the state space $L^\infty(\Omega, X_2)$, where X_2 is a real, reflexive, and separable Banach space with enough regularity to satisfy a constraint qualification; for example, if $D \subset \mathbb{R}^2$ is a bounded Lipschitz domain, one needs $X_2 = W_0^{1,p}(D)$, $p > 2$ for problem (P').

Let X_1, W, R be real, reflexive, and separable Banach spaces. Our results concern optimality theory for the general class of problems

$$(P) \quad \begin{aligned} & \underset{x := (x_1, x_2) \in X := X_1 \times L^\infty(\Omega, X_2)}{\text{minimize}} && \{j(x) := J_1(x_1) + \mathbb{E}[J_2(x_1, x_2(\cdot), \cdot)]\} \\ & \text{s.t.} \quad \begin{cases} x_1 \in C, \\ e(x_1, x_2(\omega), \omega) = 0 \text{ a.s.,} \\ i(x_1, x_2(\omega), \omega) \leq_K 0 \text{ a.s.,} \end{cases} \end{aligned}$$

where $e : X_1 \times X_2 \times \Omega \rightarrow W$ and $i : X_1 \times X_2 \times \Omega \rightarrow R$. Given a cone $K \subset R$, the partial order \leq_K is defined by $r \leq_K 0 \Leftrightarrow -r \in K$. Technical assumptions providing measurability, integrability, and convexity can be found in [1].

The central tool in our analysis is the decomposition of elements from $L^\infty(\Omega, W)$ and $L^\infty(\Omega, R)$ into absolutely continuous and singular terms. This motivates the definition of a Lagrangian with paired spaces $U := L^\infty(\Omega, W) \times L^\infty(\Omega, R)$ and $\Lambda := L^1(\Omega, W^*) \times L^1(\Omega, R^*)$:

$$(1) \quad L(x, \lambda) = j(x) + \mathbb{E}[\langle \lambda_e, e(x_1, x_2, \omega) \rangle_{W^*, W} + \langle \lambda_i, i(x_1, x_2, \omega) \rangle_{R^*, R}].$$

With $X_0 = \{x = (x_1, x_2) \in X : x_1 \in C\}$ and $\Lambda_0 := \{\lambda = (\lambda_e, \lambda_i) \in \Lambda : \lambda_i(\omega) \in K^\oplus \text{ a.s.}\}$, where K^\oplus denotes the dual cone to K , we seek saddle points

to Lagrangian L , i.e., those $(\bar{x}, \bar{\lambda}) \in X_0 \times \Lambda_0$ satisfying

$$L(\bar{x}, \lambda) \leq L(\bar{x}, \bar{\lambda}) \leq L(x, \bar{\lambda}) \quad \forall (x, \lambda) \in X_0 \times \Lambda_0.$$

Saddle points are shown to exist under the following conditions (in addition to the technical assumptions mentioned above):

- (C1) $F_{\text{ad},u}$ is bounded for all u in a neighborhood of zero or j is radially unbounded, meaning $j(x) \rightarrow \infty$ as $\|x\|_X \rightarrow \infty$.
- (C2) Strict feasibility: $0 \in \text{int dom } v$, where $v(u) := \inf_{x \in X} j(x)$ if $x \in F_{\text{ad},u} := \{x \in X : x_1 \in C, e(x_1, x_2(\omega), \omega) = u_e(\omega) \text{ a.s.}, i(x_1, x_2(\omega), \omega) \leq_K u_i(\omega) \text{ a.s.}\}$ and $v(u) = \infty$ otherwise, where $u = (u_e, u_i) \in U$.
- (C3) Relatively complete recourse: $C \subset \tilde{C} := \{x_1 \in X_1 : \exists x_2 \in L^\infty(\Omega, X_2) \text{ s.t. } e(x_1, x_2(\omega), \omega) = 0 \text{ a.s.}, i(x_1, x_2(\omega), \omega) \leq_K 0 \text{ a.s.}\}$

Additionally, we prove that saddle points are equivalent to (necessary and sufficient) Karush–Kuhn–Tucker (KKT) conditions for optimality. Notably, these conditions include an additional multiplier from the implicit nonanticipativity constraint $x_1(\omega) \equiv x_1$; as a classical stochastic optimization problem, the first stage is deterministic, i.e., not depending on ω . An advantage of obtaining Lagrange multipliers that are integrable is that one can obtain strong (almost sure) conditions for optimality, which is useful for computations, for instance via sample average approximation.

In current work, we focus on relaxing condition (C3) with the observation that the original example problem (P') does not satisfy it except for trivial choices of ψ . Without this condition, we expect the presence of singular multipliers, motivating the definition of an extended Lagrangian, where U paired with U^* :

$$(2) \quad \begin{aligned} \bar{L}(x, \lambda, \lambda^\circ) = & L(x, \lambda) + \langle \lambda_e^\circ, e(x_1, x_2(\cdot), \cdot) \rangle_{(L^\infty(\Omega, W))^*, L^\infty(\Omega, W)} \\ & + \langle \lambda_i^\circ, i(x_2, x_2(\cdot), \cdot) \rangle_{(L^\infty(\Omega, R))^*, L^\infty(\Omega, R)}. \end{aligned}$$

We again rely on the decomposition on the spaces $L^\infty(\Omega, R)$ and $L^\infty(\Omega, W)$, with \mathcal{S}_e and \mathcal{S}_i denoting their respective subspaces of singular elements. With feasible singular multipliers from the set

$$\Lambda_0^\circ = \{\lambda^\circ = (\lambda_e^\circ, \lambda_i^\circ) \in \mathcal{S}_e \times \mathcal{S}_i : \lambda_i^\circ(y) \geq 0 \forall y \in L^\infty(\Omega, R) : y \geq_K 0 \text{ a.s.}\},$$

we show that conditions (C1) and (C2) are enough to show the existence of saddle points to extended Lagrangian \bar{L} . Additionally, saddle points can be shown to be equivalent to strongly formulated KKT conditions. In view of computations, we propose solving a Moreau–Yosida regularized problem

$$(P^\gamma) \quad \begin{aligned} & \underset{x \in X}{\text{minimize}} \quad \{j^\gamma(x) := j(x) + \mathbb{E}[\beta^\gamma(-i(x_1, x_2(\cdot), \cdot))]\} \\ & \text{s.t.} \quad \begin{cases} x_1 \in C, \\ e(x_1, x_2(\omega), \omega) = 0 \quad \text{a.s.}, \end{cases} \end{aligned}$$

where $\beta^\gamma(k) = \inf_{y \in H} \{\delta_{K_H}(y) + \frac{\gamma}{2} \|k - y\|_H^2\}$ and $R \hookrightarrow H \cong H^* \hookrightarrow R^*$, where H is a Hilbert space where the projection onto $K_H := K \cap H$ can be cheaply computed. Current work involves analyzing the consistency of Problem (P $^\gamma$) as

$\gamma \rightarrow \infty$ to the original Problem (P). Additionally, we are currently working on obtaining optimality conditions for risk-averse objective functions.

FUTURE RESEARCH

These investigations will provide the theoretical framework to design algorithms. Additionally, we are interested in applications to stochastic generalized Nash equilibrium problems, where our theory can be applied in the search for variational equilibria.

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Real Time Estimation of 3D Advection Diffusion Equations

JOHN ALLEN BURNS

(joint work with James Cheung, Michael Demetriou, Nikolaos Gatsonis, Weiwei Hu, and Xin Tian)

Consider the convection diffusion equation

$$(1) \quad \frac{\partial z(t, x)}{\partial t} = \nabla \cdot [K \nabla z(t, x)] - \nabla \cdot [Kz(t, x)] + g(x)\eta(t)$$

on a domain $\Omega \subset \mathbb{R}^3$. We assume there are $p \geq 0$ sensor platforms with locations $\beta_j \in \mathbb{R}^3$ that produces the sensed output

$$(2) \quad y_j(t) = \iiint_{\Omega} c_j(x, \beta_j) z(t, x) dx + E_i v(t),$$

$c_j(x, y)$ is a kernel function. If (formally) $c_j(x, y) = \delta(x - y)$ is the delta “function” then we are assuming point sensors. Let

$$(3) \quad \boldsymbol{\beta} = [\beta_1 \ \beta_2 \ \dots \ \beta_p]^T \in \mathbb{R}^{3p} \quad \text{and} \quad \mathbf{y}(t) = [y_1(t) \ y_2(t) \ \dots \ y_p(t)]^T \in \mathbb{R}^p$$

Define $\mathcal{A} : L^2(\Omega) \rightarrow L^2(\Omega)$ on $D(\mathcal{A}) = H^2(\Omega) \cap H_0^2(\Omega)$ by

$$(4) \quad \mathcal{A}\varphi(\cdot) = \nabla \cdot [K \nabla \varphi(\cdot)] - \nabla \cdot [K\varphi(\cdot)].$$

Also, we define $\mathcal{C}(\boldsymbol{\beta}) : L^2(\Omega) \rightarrow \mathbb{R}^p$ and $\mathcal{G} : \mathbb{R}^m \rightarrow L^2(\Omega)$ by

$$(5) \quad [\mathcal{C}(\boldsymbol{\beta})\varphi(\cdot)]_j = \iint_{\Omega} c_j(x, \beta_j)\varphi(x)dx \quad \text{and} \quad \mathcal{G}\eta = g(x)\eta,$$

respectively. The corresponding distributed parameter formulation of the system is defined by

$$(6) \quad \dot{z}(t) = \mathcal{A}z(t) + \mathcal{G}\eta(t)$$

$$(7) \quad \mathbf{y}(t) = \mathcal{C}(\boldsymbol{\beta})z(t) + Ev(t)$$

We seek a (Luenberger) observer of the form

$$(8) \quad \dot{z}_e = \mathcal{A}z_e(t) + \mathcal{G}\eta(t) + \mathcal{F}(\mathbf{y}(t) - \mathcal{C}(\boldsymbol{\beta})z_e(t)),$$

where $\mathcal{F} = \mathcal{F} : \mathbb{R}^p \rightarrow L^2(\Omega)$ is a bounded linear operator. The goal is to find an observer gain operator such that the error between the state $z(t)$ and the estimated state $z_e(t)$ given by $error(t) = \|z(t) - z_e(t)\|^2$ is “asymptotically small” (see [4]).

Note that the Kalman filtering gain operator $\mathcal{F}^{Kal}(\boldsymbol{\beta})$ is a steady state Luenberger observer and given by

$$(9) \quad \mathcal{F}^{Kal}(\boldsymbol{\beta}) = \Sigma(\boldsymbol{\beta})\mathcal{C}(\boldsymbol{\beta})^*$$

where $\Sigma(\boldsymbol{\beta})$ satisfies the Riccati equation

$$(10) \quad \mathcal{A}\Sigma(\boldsymbol{\beta}) + \Sigma(\boldsymbol{\beta})\mathcal{A}^* - \Sigma(\boldsymbol{\beta})\mathcal{C}(\boldsymbol{\beta})^*\mathcal{C}(\boldsymbol{\beta})\Sigma(\boldsymbol{\beta}) + \mathcal{G}\mathcal{G}^* = 0.$$

In this case one seeks the optimal location $\boldsymbol{\beta}^{opt}$ to minimize the expected value of the mean square error

$$(11) \quad J(\boldsymbol{\beta}) = \{\mathbb{E}(\|z(t) - z_e(t, \boldsymbol{\beta})\|^2) : \boldsymbol{\beta} \in \Omega, 0 \leq t < +\infty\}$$

and

$$(12) \quad J(\boldsymbol{\beta}^{opt}) = \min_{\boldsymbol{\beta} \in \Omega} J(\boldsymbol{\beta}) = \min_{\boldsymbol{\beta} \in \Omega} Trace[\Sigma(\boldsymbol{\beta})].$$

There are (at least) two challenges to achieving real-time estimation:

1. Determining (computing) the observer gain $\mathcal{F}(\boldsymbol{\beta})$, and
2. Solving the estimation equation (8) in real-time.

In addition, we considered the case where the p sensor platforms (e.g., typically an unmanned air vehicles - UAVs) so that the flight vehicles dynamics have form

$$(13) \quad \ddot{\beta}_j(t) = f(\beta_j(t), \dot{\beta}_j(t), u_j(t)),$$

where u_j is the control input for the j^{th} UAV and $\beta_j(t) \in \mathbb{R}^3$ is the position of the UAV at time t . Including the flight dynamics requires two additional issues be resolved. Namely:

3. Determining a (feedback) guidance law for the controllers, and
4. Solving the combined flight dynamic equations (13) and estimation equation (8) in real-time.

In this talk we presented some new results where we show that by applying high order hp - finite element methods one can develop accurate numerical approximations of the Riccati equation (10) with low order finite dimensional systems. Preliminary results can be found in the paper [1, 2]. Finally, employing a computational scheme based on a simple guidance law with a CFD algorithm developed at WPI which uses a heterogeneous non-overlapping domain decomposition explicit finite volume method (NODDE-FVM-TVD-RK) one can achieve real time computation of the estimator equations using hyper-threading on a small laptop. This was achieved for one moving sensor platform with flight dynamics included. The idea is to use a Luenberger observer near the sensor location and a “naive” observer in the spatial regions outside a neighborhood of the UAV location. Details of these results will appear in the paper [3].

Open Issues and Future Work

The results described above do not use the “optimal” Kalman filter gains $\mathcal{F}^{Kal}(\beta)$. Although this choice of observer gain allows for an easy parameterizations of the optimal sensor location problem, it is not clear that in the problem with UAV dynamics that the Kalman filter is the “best” choice to achieve good and practical real time tracking. We are currently exploring other options that allow for joint optimization of sensor locations and performance that is suitable for finite (short) time intervals.

The domain decomposition method allows for the use of different observers on different subdomains. This is critical in achieving real time estimation. One open issue is whether or not one can combine adaptive hp - finite element methods to obtain a sub-optimal Kalman filter near the moving sensor platform and a crude but stabilizing Luenberger observer on the rest of the domain Ω .

Finally, we note that the same methods used in the tracking problem above should be applicable to “plume” source location problems. Further work is needed to determine if these ideas can be employed for real time source location problems.

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An Interior Point Approach for a Class of Risk-Averse PDE-Constrained Optimization Problems with Coherent Risk Measures

THOMAS M. SUROWIEC

(joint work with Sebastian Garreis and Michael Ulbrich)

PDE-constrained stochastic optimization problems offer a natural, data-driven modeling paradigm for a wide array of applications in engineering and the natural sciences. By taking cues from traditional stochastic programming and risk management, there are many ways to obtain solutions that are resilient to outlier events. One popular technique is to model risk preferences by employing risk measures in the objective functions or as part of the constraints. This leads to so-called risk-averse optimization problems. However, due to the fact that many PDE-constrained optimization problems are non-convex and a number of popular risk measures non-smooth, this convenient modeling approach presents a number of major theoretical, algorithmic, and numerical challenges.

On an abstract level, the problems of interest have the following structure:

$$\inf_{z \in Z_{\text{ad}}} \mathcal{R}[\mathcal{J}(S(z))] + \varphi(z).$$

Here, U and Z are the deterministic state and decision spaces, $S(z, \xi) \in U$ corresponds to the random field solution of the forward problem as a function of the decision variable $z \in Z$ and realization of the random variable $\xi \in \Xi \subset \mathbb{R}^d$, $\mathcal{J}(u)(\xi) = J(u(\xi), \xi)$ is the state-dependent part of objective function, $\varphi : Z \rightarrow \mathbb{R}$ is a cost or regularization term for decision z , $Z_{\text{ad}} \subset Z$ is a nonempty, closed, and convex set and $\mathcal{R} : L^1(\Xi, \mathcal{F}, \mathbb{P}) \rightarrow \mathbb{R}$ is a risk measure.

In the interest of finding a solution that performs well on average but also seeks to minimize tail events, we take as \mathcal{R} the following class of functionals

$$\mathcal{R}[X] = (1 - \lambda)\mathbb{E}[X] + \lambda\text{CVaR}_\beta[X] \quad \lambda \in (0, 1).$$

Here, \mathbb{E} is the usual expectation, $\beta \in (0, 1)$ is the “risk level”, and $\text{CVaR}_\beta[X]$ is the well-known conditional value-at-risk (also known as average value-at-risk). This is defined as the tail expectation of X beyond the β -quantile, i.e.,

$$\text{CVaR}_\beta[X] := \frac{1}{1 - \beta} \int_\beta^1 q_\alpha[X] d\alpha,$$

where $q_\alpha[X]$ is the upper α -quantile of the random variable X . In this case, it is possible to show that

$$\mathcal{R}[X] = \min \mathbb{E}[t + W] \text{ over } (t, x, W) \in \mathbb{R} \times \mathbb{R}^n \times L^1(\Xi, \mathcal{F}, \mathbb{P})$$

s.t.

$$W \geq a_i(X - t), \quad i = 1, 2, \quad \mathbb{P}\text{-}a.s.$$

for $0 \leq a_1 < 1 < a_2$ where $\lambda = 1 - a_1 \in (0, 1]$ and $\beta = \frac{a_2 - 1}{a_2 - a_1} \in (0, 1)$. This would indicate that the nonsmoothness of \mathcal{R} in the objective can be removed from the original problem by introducing the scalar variable t , slack W , and two inequality

constraints. However, the inequality constraints may be not only non-convex and high dimensional ($d \gg 1$), but they need to hold almost surely. In order to remedy this problem, yet still enforce the constraints, we suggest a log-barrier approach.

The log-barrier approach allows us to eliminate the slack W and subsequently obtain a new class of risk measures, which we call the “log-barrier risk measure” \mathcal{R}_μ . This has the general form of an optimized certainty equivalent

$$\mathcal{R}_\mu[X] = \inf_{t \in \mathbb{R}} \{t + \mathbb{E}[\hat{v}_\mu(X - t)]\},$$

where \hat{v}_μ satisfies $\hat{v}_\mu(0) = 0$, $\hat{v}'_\mu(0) = 1$, and is strictly convex. The exact form can be seen in [1]. A number of important properties can be demonstrated. For example, as a mapping from $L^1(\Xi, \mathcal{F}, \mathbb{P})$ to \mathbb{R} , \mathcal{R}_μ is finite-valued, closed, convex, invariant on constants, risk-averse, translation equivariant, and monotonic. As a mapping from $L^p(\Xi, \mathcal{F}, \mathbb{P})$ to \mathbb{R} , \mathcal{R}_μ is Hadamard differentiable for $p = 1$, continuously Fréchet differentiable for $1 < p \leq \infty$, and the differential has the form

$$\mathcal{R}'_\mu[X] = v'_\mu(X - t_\mu(X)),$$

where $t_\mu(X) = \operatorname{argmin}_t \mathbb{E}[t + \hat{v}_\mu(X - t)]$. In addition, using several techniques from the theory of variational convergence, it is possible to show that \mathcal{R}_μ Γ -converges to \mathcal{R} as $\mu \downarrow 0$.

These results can then be used to derive primal and primal-dual optimality conditions for the abstract setting under additional smooth assumptions on the objective \mathcal{J} , control-to-state mapping S , and cost functionals φ . These conditions are strongly reminiscent of the relaxed optimality conditions used in traditional interior-point methods. Using these optimality conditions, we can build primal and primal-dual interior point algorithms for the numerical solution of these challenging risk-averse optimization problems. A further consequence of the log-barrier approach is the ability to take advantage of recent computational advances for parametric PDEs using tensor-based decomposition methods. After justifying the application of Newton’s method in a fully continuous setting, we conclude with a numerical example that demonstrates the viability of the tensor-based approach.

Several open questions remain. For example, a fully intertwined numerical method that links inexact calculation of the Newton steps, adaptive sampling (where necessary), and hierarchical methods or adaptive finite elements with the interior-point parameter $\mu > 0$ has yet to be developed.

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Optimal Feedback Law Recovery by Gradient-Augmented Sparse Polynomial Regression

BEHZAD AZMI

(joint work with Dante Kalise and Karl Kunisch)

In this talk, we aim at approximating the solutions of Hamilton-Jacobi-Bellman (HJB) equations associated with a class of optimal control problems based on machine learning techniques. We are concerned with the optimal control problems which consist of minimizing

$$(1) \quad J(u; t_0, x) := \int_{t_0}^T (\ell(y(t)) + \beta \|u(t)\|_2^2) dt,$$

subject to

$$(2) \quad \begin{cases} \frac{d}{dt}y(t) = f(y(t)) + g(y(t))u(t) & \text{for } t \in (t_0, T), \\ y(t_0) = x, \end{cases}$$

where $\beta > 0$, $0 \leq t_0 < T$, and the vectors $y(t) \in \mathbb{R}^n$ and $u(t) \in \mathbb{R}^m$ stand for the state and the control, respectively. Further, we assume that the dynamics $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $g : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times m}$, and the running cost function $\ell : \mathbb{R}^n \rightarrow \mathbb{R}$ are continuously differentiable.

Here, our objective is to approximate the value function V and the optimal feedback control u^* associated to the optimal control problem (1)-(2). The value function $V : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}$ is defined by

$$(3) \quad V(t, x) := \min_{u(\cdot)} \{J(u; t, x) \text{ subject to (2)}\}.$$

It is well-known [2] that the value function is the unique solution of the following differential equation

$$(HJB) \quad \begin{cases} \partial_t V(t, x) - \frac{1}{2\beta} \nabla V(t, x)^t g(x) g^t(x) \nabla V(t, x) + \nabla V(t, x)^t f(x) + \ell(x) = 0, \\ V(T, x) = 0, \end{cases}$$

and the optimal feedback control u^* can be obtained by

$$(4) \quad u^*(t, x) = -\frac{1}{2\beta} g^t(t, x) \nabla V(t, x).$$

Due to the so-called ‘‘curse of dimensionality’’, finding the direct solutions to (HJB) is numerically intractable for high-dimensional optimal control problems. To overcome the curse of dimensionality, we present a data-driven approach [1], in which the solution of (HJB) is approximated by using orthogonal polynomials and sampling strategies. Then, by using the approximated solution of (HJB), we can derive the optimal feedback control for the corresponding optimal control problem. This approach exploits the control theoretical link between (HJB) and first-order optimality conditions via Pontryagin’s Maximum Principle and it is based on the following main elements:

- (1) Generating a random dataset consisting of different state-value pairs,
- (2) Hyperbolic cross approximation of the value function with respect to orthogonal polynomials including Chebyshev and Legendre polynomials,
- (3) Sparse recovery via a (weighted LASSO) ℓ_1 minimization decoder.

Numerical experiments are also given which reveal that enriching the dataset with gradient information reduces the number of training samples and that the sparse polynomial regression consistently yields a feedback law of lower complexity.

Future Research:

- The extension of the presented results in the context of time-dependent, and second-order stochastic control problems.
- The extension of the presented results for infinite-horizon optimal control problems by employing the receding horizon framework.

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Characterization of Generalized Derivatives for the Solution Operator of the Bilateral Obstacle Problem and a Posteriori Error Estimators for FE-Approximations of the Subgradient

STEFAN ULBRICH

(joint work with Anne-Therese Rauls)

We consider optimal control problems for bilateral obstacle problems where the control appears in a possibly nonlinear source term. The non-differentiability of the solution operator poses the main challenge for the application of efficient optimization methods and the characterization of Bouligand generalized derivatives [2, 10] of the solution operator is essential for their theoretical foundation and numerical realization. We derive specific elements of the Bouligand generalized differential if the control operator satisfies natural monotonicity properties [6, 8]. We construct monotone sequences of controls where the solution operator is Gâteaux differentiable and characterize the corresponding limit element of the Bouligand generalized differential as being the solution operator of a Dirichlet problem on a quasi-open domain. In contrast to a similar recent result for the unilateral obstacle problem [7], we have to deal with an opposite monotonic behavior of the active and strictly active sets corresponding to the upper and lower obstacle. For the reduced objective functional, we obtain two elements of the Clarke subdifferential by using an adjoint formula. Note that in the unilateral case for the particular case of the Laplace operator and distributed control in $H^{-1}(\Omega)$ the full Bouligand generalized differential has been characterized in [9].

Moreover, for the unilateral case we derive an a posteriori error estimator for Clarke subgradients of the reduced objective functional that are computed using a finite element discretization [6]. We address the inexactness that arises due to the lack of knowledge on the correct active and strictly active sets, which are, by the previous analysis, the sets determining the domain on which generalized derivatives can be computed. We focus on the generalized derivative that is obtained on the complement of the strictly active set. Using a nondegeneracy condition [5] that is well known in the literature concerning the analysis of free boundaries [1, 4], we can show that the strictly active set and the weakly active set have a suitable structure. Now, based on an L^∞ -error estimator for the discrete state, see for example [5], we derive discrete approximations of the complement of the strictly active set from the interior to use it as the domain for the discrete subgradient and from the exterior to find an upper bound for the error. The error estimator can be used to control the error in inexact bundle methods, see for example [3]. We illustrate our findings in a numerical example [6].

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Directional Differentiability and Optimal Control for Elliptic Quasi-Variational Inequalities

AMAL ALPHONSE

(joint work with Michael Hintermüller and Carlos N. Rautenberg)

We consider the issues of directional differentiability and optimal control for the quasi-variational inequality (QVI)

$$(1) \quad \begin{aligned} y \in \mathbf{K}(y) : \langle Ay - f, y - v \rangle &\leq 0 \quad \forall v \in \mathbf{K}(y), \\ \mathbf{K}(y) &:= \{v \in V : v \leq \Phi(y)\}. \end{aligned}$$

Here, V is a Hilbert space that possesses an ordering (e.g., $V = H^1(\Omega)$ with $u \leq v$ if and only if $u \leq v$ a.e. in Ω) and $\Phi: V \rightarrow V$ is a given map called the obstacle map.

Denoting by \mathbf{Q} the set-valued mapping taking the source term f into the set of solutions y (so that (1) reads $y \in \mathbf{Q}(f)$), the directional differentiability of \mathbf{Q} is not only an interesting problem by itself but is also of use for optimal control, numerics and applications. Note that the corresponding theory for variational inequalities (VIs) has been thoroughly investigated, eg. [4, 5]. Our paper [1] is, to our knowledge, the first work addressing this issue in the infinite dimensional setting. In [1], we proved that given a source term $f \geq 0$, a direction $d \geq 0$ and a function $y \in \mathbf{Q}(f)$, under certain assumptions, there exists $y^s \in \mathbf{Q}(f + sd)$ such that

$$\lim_{s \rightarrow 0^+} \frac{y^s - y}{s} = \alpha$$

where the directional derivative α satisfies

$$\alpha \in \mathcal{K}_{\mathbf{K}(y)}(y, \alpha) : \langle A\alpha - d, v - \alpha \rangle \geq 0 \quad \forall v \in \mathcal{K}_{\mathbf{K}(y)}(y, \alpha),$$

with the set $\mathcal{K}_{\mathbf{K}(y)}(y, \alpha)$ being a critical cone (the precise definition is omitted).

In [2], we extend the above result to all directions and source terms (no sign is necessary) under considerably weaker assumptions on Φ that are all local in nature. We also provide results on the convergence of solutions to the PDE

$$(2) \quad Ay_\rho + \frac{1}{\rho}(y_\rho - \Phi(y_\rho))_\rho^+ = f$$

where $(\cdot)_\rho^+$ is a regularisation of the positive part function; indeed we show that it is possible to find a subsequence (relabelled) such that $y_\rho \rightarrow y$ where $y \in \mathbf{Q}(f)$ is a solution. This provides a way to approximate solutions of QVIs. We write $y_\rho \in \mathbf{P}_\rho(f)$ to denote the solution map associated to (2).

Furthermore, we also study optimal control problems of the form

$$\min_{\substack{u \in U_{ad}, \\ y \in \mathbf{Q}(u)}} \frac{1}{2} \|y - y_d\|_H^2 + \frac{\nu}{2} \|u\|_H^2,$$

in particular we prove the existence of B-stationarity, (\mathcal{E} -almost) C-stationarity and strong stationarity points under varying sets of assumptions. For the C-stationarity, we consider the family of penalised problems

$$\min_{\substack{u \in U_{ad}, \\ y \in \mathbf{P}_\rho(u)}} \frac{1}{2} \|y - y_d\|_H^2 + \frac{\nu}{2} \|u\|_H^2,$$

derive stationarity conditions (by checking constraint qualifications) and then perform a careful analysis to pass to the limit. In the end, we obtain the \mathcal{E} -almost C-stationarity system

$$\begin{aligned} y^* + (I - \Phi'(y^*))\lambda^* + A^*p^* &= y_d, \\ Ay^* - u^* + \xi^* &= 0, \\ u &\in U_{ad} : (\nu u^* - p^*, u^* - v) \leq 0 \quad \forall v \in U_{ad}, \\ \xi^* \geq 0 \text{ in } V^*, \quad y^* &\leq \Phi(y^*), \quad \langle \xi^*, y^* - \Phi(y^*) \rangle = 0, \\ \langle \lambda^*, p^* \rangle \geq 0, \quad \langle \lambda^*, y^* - \Phi(y^*) \rangle &= 0, \\ \langle \xi^*, (p^*)^+ \rangle = \langle \xi^*, (p^*)^- \rangle &= 0, \\ \forall \tau > 0, \exists E^\tau \subset \{y^* < \Phi(y^*)\} &\text{ with } |\{y^* < \Phi(y^*)\} \setminus E^\tau| \leq \tau \text{ such that} \\ \langle \lambda^*, v \rangle = 0 \quad \forall v \in V : v = 0 &\text{ on } \Omega \setminus E^\tau, \end{aligned}$$

which can also be strengthened to C-stationarity under additional conditions. If further assumptions are available, strong stationarity conditions can also be obtained making use of the differentiability theory. Full details can be found in [2].

It is well known that — in a specific setting with certain assumptions — the QVI (1) possesses minimal and maximal solutions (denoted respectively $\mathbf{m}(f)$ and $\mathbf{M}(f)$) on some interval $[\underline{u}, \bar{u}]$:

$$\mathbf{m}(f) \leq y \leq \mathbf{M}(f) \quad \forall y \in \mathbf{Q}(f) \cap [\underline{u}, \bar{u}].$$

In [3], we address the issues of directional differentiability for these maps. We indeed show that $\mathbf{m} : V^* \rightarrow V$ is directionally differentiable in every direction $d \geq 0$:

$$\lim_{s \rightarrow 0^+} \frac{\mathbf{m}(f + sd) - \mathbf{m}(f)}{s} = \mathbf{m}'(f)(d).$$

Furthermore, $\mathbf{m}'(f)(d)$ satisfies the QVI

$$(3) \quad \alpha \in \mathcal{K}_m(\alpha) : \langle A\alpha - d, \alpha - v \rangle \leq 0 \quad \forall v \in \mathcal{K}_m(\alpha),$$

where we again omit the definition of the critical cone $\mathcal{K}_m(\alpha)$. A similar result holds for $\mathbf{M}(f)$ for directions $d \leq 0$. The proof for these results uses the above theory but some additional argumentation is necessary to derive these results. The full details are given in [3].

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Inexact Bundle Methods for Nonconvex Nonsmooth Optimization in Hilbert Spaces

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(joint work with Lukas Hertlein)

We summarize part of our results¹ [1, 2, 3] on a class of bundle methods for non-smooth nonconvex optimization problems in infinite-dimensional Hilbert spaces. Our approach can deal with inexact function value and subgradient evaluations and seems to be the first that provides a full analysis of bundle methods in an infinite-dimensional, nonconvex setting. Consider the optimization problem

$$(1) \quad \min_{u \in U} p(\iota u) + w(u) \quad \text{s.t.} \quad u \in U_{\text{ad}},$$

where $\iota : U \rightarrow V$ is linear, compact, and injective, U, V are Hilbert spaces, $p : V \rightarrow \mathbb{R}$ is Lipschitz continuous on bounded sets, $U_{\text{ad}} \subset U$ is closed and convex, and $w : U \rightarrow \mathbb{R}$ is convex, continuously differentiable, and bounded on bounded sets. Further, either w is strongly convex or U_{ad} is bounded (here, we only consider the former case). Typically, w has a simple structure, like $\frac{\alpha}{2} \|\cdot\|_V^2$. We set $f = p \circ \iota$ and $J = f + w$, and write $\|\cdot\| = \|\cdot\|_V$, $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{V^*, V}$.

This setting can be motivated by optimal control problems governed by variational inequalities (VI). For instance, if $S : H^{-1}(D) \rightarrow H_0^1(D)$ denotes the Lipschitz continuous solution operator of an obstacle problem, mapping external forces to the state, and the control enters via a linear operator $\iota : L^2(\Omega) \rightarrow H_0^1(D)$, then often ι is compact (e.g., $\iota(u) = 1_\Omega u$, $\Omega \subset D$). Considering a cost function $F(y) + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2$, where, on bounded sets, F is Lipschitz continuous and bounded, the optimal control problem can be transformed to (1) via $U = L^2(\Omega)$, $V = H^{-1}(D)$, $p = F \circ S$, $w = \frac{\alpha}{2} \|\cdot\|_{L^2(\Omega)}^2$.

Our bundle method, developed and analyzed in [1, 2, 3], extends an approach by Noll [4] in several respects, in particular, from \mathbb{R}^n to infinite-dimensional Hilbert

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spaces. In each iteration k , a bundle subproblems of the form

$$(2) \min_{z \in U_{\text{ad}}} \Psi_k(z), \quad \Psi_k(z) = \phi_k(z) + w(z) + \langle Q_k \iota(z - u_k), \iota(z - u_k) \rangle + \frac{\tau_k}{2} \|\iota(z - u_k)\|^2$$

is approximately solved to obtain a *trial iterate* \tilde{z}_k . Here, $\phi_k : U \rightarrow \mathbb{R}$ is a *cutting plane model* of p , explained below, $\tau_k > 0$ is a *proximity parameter*, and $Q_k \in \mathcal{L}(V, V^*)$ is a self-adjoint operator that can be used to model *curvature information* for p in a neighborhood of u_k (e.g., by BFGS-updates; $Q_k = 0$ is admitted as well). Further, $u_k \in U_{\text{ad}}$ is the current *serious iterate*. Suitable choices of Q_k and τ_k ensure that $\|v\|_{Q_k + \tau_k R_V} := (\langle Q_k v, v \rangle + \frac{\tau_k}{2} \|v\|^2)^{1/2}$, with $R_V \in \mathcal{L}(V, V^*)$ denoting the Riesz map, defines a norm on V that is equivalent to $\|\cdot\|$ with an equivalence constant of size $O(\max\{1, \tau_k^{1/2}\})$. The problem (2) is strongly convex and thus possesses a unique solution z_k . As mentioned, our method only requires to compute an approximate solution \tilde{z}_k . At \tilde{z}_k , an approximation \tilde{f}_k to $f(\tilde{z}_k)$ is computed. Then, by checking the ratio ρ_k between computed cost reduction and model reduction, it is decided if \tilde{z}_k can be chosen as the new serious iterate. In this case (successful iteration), we set $u_{k+1} = \tilde{z}_k$, choose Q_{k+1} , τ_{k+1} , and build the new cutting plane model ϕ_{k+1} . Otherwise (iteration unsuccessful), we choose $\tau_{k+1} \geq \tau_k$, build ϕ_{k+1} , and set $u_{k+1} = u_k$, $Q_{k+1} = Q_k$.

In the case of an unsuccessful iteration, $\tau_{k+1} = \tau_k$ is chosen if the ratio $\tilde{\rho}_k$ between ϕ_{k+1} - and ϕ_k -reduction at \tilde{z}_k is sufficiently small (i.e., the model changes sufficiently much), otherwise $\tau_{k+1} = 2\tau_k$ is chosen. If the iteration was successful, we set $\tau_{k+1} = P_k(\tau_k/2)$ if ρ_k is sufficiently large, otherwise $\tau_{k+1} = P_k(\tau_k)$; here, P_k performs some safeguarding.

The cutting planes are constructed from bundle entries $(\tilde{z}_k, \tilde{f}_k, z_k^g, \tilde{g}_k)$, where \tilde{f}_k approximates $f(\tilde{z}_k)$ and \tilde{g}_k is an approximate subgradient, provided by an oracle, that returns an element of $G(\iota z_k^g) \subset V^*$ at the *subgradient base point* $z_k^g \in U$. Typically, $z_k^g = \tilde{z}_k$ is chosen, but for more generality, also $z_k^g \neq \tilde{z}_k$ is allowed. Here, $G : V \rightrightarrows V^*$ is a set-valued mapping that *approximates* a suitable generalized differential of p . A typical choice is $G(u) = \partial p(u) + \varepsilon \bar{B}_{V^*}$, where ∂p is Clarke's subdifferential, $\varepsilon \geq 0$, and $\bar{B}_X = \{x \in X; \|x\|_X \leq 1\}$. We require that G has nonempty convex images, that it is strongly-weakly closed, and that it maps bounded sets to bounded sets. The choice of G can model inexactness in the subgradient computation, and G then replaces the subdifferential (e.g., ∂p) in the optimality conditions that we can prove for weak accumulation points of (u_k) .

Given a bundle entry $(\tilde{z}_k, \tilde{f}_k, z_k^g, \tilde{g}_k)$ and a serious iterate u_k with corresponding approximate function value $\tilde{f}_k^u \approx f(u_k)$, the associated cutting plane is defined by

$$m_k(z; u_k) = \tilde{f}_k + \langle \tilde{g}_k, \iota(z - \tilde{z}_k) \rangle - [\tilde{f}_k + \langle \tilde{g}_k, \iota(z - \tilde{z}_k) \rangle - \tilde{f}_k^u]_+ - c \|\iota(z_k^g - u_k)\|^2.$$

The two subtracted terms form the *downshift*, which ensures that $m_k(u_k; u_k) \leq \tilde{f}_k^u - c \|\iota(z_k^g - u_k)\|^2 \leq \tilde{f}_k^u$. There is a special cutting plane, the *exactness plane*, which corresponds to the bundle entry $(u_k, \tilde{f}_k^u, u_k, \tilde{g}_k^u)$, where $\tilde{g}_k^u \in G(u_k)$:

$$m_k^u(z) = \tilde{f}_k^u + \langle \tilde{g}_k^u, \iota(z - u_k) \rangle.$$

The cutting plane model is always chosen such that $\phi_k \geq m_k^u$ on U . Also, if iteration k was unsuccessful, then we require $\phi_{k+1} \geq m_k(\cdot; u_{k+1})$ and that ϕ_{k+1} majorizes the *aggregate cutting plane*, which is a certain convex combination of cutting planes contained in ϕ_k . The general form of our cutting plane model is $\phi_k(z) = \max_{m \in \mathcal{M}_k} m(z)$, where \mathcal{M}_k contains finitely many linear functions $m : U \rightarrow \mathbb{R}$, which all are convex combinations of cutting planes induced by the bundle entries computed so far. The convergence theory, however, requires only the majorization criteria stated above.

In, e.g, Noll [4], the ϵ -convexity of the cost function is assumed. We extend this as follows:

For $\epsilon > 0$, p is called ϵ - G -convex at $\bar{v} \in V$ if there exists $\delta > 0$ such that

$$p(v + s) - p(v) \geq \langle g, s \rangle - \epsilon \|s\|$$

$$\forall g \in G(v), \forall v, s \in V \text{ with } \|v - \bar{v}\| < \delta, \|v + s - \bar{v}\| < \delta, \|s\| < \delta.$$

The function p is called *approximately convex* at \bar{v} if p is ϵ - ∂p -convex at $\bar{v} \in V$ for all $\epsilon > 0$. These conditions are relatively weak. For instance, if $p = p_1 + p_2$, where p_1 is C^1 and p_2 is convex near \bar{v} , then p is approximately convex at \bar{v} .

In our convergence theory, we always assume

$$(3) \quad |\tilde{f}_k - f(\tilde{z}_k)| \leq \Delta \quad \text{and} \quad \Psi_k(\tilde{z}_k) - \Psi_k(z_k) \rightarrow 0 \quad (k \rightarrow \infty).$$

Our *first convergence result* states that, if $\tilde{z}_k^g = \tilde{z}_k$ and if suitable, implementable accuracy conditions for $\Psi_k(\tilde{z}_k)$ and \tilde{f}_k , are satisfied, the latter involving a tolerance $\epsilon_1 \geq 0$, and if $\{u \in U_{\text{ad}}; J(u) \leq J(u_0) + 2\Delta\}$ is bounded, then for any weak limit point \bar{u} of (u_k) , there holds:

If there exists a subsequence $(u_k)_K$ of unsuccessful iterations (i.e., $\rho_k < \gamma$) with $\tau_{k+1} = \tau_k$ (i.e., $\tilde{\rho}_k \geq \tilde{\gamma} > \gamma$) for all $k \in K$, $u_k \rightharpoonup_K \bar{u}$, and $\tau_k \rightarrow_K \infty$, then, if p is ϵ_2 - G -convex at $\iota\bar{u}$, the point \bar{u} is η - G -stationary for $\eta = \frac{2}{\tilde{\gamma} - \gamma}(\epsilon_1 + \epsilon_2)$:

$$(4) \quad 0 \in w'(\bar{u}) + N_{U_{\text{ad}}}(\bar{u}) + \iota^*(G(\iota\bar{u}) + \eta\bar{B}_{V^*}),$$

where $N_{U_{\text{ad}}}$ is the normal cone map of U_{ad} .

In all other cases, \bar{u} is 0- G -stationary.

This convergence theorem and other variants [1, 3] can be derived from the following general result [1]:

Define $e_k = (Q_k + \tau_k R_V)\iota(u_k - z_k)$ and, for $\bar{u} \in U$,

$$\mathcal{E}_{\bar{u}} = \{\epsilon \in [0, \infty]; \exists \text{ subsequence } K \subset \mathbb{N}_0 : \rho_k < \gamma, \tilde{\rho}_k \geq \tilde{\gamma} \ (k \in K),$$

$$\tau_k \rightarrow_K \infty, u_k \rightharpoonup_K \bar{u} \text{ in } U, \|e_k\|_{V^*} \rightarrow_K \epsilon\}.$$

Now, if (3) holds and if the set of all bundle entries used by the algorithm is bounded, then every weak limit point \bar{u} of the sequence of serious iterates (u_k) is η - G -stationary in the sense of (4), where $\eta = 0$ if $\mathcal{E}_{\bar{u}} = \emptyset$ and $\eta = \inf \mathcal{E}_{\bar{u}}$, otherwise.

For (e.g., FEM) discretizations, the accuracy requirements can be ensured using error estimates. The subproblems can be solved via their duals and the accuracy of $\Psi_k(\tilde{z}_k)$ can be controlled. The method has been applied to optimal control of obstacle problems and shows encouraging results.

For further results and details, we refer to [1, 2, 3].

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Nonlinear Observer Design Based on Minimum Energy Estimation

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(joint work with Karl Kunisch)

Estimating the state of a nonlinear perturbed dynamical system based on (output) measurements is a well-known control theoretic problem. While in the linear case, an optimal observer is given by the famous Kalman(-Bucy) filter, in the nonlinear case, constructing observers is significantly more complex and many approaches such as extended or unscented Kalman filters exist. The Mortensen observer relies on the concept of minimum energy estimation and a value function framework which is determined by a Hamilton-Jacobi-Bellman equation. In the following, an introduction to these concepts as well as a neural network based approximation technique for nonlinear observer design is provided.

STATE ESTIMATION, OBSERVER DESIGN AND THE KALMAN-BUCY FILTER

Consider a nonlinear disturbed dynamical system of the form

$$(1) \quad \begin{aligned} \dot{x}(t) &= f(x(t)) + Bv(t), & x(0) &= x_0 + \zeta, \\ y(t) &= Cx(t) + w(t), \end{aligned}$$

where $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$ and $v \in L^2(0, \infty; \mathbb{R}^m)$, $w \in L^2(0, \infty; \mathbb{R}^p)$, $\zeta \in \mathbb{R}^n$ are unknown disturbances. For given $T > 0$ and $y \in L^2(0, T; \mathbb{R}^p)$, the goal of *state estimation* is to find an estimate $\hat{x}(T)$ such that $\hat{x}(T) \approx x(T)$. If, additionally, an approximation \hat{x} of the full trajectory $x \in L^2(0, T; \mathbb{R}^n)$ is sought, one typically aims at the design of a *dynamical observer*:

$$(2) \quad \begin{aligned} \dot{\hat{x}}(t) &= \hat{f}(\hat{x}(t), \hat{y}(t) - y(t)), & \hat{x}(0) &= \hat{x}_0, \\ \hat{y}(t) &= \hat{C}\hat{x}(t), \end{aligned}$$

where the observer dynamics depend upon the current (output) prediction error $\hat{y} - y$. In the case of linear dynamics, i.e., $f(x(t)) = Ax(t)$ and Gaussian white

noise v, w , the problem is well-known and has been solved by the *Kalman-Bucy filter*, see [3].

MINIMUM ENERGY ESTIMATION

For stochastic perturbations of the nonlinear problem (1), finding the conditional posterior distribution $p(x(t) \mid \{y(\tau) : 0 \leq \tau \leq t\})$ is known to lead to the Kushner-Stratanovich or Zakai equation, see, [6, 9, 10]. Since these are (nonlinear) stochastic partial differential equations on the state space, a computational realization of the corresponding observer/filter is infeasible. As a remedy, several alternatives and approximations techniques have been proposed, one of them being the so-called *Mortensen observer*. Initially suggested as a maximum likelihood estimator ([8]), it is also known as *minimum energy estimator*, see, [4]. The typical viewpoint ([2, 7]) is to assume the disturbances v, w to be deterministic solutions to an appropriate optimal control problem. Proceeding this way, one can derive a dynamical observer of the form

$$(3) \quad \dot{\hat{x}}(t) = f(\hat{x}(t)) + (\nabla_{\xi} \mathcal{V}(t, \hat{x}(t)))^{-1} C^\top (y(t) - C\hat{x}(t)), \quad \hat{x}(0) = x_0,$$

where the value function \mathcal{V} (under regularity assumptions) satisfies a time-dependent *Hamilton-Jacobi-Bellman* equation of the form

$$(4) \quad \begin{aligned} \partial_t \mathcal{V}(t, \xi) &= -\nabla_{\xi} \mathcal{V}(t, \xi)^\top f(\xi) - \frac{1}{2} \|B^\top \mathcal{V}_{\xi}(t, \xi)\|^2 + \frac{1}{2} \|y(t) - C\xi\|^2, \\ \mathcal{V}(0, \xi) &= \frac{1}{2} \|\xi - x_0\|_{Q_0}^2. \end{aligned}$$

A LEARNING FORMULATION FOR OBSERVER DESIGN

Since naive discretizations of (4) suffer from the *curse of dimensionality*, a viable alternative is to instead consider meshless approximation techniques. One such approach relies on neural network based approximations and utilizes the underlying optimal control problems for training the network. In context of optimal feedback control, this strategy has been investigated theoretically and numerically in [5]. Motivated by these promising results, we propose to construct approximations of the form

$$\dot{\hat{x}}_{\theta}(t) = f(\hat{x}_{\theta}(t)) + (D_x h_{\theta}(t, \hat{x}_{\theta}(t)))^{-1} C^\top (y(t) - C\hat{x}_{\theta}(t)), \quad \hat{x}_{\theta}(0) = x_0,$$

where $\nabla_{\xi} \mathcal{V}(t, x) \approx g_{\theta}(t, x)$ is determined by a neural network

$$\begin{aligned} g_{\theta} : \mathbb{R}^{n+1} &\rightarrow \mathbb{R}^n, \quad g_{\theta}(z) = (g_{\theta_L} \circ g_{\theta_{L-1}} \circ \dots \circ g_{\theta_1})(z), \\ g_{\theta_i} : \mathbb{R}^{n_{i-1}} &\rightarrow \mathbb{R}^{n_i}, \quad g_{\theta_i}(z) = \sigma(W_i z + b_i) + R_i z, \quad i = 1, \dots, L-1, \\ g_{\theta_L} : \mathbb{R}^{n_{L-1}} &\rightarrow \mathbb{R}^{n_L}, \quad g_{\theta_L}(z) = W_L z, \end{aligned}$$

with parameters $\theta = (W_i, R_i, b_i)$ and an activation function σ . For the computation of the parameters $\theta = (W_i, R_i, b_i)$ we consider the following optimal control problem:

$$\min_{\theta \in \mathbb{R}^N} \frac{1}{d} \sum_{j=1}^d \left(\frac{1}{2} \|x_{\theta,j}(0)\|_{Q_0}^2 + \frac{1}{2} \int_0^T (\|B^\top h_\theta(t, x_{\theta,j}(t))\|^2 + \|y(t) - Cx_{\theta,j}(t)\|^2) dt \right)$$

s.t. $\dot{x}_{\theta,j}(t) = f(x_{\theta,j}(t)) + BB^\top h_\theta(t, x_{\theta,j}(t))$, $x_{\theta,j}(T) = \xi_j$, $j = 1, \dots, d$,

which relies on the theoretical foundation of the Mortensen observer. For typical (nonlinear) oscillators, we show numerical results of our approximations and compare them with standard nonlinear observers such as the extended Kalman filter.

CHALLENGES AND FUTURE WORK

Since the approach relies on the (inverse) Hessian of the value function along the (unknown) optimal state estimate \hat{x} , regularity properties of \mathcal{V} have to be studied. Here, recent techniques from optimal feedback control could be used. Further study should rely on an efficient numerical computation of neural network based observers for large-scale (discretized) partial differential equations.

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Control and Deep Learning: Some Connections

ENRIQUE ZUAZUA

(joint work with Borjan Geshkovski)

It is superfluous to state the impact that deep learning has had on modern technology, as it powers many tools of modern society, ranging from web search to content filtering on social networks ([1]). A key paradigm of deep learning is that of *supervised learning*, which addresses the problem of predicting from labeled data, consisting in approximating an unknown function $f(\cdot) : \mathcal{X} \rightarrow \mathcal{Y}$ from N known but possibly noisy data samples $\{\vec{x}_i, \vec{y}_i\}_{i=1}^N$ with $\vec{x}_i \in \mathcal{X} \subset \mathbb{R}^d$ and $\vec{y}_i \in \mathcal{Y}$. We shall mostly concentrate on *classification tasks*, wherein $\mathcal{Y} = \{1, \dots, m\}$.

The workhorse behind the recent successes of deep learning are models called *deep neural networks* for providing an approximation f_{approx} of the unknown function f ; these are parametrized computational architectures which propagate each individual sample \vec{x}_i of the input data across a sequence of linear parametric operators and simple nonlinearities. A canonical example of such models is the *perceptron*, parametrized as

$$(1) \quad f_{\text{approx}}(x) = \sum_{j=1}^d w_{1,j} \sigma(w_{2,j}x + b_j)$$

where $w_1 \in \mathbb{R}^d$, $w_2 \in \mathbb{R}^{d \times d}$ and $b \in \mathbb{R}^d$ are unknown parameters, with $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ being a globally Lipschitz continuous function, defined element-wise, the so-called *activation function*.

A by-now classical result, Cybenko's *universal approximation theorem* ([2]) ensures that the set of functions which can be represented by formula (1) is a dense subset of $C^0([-1, 1]^d)$. This theory has since flourished, and universal approximation results have been shown for more compound models than (1) (see [3]).

In practice however, one looks to use models wherein the compositions are iterated over multiple layers. A staple of modern neural networks are the so-called *residual neural networks* (ResNets, [4]) which may often be cast as schemes of the mould

$$(2) \quad \begin{cases} \mathbf{x}_i^{k+1} = \mathbf{x}_i^k + w_1^k \sigma(w_2^k \mathbf{x}_i^k + b^k) & \text{for } k \in \{0, \dots, N_{\text{layers}} - 1\} \\ \mathbf{x}_i^0 = \vec{x}_i \end{cases}$$

for all $i \in [N]$, where $[N] := \{1, \dots, N\}$, $w_1^k, w_2^k \in \mathbb{R}^{d \times d}$ and $N_{\text{layers}} \geq 1$ designates the number of layers referred to as the *depth*. Due to the inherent dynamical nature of ResNets, several recent works have aimed at studying an associated continuous-time formulation in some detail, a trend started with the work [5]. This is motivated by the simple observation that for any $i \in [N]$ and for $T > 0$, (2) is roughly the forward Euler approximation of the neural ordinary differential equation (neural ODE)

$$(3) \quad \begin{cases} \dot{\mathbf{x}}_i(t) = w_1(t) \sigma(w_2(t) \mathbf{x}_i(t) + b(t)) & \text{for } t \in (0, T) \\ \mathbf{x}_i(0) = \vec{x}_i \in \mathbb{R}^d. \end{cases}$$

It should be noted that the origins of continuous-time supervised learning go back to the 1980s – in [6] back-propagation algorithms are connected to the adjoint method arising in optimal control (see also [7, 8]).

One readily sees that the parameters w_2, w_1, b in the neural ODE play the role of *controls*, and thus, the supervised learning problem may be seen as a compound and high-dimensional simultaneous control problem.

This is the viewpoint adopted by our group. And here we present some of our main findings.

We first analyze neural ODEs from a control theoretical perspective to obtain a fundamental understanding of the working mechanisms behind the processes of classification (more precisely, how the neural ODE flow manages separation of the different classes of data according to their labels).

These objectives are tackled and achieved from the perspective of the simultaneous control of systems of neural ODEs. Namely, in [9] we prove that both separation and universal approximation (to arbitrary L^∞_{loc} or L^2_{loc} functions) are valid properties for the controlled neural ODE flow by means of genuinely nonlinear and constructive proofs, allowing us to also estimate the complexity of the developed control strategies. Indeed, the nonlinear nature of the activation function allows deforming half of the phase space while the other half remains invariant, a property that classical models in mechanics do not fulfill. This very property allows to build elementary controls inducing specific dynamics and transformations whose concatenation, along with properly chosen hyperplanes, allows achieving our goals in finitely many steps. We also present the counterparts in the context of the control of neural transport equations, establishing a link between optimal transport and deep neural networks.

In practical applications however, the time-dependent parameters/controls are found by minimizing some cost functional rather than explicitly, via a process commonly referred to as *training*. Due to the ODE reformulation of ResNets, the training process is nothing else than an optimal control problem which consists in finding optimal parameters steering all of the network outputs $P\mathbf{x}_i(T)$ as close as possible to the corresponding labels \vec{y}_i , where $P: \mathbb{R}^d \rightarrow \mathbb{R}^m$ is a given affine and surjective map (e.g., a random matrix) which serves to match dimensions.

In [10, 11], we propose the training problem consisting in minimizing

$$(4) \quad \frac{1}{N} \sum_{i=1}^N \text{loss}(P\mathbf{x}_i(T), \vec{y}_i) + \int_0^T \|\mathbf{x}_i(t) - \bar{\mathbf{x}}_i\|^2 dt + \|u\|_{H^1(0,T;\mathbb{R}^{d_u})}^2,$$

where $\text{loss}(\cdot, \cdot)$ is a given continuous and nonnegative function which, in classification tasks (for simplicity, say $m = 2$), is usually $\text{loss}(x, y) := \|\sigma(x) - y\|^2$ or $\text{loss}(x, y) = \log(1 + \exp(-yx))$, and $\bar{\mathbf{x}}_i \in P^{-1}(\{\vec{y}_i\})$.

As each time-step of a discretization to (3) may be seen to represent a different layer of the ResNet (2), the time horizon $T > 0$ in (3) may serve as an indicator of the number of layers N_{layers} in the discrete-time context (2). A good understanding of the dynamics of the learning problem over longer time horizons would lead

to potential rules for choosing the number of layers, and enlighten the possible generalization properties when the number of layers is large.

In [10, 12], under specific controllability assumptions on the neural ODE (which are addressed in [9]), but without any smallness assumptions on the data, targets, or smoothness assumptions on the dynamics (we only assume $\sigma \in \text{Lip}(\mathbb{R})$), we conclude that the optimal controls $u_T = [w_{1,T}, w_{2,T}, b_T]$ and associated optimal trajectories \mathbf{x}_T satisfy

$$(5) \quad \frac{1}{N} \sum_{i=1}^N \text{loss}(P_{\mathbf{x}_{T,i}}(t), \vec{y}_i) + \|\mathbf{x}_{T,i}(t) - \bar{\mathbf{x}}_i\| \leq C e^{-\mu t}$$

and, moreover

$$(6) \quad \|u_T(t)\| \leq C e^{-\mu t}$$

for some constant $C, \mu > 0$ independent of T and for all $t \in [0, T]$. This is a manifestation of the so-called *turnpike property*, well-known in optimal control and economics ([13]).

Outlook. In the above presented works, we have studied a variety of supervised learning tasks from the continuous-time control theoretical perspective, allowing us to obtain fundamental understanding of the working mechanisms and properties that deep learning. We have, however, focused solely on supervised learning tasks, namely, wherein the dataset is labeled. A major challenge which ought to be formulated and addressed in a more control theoretical framework is the topic of *unsupervised learning*, wherein one only disposes of unlabeled data $\{\vec{x}_i\}$.

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Well-Posedness and Optimal Control of a Complex PDE-System Modelling Tumor Growth

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(joint work with Andrea Signori and Jürgen Sprekels)

In this note we recall some results on the well-posedness and optimal control for a complex PDE-system arising from an extended model of phase field type for tumor growth. In the model, the key assumption is that the tumor cells are submerged in a nutrient-rich environment which is the primary source of nourishment for the tumorous cells: this is a reasonable assumption at least for young tumors (avascular tumors). A four-species PDE system (tumor cells, healthy cells, nutrient-rich concentration, nutrient-poor concentration - see [4]) is considered, which couples a viscous Cahn–Hilliard equation with source term for the tumor with a reaction-diffusion equation for the surrounding nutrient. The chemotaxis effects are taken into account and the analysis for a singular potential is developed.

In the continuum model, the sharp interfaces are replaced by a narrow transition layer modelling the adhesive forces among the cell species: a diffuse interface separates tumor and healthy cell regions. Indeed, the proliferating tumor cells are surrounded by (healthy) host cells and by a nutrient. The variable φ is used for the difference in volume fraction, so that $\varphi = 1$ represents the tumor phase and $\varphi = -1$ is for the healthy tissue phase, while σ stands for the concentration of the nutrient. Based on the Cahn–Hilliard approach, an additional variable μ plays the role of the chemical potential.

The system we address in a bounded domain $\Omega \subset \mathbb{R}^3$ and a time interval $(0, T)$ is (cf. [2])

$$(1) \quad \alpha \partial_t \mu + \partial_t \varphi - \Delta \mu = (P\sigma - A - u)h(\varphi) \quad \text{in } Q,$$

$$(2) \quad \mu = \beta \partial_t \varphi - \Delta \varphi + F'(\varphi) - \chi \sigma \quad \text{in } Q,$$

$$(3) \quad \partial_t \sigma - \Delta \sigma = \Delta(-\chi \varphi) + B(\sigma_s - \sigma) - D\sigma h(\varphi) + w \quad \text{in } Q,$$

$$(4) \quad \partial_n \mu = \partial_n \varphi = \partial_n \sigma = 0 \quad \text{on } \Sigma,$$

$$(5) \quad \mu(0) = \mu_0, \varphi(0) = \varphi_0, \sigma(0) = \sigma_0 \quad \text{in } \Omega,$$

where $\Gamma = \partial\Omega$, $Q = \Omega \times (0, T)$, $\Sigma := \Gamma \times (0, T)$ and ∂_n indicates the outward normal derivative to Γ .

Here, α and β denote two relaxation positive coefficients (that can go to zero with consequences on the limit system – see [1] and its references); A, B, D, P denote positive rate values standing for apoptosis, nutrient supply, nutrient consumption, and proliferation, respectively; u and w are source terms acting as control variables in the system; $h(\cdot)$ denotes an interpolation function between -1

and 1 such that $h(-1) = 0$ and $h(1) = 1$, so that the mechanisms ruled by the terms $(P\sigma - A - u)h(\varphi)$ and $D\sigma h(\varphi)$ are switched off in the healthy case $\varphi = -1$, and fully active in the tumorous case $\varphi = 1$.

The constant coefficient χ is referred to chemotaxis; indeed, the contributions $-\chi\sigma$ in (2) and $\Delta(-\chi\varphi)$ in (3) give account of pure chemotaxis and active transport, both related to the movement of cells towards regions of increasing or decreasing concentration. The term σ_s is nonnegative and models concentration in a pre-existing vasculature.

Finally, the term F' is the derivative of a double-well nonlinearity. Typical examples for this nonlinearity are the regular potential

$$(6) \quad F_{reg}(r) = \frac{1}{4}(r^2 - 1)^2 \quad \text{for } r \in \mathbb{R},$$

and, more relevant for applications, the logarithmic potential

$$(7) \quad F_{log}(r) = (1 + r) \ln(1 + r) + (1 - r) \ln(1 - r) - kr^2 \quad \text{for } r \in (-1, 1),$$

where $k > 1$ so that F_{log} is nonconvex. About F we set the general assumptions

- (F1) $F = F_1 + F_2$, where $F_1 : \mathbb{R} \rightarrow [0, +\infty]$ is convex and l.s.c. with $F_1(0) = 0$.
- (F2) There exist r_-, r_+ , with $-\infty \leq r_- < 0 < r_+ \leq +\infty$, such that the restriction of F_1 to (r_-, r_+) is differentiable with derivative F'_1 .
- (F3) $F_2 \in C^3(\mathbb{R})$ and F'_2 is Lipschitz continuous.
- (F4) $F|_{(r_-, r_+)} \in C^3(r_-, r_+)$ and $\lim_{r \rightarrow r_{\pm}} F'(r) = \pm\infty$.

Existence and uniqueness of a strong solution of (1)–(5) are ensured by this result, which is proved in [2].

Theorem 1. *Assume (F1) – (F4), $h \in C^2(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$ positive on (r_-, r_+) , σ_s given, $u, w \in L^\infty(Q)$,*

$$\varphi_0 \in H_n^2(\Omega), \quad \varphi_0 \in \text{domain}(F_1) \text{ a.e. in } \Omega, \quad \mu_0, \sigma_0 \in H^1(\Omega) \cap L^\infty(\Omega).$$

Then the problem (1)–(5) admits a solution such that

$$\begin{aligned} \varphi &\in W^{1,\infty}(0, T; L^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^2(\Omega)), \\ \mu, \sigma &\in H^1(0, T; L^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)) \cap L^\infty(Q), \end{aligned}$$

where $H_n^2(\Omega) := \{f \in H^2(\Omega) : \partial_n f = 0 \text{ on } \Sigma\}$. In addition, if $r_- < \inf \varphi_0 \leq \sup \varphi_0 < r_+$, there exist some constants r_ and r^* , $r_- < r_* \leq r^* < r_+$, such that $r_* \leq \varphi \leq r^*$ a.e. in Q and consequently*

$$\|\varphi\|_{L^\infty(Q)} + \max_{i=1,2,3} \|F^{(i)}(\varphi)\|_{L^\infty(Q)} \leq K$$

for some positive constant K . Moreover, let $(\mu_i, \varphi_i, \sigma_i)$, $i = 1, 2$, be two solutions to (1)–(5) obtained as above, with initial data $(\mu_0^i, \varphi_0^i, \sigma_0^i)$ and control terms (u_i, w_i) ,

$i = 1, 2$. Then, we have that

$$\begin{aligned} & \|\mu_1 - \mu_2\|_{H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))} \\ & + \|\varphi_1 - \varphi_2\|_{H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))} \\ & + \|\sigma_1 - \sigma_2\|_{H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))} \\ & \leq K (\|\mu_0^1 - \mu_0^2\|_{H^1(\Omega)} + \|\varphi_0^1 - \varphi_0^2\|_{H^1(\Omega)} + \|\sigma_0^1 - \sigma_0^2\|_{H^1(\Omega)} \\ & + \|u_1 - u_2\|_{L^2(Q)} + \|w_1 - w_2\|_{L^2(Q)}) \end{aligned}$$

for another constant K depending only on data and structural assumptions.

About the optimal control problem, let us consider the tracking-type cost functional

$$\mathcal{J}(\varphi, u, w) := \frac{\gamma_1}{2} \int_{\Omega} |\varphi(T) - \varphi_{\Omega}|^2 + \frac{\gamma_2}{2} \int_Q |\varphi - \varphi_Q|^2 + \frac{\gamma_3}{2} \int_Q |u|^2 + \frac{\gamma_4}{2} \int_Q |w|^2,$$

with φ being the first component of the solution to the state system (1)–(5), and with the control box

$$\mathcal{U} := \{(u, w) \in (L^\infty(Q))^2 : u_* \leq u \leq u^*, w_* \leq w \leq w^*\},$$

where $u_*, u^*, w_*, w^* \in L^\infty(Q)$, $\varphi_{\Omega} \in L^2(\Omega)$, $\varphi_Q \in L^2(Q)$. In fact, the control problem is motivated by the search for a strategy how to apply the controls u , w (nutrients, therapy, drug, ...) to the system in order that L^2 -amount of substances supplied (which is restricted by the L^∞ -constraints in \mathcal{U}) does not inflict any harm on the patient; on the other hand, the final distribution and desired evolution of the tumor cells (expressed by the target functions φ_{Ω} and φ_Q) have to be realized in the best possible way. The values of the coefficients γ_i , $i = 1, 2, 3, 4$, have to be chosen in order to set precisely the targets, which could range from *avoiding unnecessary harm to the patient to qualifying the approximation of φ_{Ω} and φ_Q* . Notice that the setting **(F1)**–**(F4)** for the potential F turns out to be quite general and allows us to study the optimal control problem also in the case of the logarithmic potential (7).

In [2] we proved a variety of results, in particular we could discuss the existence of optimal controls, show the Fréchet differentiability of the control-to-state operator in a suitable framework, and derive the first-order necessary conditions of optimality in terms of a variational inequality involving the adjoint problem.

Finally, let us mention the contribution [5], devoted to the study of directional sparsity effects, by including a non-differentiable (but convex) term like some L^1 -penalization in the cost functional, and the recent paper [3], which deals with the second-order sufficient conditions for optimality and it investigates them in depth.

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Optimal Control of Perfect Plasticity

CHRISTIAN MEYER

(joint work with Stephan Walther)

We consider two optimal control problems governed by the system of perfect plasticity. The first problem is a *stress tracking* problem and reads as follows:

$$\left(P_\sigma \right) \left\{ \begin{array}{l}
 \min \quad \frac{1}{2} \|\sigma(T) - \sigma_d\|_{\mathbb{L}^2(\Omega)}^2 + \frac{\alpha}{2} \|\partial_t \ell\|_{L^2(0,T;\mathcal{X}_c)}^2 \\
 \text{s.t.} \quad \textit{Equilibrium condition:} \\
 \qquad \qquad \sigma(t) \in \mathcal{E} := \{ \tau \in \mathbb{L}^2(\Omega) : \langle \tau, \nabla^s \varphi \rangle_{\mathbb{L}^2} = 0 \ \forall \varphi \in \mathbf{H}_D^1(\Omega) \} \\
 \qquad \qquad \textit{Yield condition:} \\
 \qquad \qquad \sigma(t) \in \mathcal{K} := \{ \tau \in \mathbb{L}^2(\Omega) : \tau(x) \in K \ \text{f.a.a.} \ x \in \Omega \} \\
 \qquad \qquad \textit{Flow rule:} \\
 \qquad \qquad \langle \mathbb{C}^{-1} \partial_t \sigma(t) - \nabla^s \partial_t u_D(t), \tau - \sigma(t) \rangle_{\mathbb{L}^2} \geq 0 \quad \forall \tau \in \mathcal{E} \cap \mathcal{K} \\
 \qquad \qquad \textit{Initial condition:} \quad \sigma(0) = \sigma_0 \\
 \text{and} \quad u_D = G(\ell) + \mathbf{a} \quad \text{with} \quad \ell(0) = \ell(T) = 0.
 \end{array} \right.$$

Herein, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a bounded Lipschitz domain that, together with its boundary $\Gamma_D \cup \Gamma_N$ is regular in the sense of Gröger [2], and $T > 0$ is a given final time. Moreover, $\mathbb{L}^2(\Omega) := L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})$ and

$$\mathbf{H}_D^1(\Omega) := \overline{\{ \psi|_\Omega : \psi \in C_0^\infty(\mathbb{R}^n), \text{supp}(\psi) \cap \Gamma_D = \emptyset \}}^{\mathbf{H}^1(\Omega; \mathbb{R}^n)}.$$

The variable $\sigma : [0, T] \times \Omega \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$ denotes the stress field of the body occupying the domain Ω and represents the state variable of the problem. The Dirichlet displacement u_D serves as control variable and is itself controlled by a pseudo force ℓ through a given linear and bounded operator G that maps the control space \mathcal{X}_c compactly to $\mathbf{H}^1(\Omega)$. A possible example for such an operator is the solution operator of linear elasticity. The set $K \subset \mathbb{R}_{\text{sym}}^{d \times d}$ is the set of feasible stresses and is assumed to be closed and convex, and the elasticity tensor $\mathbb{C} : \mathbb{R}_{\text{sym}}^{d \times d} \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$ is a linear and coercive mapping. Furthermore, $\sigma_0 \in \mathbb{L}^p(\Omega)$, $p > d$, is a fixed initial stress distribution. Finally, $\alpha > 0$, $\mathbf{a} \in H^1(0, T; \mathbf{H}^1(\Omega))$, and $\sigma_d \in \mathbb{L}^2(\Omega)$ are given data. The motivation for the above optimization problem is to deform the Dirichlet part of a workpiece in a prescribed manner (given by \mathbf{a}) and at the same

time to minimize the deviation of the stress field at end time to a given desired stress field σ_d .

Based on results of [4], the existence and uniqueness of solutions to the state equation in (P_σ) can be shown. The associated solution operator is Lipschitz continuous, which allows to establish the existence of globally optimal solutions to (P_σ) by the standard direct method of the calculus of variations. Due to the flow rule inequality however, the solution operator is not Gâteaux-differentiable and therefore, the application of gradient-based optimization algorithms off the shelf is not possible. Following a well-established approach, cf. e.g. [9], we employ the Yosida regularization (resp. viscous approximation) of the flow rule accompanied by a further smoothing in order to obtain a differentiable mapping. At this point, the higher integrability results from [3] are decisive. Standard arguments show that sequences of global minimizers of the regularized optimal control problems admit (weak = strong) accumulation points for regularization and smoothing parameter tending to zero and every such accumulation point is a global solution of (P_σ) . Numerical examples illustrate the feasibility of this approach, see [5].

The second problem is the following *displacement tracking problem*:

$$(P_u) \left\{ \begin{array}{l} \min \quad J(u, u_D) := \int_0^T \|\nabla^s \partial_t u(t) - \mu(t)\|_{\mathfrak{M}(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})}^2 \\ \quad \quad \quad + \|\partial_t u(t) - v(t)\|_{L^1(\Omega)}^2 dt + \frac{\alpha}{2} \|u_D\|_{H^1(0,T; \mathbf{H}^2(\Omega))}^2 \\ \text{s.t.} \quad \textit{Equilibrium and yield condition:} \quad \sigma(t) \in \mathcal{E} \cap \mathcal{K}, \\ \quad \quad \textit{Flow rule:} \quad \forall \tau \in \Sigma \cap \mathcal{K} : \\ \quad \quad \int_{\Omega} \mathbb{C}^{-1} \partial_t \sigma(t) : (\tau - \sigma(t)) dx + \int_{\Omega} \partial_t u(t) \cdot \text{div} (\tau - \sigma(t)) dx \\ \quad \quad \geq \int_{\Omega} \nabla^s \partial_t u_D(t) : (\tau - \sigma(t)) + \partial_t u_D(t) \cdot \text{div} (\tau - \sigma(t)) dx, \\ \quad \quad \textit{Initial condition:} \quad u(0) = u_0, \quad \sigma(0) = \sigma_0, \\ \text{and} \quad u_D(0) = u_0 \text{ on } \Gamma_D. \end{array} \right.$$

Here we assume that we can directly control the Dirichlet data u_D . The state now consists of two variables, the stress (as before) and the displacement $u \in H_w^1(0, T; BD(\Omega))$, where $BD(\Omega)$ is the *space of bounded deformation*, see e.g. [8], which lacks the Radon-Nikodým property such that the displacement is only weakly measurable in time. Now the aim of the optimization is to control the Dirichlet displacement in order to reach a desired strain rate μ and a desired displacement rate v . Existence of solutions to the state equation has been established in [7, 1], but classical counterexamples show that the displacement is in general not unique (in contrast to the stress). We underline that the safe-load condition, which is needed to guarantee the existence of solutions, is automatically fulfilled in case of (P_u) , since we have no external loads, but use the Dirichlet data as control variable. Due to the non-uniqueness of solutions to the state equation, (P_u) is strictly speaking no optimal control problem, but rather an optimization problem in function space. Nevertheless, based on continuity properties of the solution set

of the state equation, one again establishes the existence of optimal solutions by means of the direct method. The approximation of optimal solutions via Yosida regularization of the flow rule is however by far more complicated compared to the stress tracking problem. In particular, the so-called *reverse approximation property*, i.e., the construction of a recovery sequence for an optimal solution of (P_u) , which is feasible for the regularized problems, is challenging. The construction of such a sequence requires an additional control variable in terms of distributed loads that are forced to vanish in the regularization limit by means of a tailored penalty term within the objective. Unfortunately, this is still not sufficient for the construction of a recovery sequence and we were only able to establish the existence of such a sequence under additional fairly restrictive regularity assumptions that have to be fulfilled by at least one optimal solution to (P_u) , see [6] for details. The weakening of these assumptions is subject to future research.

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Semiglobal Oblique Projection Exponential Dynamical Observers for Nonautonomous Semilinear Parabolic-like Equations

SÉRGIO S. RODRIGUES

Let us be given a scalar parabolic equation as

$$(1) \quad \frac{\partial}{\partial t} y + (-\Delta + \mathbf{1})y + ay + b \cdot \nabla y - y^3 = f, \quad \mathcal{G}y|_{\partial\Omega} = g,$$

evolving in a bounded, convex polygon (polyhedron) $\Omega \subset \mathbb{R}^3$. The functions $a = a(t, x) \in \mathbb{R}$, $b = b(t, x) \in \mathbb{R}^3$, $f = f(t, x) \in \mathbb{R}$, and $g = g(t, x) \in \mathbb{R}$ are given and known, for $(t, x) \in [0, +\infty) \times \Omega$. By $\mathbf{1}$ we denote the identity operator, and \mathcal{G} stands for either Dirichlet or Neumann boundary conditions, $\mathcal{G} \in \{\mathbf{1}, \frac{\partial}{\partial \mathbf{n}}\}$.

The state $y = y(t, x)$, and in particular the initial state $y(0, x)$, is unknown.

The main goal is to obtain an estimate $\hat{y} = \hat{y}(t, x)$ for the state $y = y(t, x)$.

Motivation. Obtaining an estimate \hat{y} for the state y is of interest for applications, for example, in the implementation of feedback controls, where the control u is a function of the state $u = K(y)$. Since y is usually unknown, the approximated feedback $\hat{u} = K(\hat{y})$ is used instead.

The sensors. For the construction of such state estimate we can use a Luenberger-type observer based on a finite number of sensor measurements.

Let us consider, as sensors, the indicator functions in the set

$$(2) \quad W_S := \{\mathbf{1}_{\omega_{S,i}} \mid 1 \leq i \leq S\} \subset L^2(\Omega), \quad \mathcal{W}_S = \text{span}W_S, \quad \dim \mathcal{W}_S = S,$$

where $\omega_{S,i} \subseteq \Omega$, and we take average-like measurements as

$$w_{S,i}(t) := (\mathbf{1}_{\omega_{S,i}}, y(t, \cdot))_{L^2} = \int_{\omega_{S,i}} y(t, x) \, dx.$$

The vector $w(t) \in \mathbb{R}^{S \times 1}$, $w(t) = \begin{bmatrix} w_{S,1}(t) \\ w_{S,2}(t) \\ \vdots \\ w_{S,S}(t) \end{bmatrix} =: \mathcal{Z}_S y$ is called the output.

The result. For an arbitrary pair (μ, R) of positive constants. the estimate $\hat{y}(t)$ given by the Luenberger observer/estimator

$$(3a) \quad \frac{\partial}{\partial t} \hat{y} + (-\nu \Delta + \mathbf{1}) \hat{y} + a \hat{y} + b \cdot \nabla \hat{y} - \hat{y}^3 = f + \mathcal{I}(\mathcal{Z}_S \hat{y} - \mathcal{Z}_S y), \quad \mathcal{G} \hat{y}|_{\partial \Omega} = g,$$

with an output injection operator \mathcal{I} in the explicit form

$$(3b) \quad \mathcal{I} := -\lambda A^{-1} P_{\mathcal{W}_S}^{\widetilde{\mathcal{W}}_S^\perp} A^2 P_{\widetilde{\mathcal{W}}_S}^{\mathcal{W}_S} \mathbf{Z}_S,$$

converges exponentially to the state $y(t)$ as time increases, as

$$(4) \quad |\hat{y}(t, \cdot) - y(t, \cdot)|_{H^1(\Omega)} \leq e^{-\mu t} |\hat{y}(0, \cdot) - y(0, \cdot)|_{H^1(\Omega)}, \quad t \geq 0,$$

provided that $|\hat{y}(0, \cdot) - y(0, \cdot)|_{H^1(\Omega)} \leq R$ and that $\lambda > 0$ and $S \in \mathbb{N}_+$ are both large enough. Here $\hat{y}(0, \cdot)$ can be chosen/set as an initial guess we might have for $y(0, \cdot)$, S is the number of “appropriately” placed sensors as (2), and $\widetilde{\mathcal{W}}_S$ is an “appropriate” auxiliary space. Namely, it is required that

$$(5) \quad L^2(\Omega) = \mathcal{W}_S \oplus \widetilde{\mathcal{W}}_S^\perp, \quad \text{and} \quad \lim_{S \rightarrow +\infty} \min_{Q \in \text{D}(A) \cap \mathcal{W}_S^\perp} \frac{|AQ|_{L^2(\Omega)}}{|Q|_{H^1(\Omega)}} = +\infty,$$

where $A = -\nu \Delta + \mathbf{1}$ is the shifted Laplacian operator under the respective (Neumann or Dirichlet) boundary conditions. The operator \mathbf{Z}_S is defined by $P_{\mathcal{W}_S}^{\mathcal{W}_S} z = \mathbf{Z} \mathbf{Z}_S z$. Finally for X and Y closed subspaces of $L^2(\Omega) = X \oplus Y$, P_X^Y denotes the oblique projection in $L^2(\Omega)$ onto X along Y , defined as follows: we write $h \in L^2(\Omega)$ as $h = h_X + h_Y$ with $(h_X, h_Y) \in X \times Y$ and set $P_X^Y h := h_X$.

Remarks. The auxiliary space $\widetilde{\mathcal{W}}_S$ is needed due to a regularity detail. If the sensors satisfy $\mathcal{W}_S \subset D(A)$, then we can take $\widetilde{\mathcal{W}}_S = \mathcal{W}_S$.

The direct sum in (5) is satisfied if $\widetilde{\mathcal{W}}_S = \text{span}\{\psi_{S,i} \mid 1 \leq i \leq S\} \subset D(A)$ where $\psi_{S,i}$ is close enough to $\mathbf{1}_{\omega_{S,i}}$ in $L^2(\Omega)$ norm.

The divergent limit condition in (5) is satisfiable for convex polygonal domains. The result also holds for more general nonlinearities.

For more details we refer to [1]. See also [2] for the linear case.

Simulations. We consider the case of 4, 9, and 16 sensors as indicator functions of the subrectangles as in Figure 1. As auxiliary set $\widetilde{\mathcal{W}}_S$ we take bump-like functions “approximating” such indicator functions.

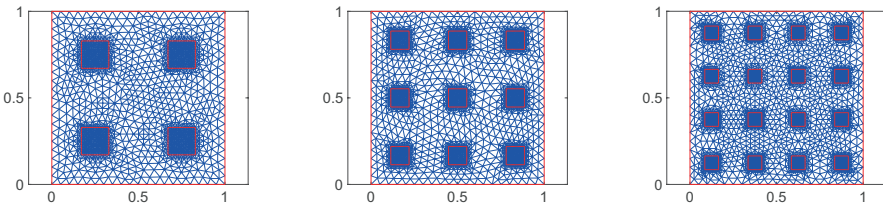


FIGURE 1. Locations of sensors in cases $S_\sigma \in \{4, 9, 16\}$.

In the figures, the number of sensors is denoted by S_σ . The simulations correspond to an academic dynamical system inspired by the error $z = \widehat{y} - y$ dynamics,

$$\begin{aligned} \frac{\partial}{\partial t} z + (-\nu \Delta + \mathbf{1})z + az + b \cdot \nabla z - |z|_{\mathbb{R}}^3 z + \left(\frac{\partial}{\partial x_1} z - 2\frac{\partial}{\partial x_2} z\right)z &= \mathcal{I}Z_S z \\ z(0, x) = \frac{2-x_1 x_2}{|2-x_1 x_2|_{H^1(\Omega)}}, \quad \frac{\partial z}{\partial \mathbf{n}} \Big|_{\partial \Omega} &= 0. \end{aligned}$$

As parameters we take,

$$\nu = 0.1, \quad a = -2 + x_1 - |\sin(t + x_1)|_{\mathbb{R}}, \quad b = \begin{bmatrix} x_1 + x_2 \\ \cos(t)x_1 x_2 \end{bmatrix}.$$

In Figure 2 we see that without output injection, $\lambda = 0$, the norm of the “error” blows up in finite time. With 4 measurements we can delay but not avoid the blow up of the norm (the simulations with $S_\sigma = 4$ have been run up to time $T = 15$, the fact that the figure does not show the plot up to $t = 15$, means that the norm blew up, around time $t \approx 10$). On the other hand, Figure 3 shows that, with 9 and 16 measurements we obtain the stability of the norm.

Open problems. It would be interesting to:

- construct an analogous explicit output injection for boundary sensors,
- investigate optimal sensors positions maximizing $\min_{Q \in D(A) \cap \mathcal{W}_S^\perp} \frac{|AQ|_{L^2(\Omega)}}{|Q|_{H^1(\Omega)}}$, in (5).

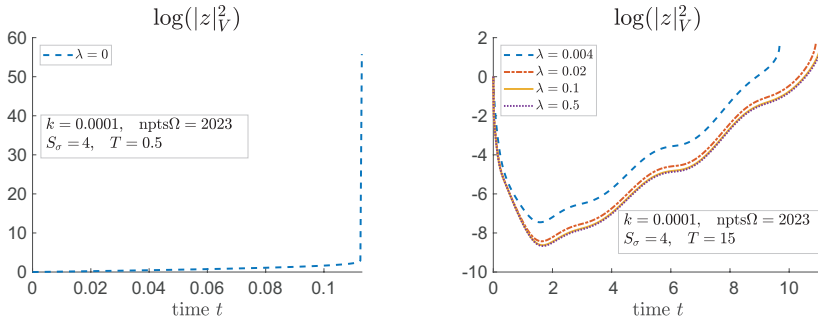


FIGURE 2. The free dynamics and the case of 4 sensors.

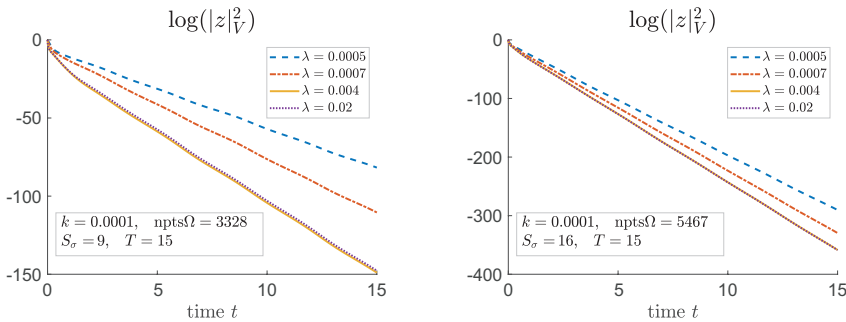


FIGURE 3. The case of 9 and 16 sensors.

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Numerical Analysis of Sparse Initial Data Identification for Parabolic Problems

BORIS VEXLER

(joint work with Dmitriy Leykekhman and Daniel Walter)

In this talk we discuss the problem of identification of initial data for a homogeneous heat equation from an observation of the terminal state. This problem is known to be exponentially ill-conditioned. Under the assumption that the unknown initial state is sparse, we formulate the problem as a PDE-constrained optimal control problem on a measure space for the control variable as follows:

$$\text{minimize } \frac{1}{2} \|u(T) - u_d\|_{L^2(\Omega)}^2 + \alpha \|q\|_{\mathcal{M}(\Omega)},$$

for $q \in \mathcal{M}(\Omega)$, subject to

$$\begin{aligned} \partial_t u - \Delta u &= 0 && \text{in } (0, T) \times \Omega, \\ u &= 0 && \text{on } (0, T) \times \partial\Omega, \\ u(0) &= q && \text{in } \Omega. \end{aligned}$$

Here, $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) is a convex polygonal / polyhedral domain, $\mathcal{M}(\Omega)$ is the space of regular Borel measures, which can be identified with the dual space of continuous functions, i.e. $\mathcal{M}(\Omega) = C_0(\Omega)^*$, $u_d \in L^2(\Omega)$ is the desired terminal state. The terminal time is denoted by $T > 0$ and the cost parameter by $\alpha > 0$.

A similar problem, which is equivalent to the problem described above, is analyzed in [1]. There, optimality conditions and structural properties of the optimal control are derived, and finite element discretization is considered. However, only plain convergence result (without rates) is shown. The goal of my talk is to present numerical analysis with convergence rates for a space-time finite element discretization.

The optimal control problem under consideration possesses a unique solution consisting of the optimal control $\bar{q} \in \mathcal{M}(\Omega)$ and the corresponding optimal state $\bar{u} \in L^r(0, T; W^{1,p}(\Omega))$ with $\bar{u}(T) \in H^2(\Omega) \cap H_0^1(\Omega)$. It is characterized by the following optimality system involving the adjoint state $\bar{z} \in W(0, T)$ with $\bar{z}(0) \in H^2(\Omega) \cap H_0^1(\Omega) \hookrightarrow C_0(\Omega)$,

$$(1a) \quad \begin{aligned} \partial_t \bar{u} - \Delta \bar{u} &= 0 && \text{in } (0, T) \times \Omega, \\ \bar{u} &= 0 && \text{on } (0, T) \times \partial\Omega, \\ \bar{u}(0) &= \bar{q} && \text{in } \Omega, \end{aligned}$$

$$(1b) \quad \begin{aligned} -\partial_t \bar{z} - \Delta \bar{z} &= 0 && \text{in } (0, T) \times \Omega, \\ \bar{z} &= 0 && \text{on } (0, T) \times \partial\Omega, \\ \bar{z}(T) &= \bar{u}(T) - u_d && \text{in } \Omega, \end{aligned}$$

$$(1c) \quad -\langle q - \bar{q}, \bar{z}(0) \rangle \leq \alpha (\|q\|_{\mathcal{M}(\Omega)} - \|\bar{q}\|_{\mathcal{M}(\Omega)}) \quad \text{for all } q \in \mathcal{M}(\Omega).$$

This optimality system implies that $\|z(0)\|_{C_0(\Omega)} \leq \alpha$ and the following support condition for the optimal control $\bar{q} = \bar{q}^+ - \bar{q}^-$ holds:

$$\text{supp } \bar{q}^+ \subset \Omega^+ = \{x \in \Omega \mid \bar{z}(0, x) = -\alpha\}, \quad \text{supp } \bar{q}^- \subset \Omega^- = \{x \in \Omega \mid \bar{z}(0, x) = \alpha\},$$

see [1] and [2] for the elliptic case. This condition leads to sparsity of \bar{q} since the sets Ω^\pm are the sets of measure zero. This is due to the fact that Ω^\pm lie in the interior of Ω and $z(0)$ is analytic there.

We discretize the problem using discontinuous Galerkin method dG(r) of order r in time and usual conforming cG(1) finite elements in space. The corresponding discrete space is called X_{kh} with k being the maximal time step and h the maximal mesh size, see, e.g., [5] for details of this notation in the context of optimal

control problems. The control variable is discretized using the space $M_h \subset \mathcal{M}(\Omega)$ being the span of Dirac functionals δ_{x_i} corresponding to all interior nodes of the underlying finite element mesh. This results in the discrete problem

$$\text{minimize } \frac{1}{2} \|u_{kh}(T) - u_d\|_{L^2(\Omega)}^2 + \alpha \|q_{kh}\|_{\mathcal{M}(\Omega)},$$

for $q_{kh} \in M_h$, subject to $u_{kh} \in X_{kh}$ and

$$B(u_{kh}, \varphi_{kh}) = \langle q_{kh}, \varphi_{kh}(0) \rangle \quad \text{for all } \varphi_{kh} \in X_{kh},$$

where B is the standard bilinear form used for formulation of dG(r) discretization in time. For the error in the optimal state we first prove the following suboptimal error estimate

$$(2) \quad \|\bar{u}(T) - \bar{u}_{kh}(T)\|_{L^2(\Omega)} \leq c(T) |\ln h|^{\frac{1}{2}} |\ln k|^{\frac{1}{2}} \left(k^{r+\frac{1}{2}} + h\right).$$

For the optimal control no convergence of $\|\bar{q} - \bar{q}_{kh}\|_{\mathcal{M}(\Omega)}$ can be expected. We show (cf. also [1]) that

$$\bar{q}_{kh} \xrightarrow{*} \bar{q} \text{ in } \mathcal{M}(\Omega) \quad \text{and} \quad \|\bar{q}_{kh}\|_{\mathcal{M}(\Omega)} \rightarrow \|\bar{q}\|_{\mathcal{M}(\Omega)}, \quad (k, h) \rightarrow 0.$$

Under the following additional structural assumption we can provide further information on the convergence of support points and improve the estimate (2).

Assumption. We assume that

- (1) $\text{supp } \bar{q} = \{x \in \Omega \mid |\bar{z}(0, x)| = \alpha\} = \{x_1, x_2, \dots, x_N\}$,
- (2) For x_i with $\bar{z}(0, x_i) = -\alpha$ the Hessian matrix $\nabla_x^2 \bar{z}(0, x_i)$ is positive definite,
- (3) For x_i with $\bar{z}(0, x_i) = \alpha$ the Hessian matrix $\nabla_x^2 \bar{z}(0, x_i)$ is negative definite.

This assumption states that the minima and maxima of $\bar{z}(0)$ fulfill standard second order sufficient optimality conditions. A similar assumption can be found in the literature in the context of optimal control problems with state constraints, see, e. g., [6]. Under this assumption we know that the optimal control \bar{q} is a linear combination of Dirac delta functions, i.e.

$$\bar{q} = \sum_{i=1}^N \beta_i \delta_{x_i}$$

with

$$\beta_i > 0 \quad \text{for } \bar{z}(0, x_i) = -\alpha \quad \text{and} \quad \beta_i < 0 \quad \text{for } \bar{z}(0, x_i) = \alpha.$$

For the discrete control \bar{q}_{kh} we can prove the following: There are $\varepsilon > 0$, $k_0, h_0 > 0$ such that for all $k < k_0$ and $h < h_0$

- (1) $\text{supp } \bar{q}_{kh} \cap B_\varepsilon(x_i) \neq \emptyset, \quad i = 1, 2, \dots, N$,
- (2) $\text{supp } \bar{q}_{kh} \subset \cup_i B_\varepsilon(x_i)$. Moreover, we can estimate the distance between any support point $x_{ij,kh} \in B_\varepsilon(x_i)$ of $\text{supp } \bar{q}_{kh}$ and x_i by

$$|x_i - x_{ij,kh}| \leq c(T) |\ln h| |\ln k|^{\frac{1}{2}} (k^{2r+1} + h).$$

Moreover, the corresponding coefficients converges to β_i with the same rate and the estimate (2) is improved to

$$\|\bar{u}(T) - \bar{u}_{kh}(T)\|_{L^2(\Omega)} \leq c(T) |\ln h| |\ln k|^{\frac{1}{2}} (k^{2r+1} + h),$$

see [4] for details.

The main tool used in the proof are sharp smoothing type pointwise finite element error estimates for homogeneous parabolic equations [4], which are based on smoothing estimates and discrete maximal parabolic regularity from [3].

Currently we are working on the extension of these results in several direction. We investigate higher order spacial discretization allowing for more precise identification of the positions x_i of the unknown Diracs. Moreover, we consider a problem with only finitely many pointwise measurements of the final state, i.e. replacing the original problem by

$$\text{minimize } \frac{1}{2} \sum_{k=1}^K (u(T, \xi_k) - u_d^k)^2 + \alpha \|q\|_{\mathcal{M}(\Omega)},$$

for $q \in \mathcal{M}(\Omega)$, subject to

$$\begin{aligned} \partial_t u - \Delta u &= 0 && \text{in } (0, T) \times \Omega, \\ u &= 0 && \text{on } (0, T) \times \partial\Omega, \\ u(0) &= q && \text{in } \Omega \end{aligned}$$

with some measurement points ξ_k and the data vector $u_d \in \mathbb{R}^K$.

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Optimal Control of Quasilinear Partial Differential Equations

IRA NEITZEL

(joint work with Fabian Hoppe)

In this talk, we discuss results on second-order sufficient optimality conditions for control problems with quasilinear parabolic state equation, eventually, presenting recent results for certain state-constrained problems obtained by Hoppe and the speaker in [7].

The first part of the talk reviews earlier results for purely control constrained problems by Bonifacius and the speaker [1], and provides a brief comparison with a similar setting that has been analyzed by Casas and Chrysafinos in [3]. The main differences between the two settings include certain aspects regarding the quasilinear operators, the types of controls discussed, and smoothness assumptions on the domain. In the second part of the talk, we eventually present the challenges appearing in the discussion and analysis of second order sufficient conditions in the presence of certain additional types of state constraints, see [7]. We make use of both settings from [1] and [3] and show how they allow for different types of constraints.

More precisely, a motivating model problem with both control and state constraints is given by

$$\begin{aligned} & \text{Minimize } J(u, q) \\ & \partial_t u + A(u)u = Bq \quad \text{in } I \times \Omega, \\ & u|_{\Gamma_D} = 0, \quad \text{in } I \times \Gamma_D, \\ & u(0) = u_0, \quad \text{in } \Omega \\ & q_a \leq q \leq q_b, \quad u \in U_{\text{ad}}, \end{aligned}$$

where J is a typical tracking type objective function for the state u and control q . The latter is allowed to act in the whole domain or on a Neumann part of the boundary, either depending on space and time or purely on time. This is encoded in the control-operator B . In either case, L^∞ -bounds q_a and q_b are prescribed. $A(u)$ is a uniformly elliptic operator of the form

$$A(u) = -\nabla \cdot \xi(u)\mu\nabla.$$

For the precise conditions we refer to [1, 7].

Since the meanwhile classical work of Casas [2], it is well known that pointwise state constraints introduce specific challenges in the analysis, numerical analysis, and numerical solution of such control problems. In essence, classical techniques to prove necessary optimality conditions often rely on existence of a so called (linearized) Slater point, and the space of continuous functions is then usually used. This leads to the appearance of measures in the optimality conditions, influencing the regularity of the adjoint state. In some cases, see [4] for some control problems with linear and semilinear partial differential equations, the regularity of the Lagrange multipliers and thus the adjoint state can be improved.

For quasilinear problems, the regularity of the adjoint state proved to be a challenge even with regular right-hand-sides. An intuitive explanation for this challenge is the following formal calculation. For $A(u)$ defined as above, a formal derivation of the adjoint equation for the adjoint state z leads to the following expression

$$-\partial_t z + A(u)^* z + A'(u)^* z = J_u(u, q),$$

combined with terminal and boundary conditions, where

$$A'(u)v = -\nabla \cdot \xi'(u)v\mu\nabla u.$$

Thus, in contrast to linear and semilinear equations, the state and the gradient of the state appear in the differential operator itself. A careful regularity analysis of e.g. the linear equation and the adjoint equation has been carried out in [1], starting with and based on results from e.g. [8, 6]. For further details, we refer to [1].

While these results allowed to obtain first order necessary optimality conditions also for problems with pointwise state constraints, the presence of the latter still leads to several challenges and difficulties when it comes to discussing second order sufficient conditions. First, an abstract result without two-norm discrepancy is obtained in [7], extending techniques and ideas from [5]. When applying this to the model problem with additional state constraints, we build upon both results and settings in [1] and [3].

While the motivation is a setting of pointwise in space and time constraints, i.e.

$$U_{\text{ad}} = \{u \in C(\bar{I} \times \bar{\Omega}) : u_a(t, x) \leq u(t, x) \leq u_b(t, x) \forall (t, x) \in \bar{I} \times \bar{\Omega}\},$$

these can only be handled in the regularity setting of [3] for certain types of control. If for instance the domains are less smooth and the regularity setting from [1] is used, it is possible to consider averaged-in-time state constraints given by

$$U_{\text{ad}} = \{u \in L^1(I, C(\bar{\Omega})) : u_a(x) \leq \int_0^T u(t, x) dt \leq u_b(x) \forall x \in \bar{\Omega}\}.$$

Interestingly, averaged-in-space but pointwise-in-time state constraints cannot be handled in the same setting.

The talk aims at pointing out the challenges and difficulties in the derivation of second order sufficient conditions that lead to an interplay of regularity assumptions vs. type of state constraints vs. type of controls that can be covered by the theory.

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Nonconvex Regularization in Spaces of Measures for Minimal Width Neural Networks

KONSTANTIN PIEPER

(joint work with Armenak Petrosyan)

Classical training procedures for neural networks based on gradient descent applied to (regularized) loss functions can be interpreted through the lens of function-space and PDE-constrained optimization. This is accomplished by viewing the neural network $\mathcal{N}: \mathbb{R}^d \rightarrow \mathbb{R}$ as an unknown function parametrized by an unknown number of weights Θ and interpreting the regularization term as a function-space penalty on the underlying network. In this talk we consider the construction of shallow ReLU networks

$$\mathcal{N}_\Theta(x) = \sum_{n=1, \dots, N} c_n \sigma(a_n \cdot x + b_n), \quad \text{where } \sigma(z) = \max\{z, 0\},$$

through the minimization of a loss function with standard weight-decay regularization,

$$\min_{\Theta = \{(a_n, b_n, c_n) \mid n=1, \dots, N\} \subset \mathbb{R}^{d+2}} l(\mathcal{N}_\Theta) + \alpha \|\Theta\|_{\mathbb{R}^{N \times (d+2)}}^2,$$

where l is a loss term that measures the discrepancy of the output of the network to the data in the training set. This turns out to correspond to an optimization problem on a space of measures [1, 2], given as

$$\min_{\mu \in M(\mathbb{S}^d)} l(\mathcal{N}\mu) + \alpha \|\mu\|_{M(\mathbb{S}^d)},$$

where $M(\mathbb{S}^d)$ is the set of regular Borel measures on the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ and $\|\cdot\|_{M(\mathbb{S}^d)}$ the associated total variation (TV) norm. Moreover, the network is given by

$$\mathcal{N}\mu = \int_{\mathbb{S}^d} \sigma(a \cdot x + b) d\mu(a, b),$$

and the equivalence is realized through the atomic measures $\mu = \sum_{n=1}^N c_n \delta_{(a_n, b_n)}$. The sparsity-promoting regularization term on the measure representing the network can be additionally interpreted as a derivatives based regularizer on the network itself [3, 4], which helps interpret the structure of optimal networks and sheds light on questions connected to how well different classes of functions can

be approximated. We also point out the close connection of this problem to a PDE-constrained problem that arises by introducing the function represented by the network $u = \mathcal{N}\mu$ as an additional optimization variable:

$$\begin{aligned} \min_{\mu \in M(\mathbb{S}^d), u: \mathbb{R}^d \rightarrow \mathbb{R}} \quad & l(u) + \alpha \|\mu\|_{M(\mathbb{S}^d)} \\ \text{subject to} \quad & \Delta u = \mathcal{R}^* \{ \|a\| d\mu \} \quad \text{on } \mathbb{R}^d, \end{aligned}$$

where \mathcal{R}^* is the adjoint Radon transform.

However, a closer analysis of the optimality conditions and numerical experiments reveal that the optimal solutions tend to correspond to networks that are wider than necessary and can even lead to infinite width networks. This is caused by a clustering of similar neurons in the presence of many data points that can even lead to a non-atomic optimal solution of the measures space problem in the infinite data case. To remedy this, we study a different class of nonconvex regularizers that preserve many of the functional-analytic properties of the TV-norm, but lead to much sparser optimal solutions [5]. The new formulation is given as

$$\min_{\mu \in M(\mathcal{S}^d)} l(\mathcal{N}\mu) + \alpha \Phi(\mu),$$

where the regularization functional Φ is the weak-* lower-semicontinuous extension of

$$\Phi \left(\sum_{n=1}^N c_n \delta_{(a_n, b_n)} \right) = \sum_{n=1}^N \phi(|c_n|),$$

and ϕ is a suitably regular concave function with $\phi(0) = 0$, $\phi'(0) = 1$; e.g., $\phi(z) = \log(1+z)$. The nonconvex formulation provides smaller networks of comparable accuracy and structure. We rely on a concept of local minimizers/stationary solutions and we show that such solutions are free of clustering and always finite, even in the presence of infinite data, and fulfill the same approximation guarantees as the global solutions of the convex (TV) problem. Moreover, we describe how such optimal networks can be obtained in practice by extending generalized conditional gradient methods to the nonconvex case: Here, we combine proximal-gradient based optimization of finite-dimensional loss functions (corresponding to finite atomic measures) together with adaptive pruning and greedy insertion of new neurons to the network. With this, we are able to construct smaller networks of similar approximation quality in shorter time than for the (TV) based approach.

We also point out several open problems and questions for further research, such as a more detailed study of the structure of local minimizers of the nonconvex problem (e.g., second order optimality conditions and quantitative bounds on the number of atoms) and the potential influence of different notions of locality in the space of measures on the minimizers. Moreover, we motivate the desire to extend the concepts mentioned above to deeper networks due to their better approximation properties with fewer neurons for certain classes of functions.

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Sequential Action Control for Stabilization of PDE-Dynamical Systems

FALK M. HANTE

(joint work with Yan Brodskyi and Arno Seidel)

1. MOTIVATION AND RECENT CONTRIBUTIONS

Data is playing an increasingly important role in modeling, simulation and optimization of systems governed by partial differential equations (PDEs). A nontrivial and relevant example are energy distribution systems, where an information layer based on a wide installation of sensors is being added to the physical network for data collection and analysis of flows governed by a coupling of balance laws on graphs [6, 12]. Feedback control based on optimality principles such as model predictive control (MPC) provides the flexibility to incorporate measurements and state estimation techniques for typical control tasks such as stabilization e.g. at steady states [5] or state-tracking e.g. towards a turnpike [4]. However, at least for large scale energy networks, MPC in its original form repeatedly solving stage problems

$$\begin{aligned} \min J_1(u) &= \int_{t_0}^{t_0+T} l_1(y(s)) ds + m(y(t_0 + T)) \\ \dot{y}(t) &= Ay(t) + f(t, y(t))u(t), \quad u(t) \in U, \quad t \in (t_0, t_0 + T) \\ y(t_0) &= y_0, \end{aligned}$$

for states y and controls u in Hilbert spaces H and U on a prediction horizon $[t_0, t_0 + T]$ as in [9] is computationally challenging. For control and stabilization of PDEs, we therefore propose and analyse in [3] a variant of a moving horizon scheme called sequential action control (SAC) going back to [2]. Given a reference control u_1 , this real-time iteration scheme consists of (i) predicting the nominal dynamics of the state and adjoint state for u_1 on $[t_0, t_0 + T]$, (ii) computing control actions $u^*(t)$ on $[t_0, t_0 + T]$ using adjoint information, (iii) selecting an application

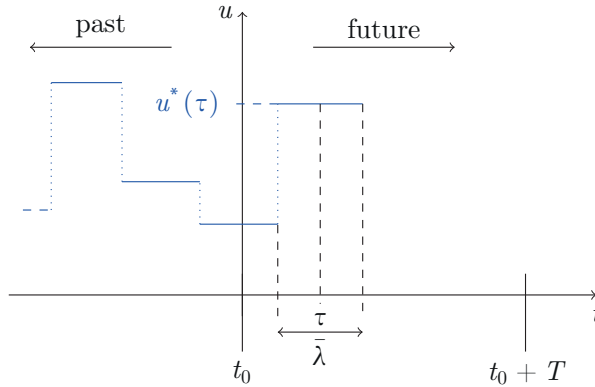


FIGURE 1. Illustration of sequential action control.

time τ and an action’s duration $\bar{\lambda}$, before applying $u \equiv u^*(\tau)$ on $[\tau - \frac{\bar{\lambda}}{2}, \tau + \frac{\bar{\lambda}}{2}]$ with $u = u_1$ elsewhere and updating t_0 , cf. Figure 1. The control values $u^*(\tau)$ are chosen as

$$(1) \quad u^*(\tau) := \arg \min_{u \in U} l_2(u; \tau) := \frac{1}{2} \left[\frac{dJ_1}{d\lambda^+}(\tau, u) - \alpha_d \right]^2 + \frac{1}{2} \langle u, Ru \rangle_U,$$

for any $\tau \in (t_0, t_0 + T)$, where

$$\frac{dJ_1}{d\lambda^+}(\tau, v) = \lim_{\lambda \downarrow 0} \frac{J_1(u_{\lambda, \tau, v}) - J_1(u_1)}{\lambda}$$

is the variation of J_1 corresponding to Pontryagin’s needle variation [10]

$$u_{\lambda, \tau, v} = \begin{cases} u_1(t), & t \notin [\tau - \frac{\lambda}{2}, \tau + \frac{\lambda}{2}] \\ v, & t \in [\tau - \frac{\lambda}{2}, \tau + \frac{\lambda}{2}] \end{cases},$$

$\alpha_d < 0$ is a parameter in order to obtain a reduction for the cost of the current prediction and R is a regularization parameter. From results in [11], we get that

$$\frac{dJ_1}{d\lambda^+}(\tau, v) = \langle p(\tau), f(\tau, y(\tau))(v - u_1(\tau)) \rangle_{H^*, H},$$

where p satisfies the adjoint PDE

$$\begin{aligned} \dot{p}(t) &= -A^*p(t) - ((f(t, y(t))u_1(t))_y)^*p(t) - (l_1)_y(y(t)) \\ p(t_0 + T) &= m_y(y(t_0 + T)), \end{aligned}$$

so that $u^*(\tau)$ can be explicitly obtained using first order conditions on l_2 for any fixed τ . Hence, the scheme qualifies for late lumping approaches and thus discretization grid independent qualitative analysis.

For linear-quadratic problems we show that the closed-loop feedback obtained from SAC can be analyzed in first order as a linear feedback with the solution of

a Lyapunov-equation. Prototypically, we consider the stabilization of an unstable heat equation from [1]. Our results show that SAC stabilizes the problem at the origin and outperforms the standard linear quadratic regulator both in the needed computation time and in robustness with respect to uncertainty in parameters. Details are available in [3].

Finally, we observe that the control principle can be extended with methods from [7, 8, 11] to switched systems and mixed-integer control problems being motivated, for example, by operation of valves in gas networks. The proposed framework indeed provides a rigorous link between variational principles for PDEs and mixed-integer programming for solving (1).

2. OPEN QUESTIONS AND TOPICS FOR FUTURE RESEARCH

We note that guarantees for SAC-type feedback in case of partial state observation, boundary control, nonlinear PDEs and other advanced topics are still to be investigated. Beyond that, the motivating application of control and stabilization for energy networks presents a number of further challenges in the context of PDE-control such as methods for robustification, coupling with market leading to multi-level optimization problems and advanced aspects of coupling discrete and continuous control concerning, for example, methods to deal with changing network topologies or combinatorial constraints.

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Constructive Exact Controls for some Semilinear PDEs

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Let Ω be a bounded domain of \mathbb{R}^d , $d \in \{2, 3\}$ with $C^{1,1}$ boundary and $\omega \subset\subset \Omega$ be a non empty open set. Let $T > 0$ and denote $Q_T := \Omega \times (0, T)$, $q_T := \omega \times (0, T)$ and $\Sigma_T := \partial\Omega \times (0, T)$. We consider the semilinear wave equation

$$(1) \quad \begin{cases} \square y + g(y) = f1_\omega, & \text{in } Q_T, \\ y = 0, & \text{on } \Sigma_T, \\ (y(\cdot, 0), y_t(\cdot, 0)) = (u_0, u_1), & \text{in } \Omega, \end{cases}$$

where $(u_0, u_1) \in \mathbf{V} := H_0^1(\Omega) \times L^2(\Omega)$ is the initial state of y , $f \in L^2(q_T)$ is a control function and $\square y := \partial_{tt}y - \Delta y$. $g : \mathbb{R} \rightarrow \mathbb{R}$ is a function of class C^1 such that $|g(r)| \leq C(1 + |r|) \ln(2 + |r|)$ for every $r \in \mathbb{R}$ and some $C > 0$. (1) has a unique global weak solution in $C([0, T]; H_0^1(\Omega)) \cap C^1([0, T]; L^2(\Omega))$ (see [2]). The exact controllability for (1) in time T is formulated as follows: for any $(u_0, u_1), (z_0, z_1) \in \mathbf{V}$, find a control function $f \in L^2(q_T)$ such that the weak solution of (1) satisfies $(y(\cdot, T), \partial_t y(\cdot, T)) = (z_0, z_1)$. This problem has been solved by Fu, Yong and Zhang:

Theorem 1. [Fu, Yong, Zhang, 2007] For any $x_0 \in \mathbb{R}^d \setminus \overline{\Omega}$, let $\Gamma_0 = \{x \in \partial\Omega, (x - x_0) \cdot \nu(x) > 0\}$ and, for any $\epsilon > 0$, let $\mathcal{O}_\epsilon(\Gamma_0) = \{y \in \mathbb{R}^d \mid |y - x| \leq \epsilon \text{ for } x \in \Gamma_0\}$. Assume

(H₀) $T > 2 \max_{x \in \overline{\Omega}} |x - x_0|$ and $\omega = \mathcal{O}_\epsilon(\Gamma_0) \cap \Omega$ for some $\epsilon > 0$,

(H₁) $\limsup_{|r| \rightarrow \infty} \frac{|g(r)|}{|r| \ln^{1/2} |r|} = 0$,

then (1) is exactly controllable in time T .

Γ_0 is the star-shaped part of the whole boundary of Ω introduced in [11]. Theorem 1 extends to the multi-dimensional case the result of [15] devoted to the one dimensional case. The proof given in [5] is based on a fixed point argument introduced in [15]: it is shown that the operator $K : L^\infty(0, T; L^d(\Omega)) \rightarrow L^\infty(0, T; L^d(\Omega))$ where $y_\xi := K(\xi)$ is a controlled solution through the control function f_ξ (of minimal $L^2(q_T)$ -norm) of the linear boundary value problem

$$\begin{cases} \square y_\xi + y_\xi \widehat{g}(\xi) = -g(0) + f_\xi 1_\omega, & \text{in } Q_T, \\ y_\xi = 0, & \text{on } \Sigma_T, \\ (y_\xi(\cdot, 0), \partial_t y_\xi(\cdot, 0)) = (u_0, u_1), & \text{in } \Omega, \end{cases} \quad \widehat{g}(r) := \begin{cases} \frac{g(r) - g(0)}{r} & r \neq 0, \\ g'(0) & r = 0 \end{cases},$$

satisfying $(y_\xi(\cdot, T), y_{\xi,t}(\cdot, T)) = (z_0, z_1)$ has a fixed point. The existence of a fixed point for the compact operator K is obtained by using the Leray-Schauder's degree theorem: it is shown under the growth assumption (\mathbf{H}_1) that there exists a constant $M = M(\|u_0, u_1\|_{\mathbf{V}}, \|z_0, z_1\|_{\mathbf{V}})$ such that K maps the ball $B_{L^\infty(0,T;L^d(\Omega))}(0, M)$ into itself.

Our goal is to construct an explicit sequence $(f_k)_{k \in \mathbb{N}}$ that converges strongly to an exact control for (1). The controllability of nonlinear partial differential equations has attracted a large number of works in the last decades (see [3]). However, as far as we know, few are concerned with the approximation of exact controls for nonlinear partial differential equations, and the construction of convergent control approximations for nonlinear equations remains a challenge.

A first idea that comes to mind is to consider the Picard iterations $(y_k)_{k \in \mathbb{N}}$ associated with the operator K defined by $y_{k+1} = K(y_k)$, $k \geq 0$ initialized with any element $y_0 \in L^\infty(0, T; L^d(\Omega))$. Such a strategy usually fails since the operator K is in general not contracting, even if g is globally Lipschitz.

Given any initial data $(u_0, u_1) \in \mathbf{V}$, we design an algorithm providing a sequence $(y_k, f_k)_{k \in \mathbb{N}}$ converging to a controlled pair for (1), under assumptions on g that are slightly stronger than (\mathbf{H}_1) . Moreover, after a finite number of iterations, the convergence is super-linear. This is done by introducing a least-squares functional measuring how much a pair $(y, f) \in \mathcal{A}$ is close to a controlled solution for (1) and then by determining a particular minimizing sequence enjoying the announced property. We define the Hilbert space \mathcal{H}

$$\mathcal{H} = \left\{ (y, f) \in L^2(Q_T) \times L^2(Q_T) \mid \square y \in L^2(Q_T), (y(\cdot, 0), \partial_t y(\cdot, 0)) \in \mathbf{V}, y = 0 \text{ on } \Sigma_T \right\}.$$

Then, for any $(u_0, u_1), (z_1, z_1) \in \mathbf{V}$, we define the subspaces of \mathcal{H}

$$\begin{aligned} \mathcal{A} &= \left\{ (y, f) \in \mathcal{H} \mid (y(\cdot, 0), \partial_t y(\cdot, 0)) = (u_0, u_1), (y(\cdot, T), \partial_t y(\cdot, T)) = (z_0, z_1) \right\}, \\ \mathcal{A}_0 &= \left\{ (y, f) \in \mathcal{H} \mid (y(\cdot, 0), \partial_t y(\cdot, 0)) = (0, 0), (y(\cdot, T), \partial_t y(\cdot, T)) = (0, 0) \right\} \end{aligned}$$

and consider the following non convex extremal problem

$$(2) \quad \inf_{(y,f) \in \mathcal{A}} E(y, f), \quad E(y, f) := \frac{1}{2} \|\square y + g(y) - f 1_\omega\|_2^2$$

observing that any zero $(y, f) \in \mathcal{A}$ of E is a solution of the controllability problem. Our main result is

Theorem 2. [Lemoine, Münch, 2021] Assume for some $s \in (0, 1)$

$$(\overline{\mathbf{H}}_s) \quad [g']_s := \sup_{\substack{a, b \in \mathbb{R} \\ a \neq b}} \frac{|g'(a) - g'(b)|}{|a - b|^s} < +\infty,$$

$$(\mathbf{H}_2) \quad \text{There exists } \alpha \geq 0 \text{ and } \beta \in [0, \sqrt{\frac{s}{2C(2s+1)}}) \text{ such that } |g'(r)| \leq \alpha + \beta \ln^{1/2}(1 + |r|) \text{ for every } r \text{ in } \mathbb{R}.$$

Then, for any $(y_0, f_0) \in \mathcal{A}$, the sequence $(y_k, f_k)_{k \in \mathbb{N}}$ defined by

$$(3) \quad \begin{cases} (y_0, f_0) \in \mathcal{A}, \\ (y_{k+1}, f_{k+1}) = (y_k, f_k) - \lambda_k(Y_k^1, F_k^1), \quad k \in \mathbb{N}, \\ \lambda_k = \operatorname{argmin}_{\lambda \in [0,1]} E((y_k, f_k) - \lambda(Y_k^1, F_k^1)), \end{cases}$$

where $(Y_k^1, F_k^1) \in \mathcal{A}_0$ is the solution of minimal control norm of

$$(4) \quad \begin{cases} \square Y_k^1 + g'(y_k)Y_k^1 = F_k^1 1_\omega + \square y_k + g(y_k) - f_k 1_\omega, & \text{in } Q_T, \\ Y_k^1 = 0, & \text{on } \Sigma_T, \\ (Y_k^1(\cdot, 0), \partial_t Y_k^1(\cdot, 0)) = (0, 0), & \text{in } \Omega \end{cases}$$

strongly converges to a pair $(\bar{y}, \bar{f}) \in \mathcal{A}$ satisfying (1). Moreover, the convergence is at least linear and is at least of order $1 + s$ after a finite number of iterations.

As far as we know, the method described here is the first one providing an explicit, algorithmic construction of exact controls for semilinear wave equations with non Lipschitz nonlinearity and defined over multi-dimensional bounded domains. It extends the one-dimensional study addressed in [14]. The parabolic case can be addressed as well: for semilinear heat equation, we mention [6] for $d \in \{2, 3\}$ with Lipschitz nonlinearity and [10] for $d = 1$ and non Lipschitz nonlinearity. These works devoted to controllability problems takes their roots in [9, 7] concerned with the direct problem for the Navier-Stokes equation: they refine the analysis performed in [8, 12] inspired from the seminal contribution [1].

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Obstacle Problems in Electromagnetic Shielding

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Electromagnetic (EM) shielding is a physical process of canceling or redirecting EM waves in a certain domain of interest by means of obstacles made of conducting or magnetic materials. It was first discovered by Michael Faraday in 1836, who experimentally verified that a conductive enclosure (Faraday cage) is able to eliminate the effect of an external electric field by charge cancellation on the boundary and leaving zero field inside the cage. On the other hand, a specific magnetic material can realize shielding by diverting the external magnetic flux to another direction. Typical materials used in Faraday shielding are conductive sheet metals and metallic alloys, whereas ferromagnetic materials are widely used for magnetic obstacles. Today, EM shielding is indispensable not only for high-technological applications but also for our daily used applications such as microwave ovens, mobile phones, aircraft, shielded cable wires, circuits, and many other electronic devices.

From the mathematical point of view, EM shielding falls into the class of obstacle problems (cf. Duvaut and Lions [1]). More precisely, in the free region, the EM waves satisfy the fundamental Maxwell equations, whereas in the shielded area obstacle constraints are applied to the fields. To formulate the corresponding mathematical formulation, let us denote by $\Omega \subset \mathbb{R}^3$ an open set (not necessarily connected, Lipschitz, or bounded) representing the hold all domain and set

$$\begin{aligned} \mathbf{H}(\mathbf{curl}) &:= \{ \mathbf{q} \in \mathbf{L}^2(\Omega) \mid \mathbf{curl} \mathbf{q} \in \mathbf{L}^2(\Omega) \} \\ \mathbf{H}_0(\mathbf{curl}) &:= \text{closure of } \mathbf{C}_0^\infty(\Omega) \text{ w.r.t. } \|\cdot\|_{\mathbf{H}(\mathbf{curl})}, \end{aligned}$$

where $\mathbf{L}^2(\Omega)$ denotes the space of all (equivalence classes of) \mathbb{R}^3 -valued Lebesgue square-integrable functions. Furthermore, let $(0, 0) \in \mathbf{K} \subset \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega)$ be a convex and closed subset standing for the underlying feasible (constraint) set. Then, given initial data $(\mathbf{E}_0, \mathbf{H}_0) \in \{ \mathbf{H}_0(\mathbf{curl}) \times \mathbf{H}(\mathbf{curl}) \} \cap \mathbf{K}$ and an applied current source $\mathbf{f} \in W^{1,\infty}((0, T), \mathbf{L}^2(\Omega))$, we look for $(\mathbf{E}, \mathbf{H}) \in W^{1,\infty}((0, T), \mathbf{L}^2(\Omega))$

$\times L^2(\Omega)$) such that

$$(1) \quad \left\{ \begin{array}{l} \int_0^T \int_{\Omega} \epsilon \partial_t \mathbf{E} \cdot (\mathbf{v} - \mathbf{E}) + \mu \partial_t \mathbf{H} \cdot (\mathbf{w} - \mathbf{H}) - \mathbf{H} \cdot \mathbf{curl} \mathbf{v} + \mathbf{E} \cdot \mathbf{curl} \mathbf{w} \, dx \, dt \\ \geq \int_0^T \int_{\Omega} \mathbf{f} \cdot (\mathbf{v} - \mathbf{E}) \, dx \, dt \\ \forall (\mathbf{v}, \mathbf{w}) \in L^2((0, T), \mathbf{H}_0(\mathbf{curl}) \times \mathbf{H}(\mathbf{curl})), (\mathbf{v}, \mathbf{w})(t) \in \mathbf{K} \text{ a.e. } t \in (0, T) \\ (\mathbf{E}, \mathbf{H})(t) \in \mathbf{K} \text{ for all } t \in [0, T] \\ (\mathbf{E}, \mathbf{H})(0) = (\mathbf{E}_0, \mathbf{H}_0). \end{array} \right.$$

Here, the electric permittivity and the magnetic permeability $\epsilon, \mu : \Omega \rightarrow \mathbb{R}^{3 \times 3}$ are assumed to be of class $L^\infty(\Omega)^{3 \times 3}$, symmetric, and uniformly positive definite in the sense that there exist positive constants $\underline{\epsilon}, \underline{\mu} > 0$ such that

$$\xi^T \epsilon(x) \xi \geq \underline{\epsilon} |\xi|^2 \quad \text{and} \quad \xi^T \mu(x) \xi \geq \underline{\mu} |\xi|^2 \quad \text{for a.e. } x \in \Omega \text{ and all } \xi \in \mathbb{R}^3.$$

In [3, Theorem 1], the author proved an existence result for (1) built on [2, Theorem 3.11]. The developed result yields only existence in $W^{1, \infty}((0, T), L^2(\Omega) \times L^2(\Omega))$ without the global \mathbf{curl} regularity, i.e., $(\mathbf{E}, \mathbf{H}) \in L^2((0, T), \mathbf{H}_0(\mathbf{curl}) \times \mathbf{H}(\mathbf{curl}))$ is not guaranteed. Nonetheless, the solution is still physically reasonable as it turns to obey the physical electromagnetic laws in the free regions. More precisely, if we denote the electric (resp. magnetic) free region by the open (possibly empty) subset $\Omega_E \subset \Omega$ (resp. $\Omega_H \subset \Omega$), i.e., if

$$(\mathbf{v}, \mathbf{w}) \in \mathbf{K} \Rightarrow (\tilde{\mathbf{v}}, \tilde{\mathbf{w}}) \in \mathbf{K} \quad \forall \tilde{\mathbf{v}} = \begin{cases} \mathbf{v}_E & \text{in } \Omega_E \\ \mathbf{v} & \text{elsewhere} \end{cases} \quad \tilde{\mathbf{w}} = \begin{cases} \mathbf{w}_H & \text{in } \Omega_H \\ \mathbf{w} & \text{elsewhere} \end{cases}$$

holds for any $(\mathbf{v}_E, \mathbf{w}_H) \in L^2(\Omega_E) \times L^2(\Omega_H)$, then every solution $(\mathbf{E}, \mathbf{H}) \in W^{1, \infty}((0, T), L^2(\Omega) \times L^2(\Omega))$ of (1) fulfils the Maxwell-Ampère equation in Ω_E and the Faraday law in Ω_H :

$$(2) \quad \begin{cases} \epsilon \partial_t \mathbf{E} - \mathbf{curl} \mathbf{H} = \mathbf{f} & \text{a.e. in } \Omega_E \times (0, T) \\ \mu \partial_t \mathbf{H} + \mathbf{curl} \mathbf{E} = 0 & \text{a.e. in } \Omega_H \times (0, T). \end{cases}$$

In particular, every solution to (1) enjoys the local regularity properties

$$\mathbf{curl} \mathbf{E} \in L^\infty((0, T), L^2(\Omega_H)) \quad \text{and} \quad \mathbf{curl} \mathbf{H} \in L^\infty((0, T), L^2(\Omega_E)),$$

and if $\Omega_H = \Omega$ then the electric boundary condition is fully recovered, i.e., $\mathbf{E} \in L^\infty((0, T), \mathbf{H}_0(\mathbf{curl}))$. All these results were proven in [3, Theorem 1].

The uniqueness analysis of (1) turns out to be more challenging and requires a careful treatment. We notice that energy arguments are not applicable due to the poor regularity of the solution. Under a structural assumption on the feasible set \mathbf{K} (see [3, Assumption 1.1]), the author established a uniqueness result [3, Theorem 2]. The proof is based on a local $\mathbf{H}(\mathbf{curl})$ -regularity analysis with respect to the constraint set under Assumption 1.1, in particular under a separation ansatz between the electric and magnetic obstacle sets. As shown there, the uniqueness holds also true if $\Omega_H = \Omega$ (pure electric obstacle problem) or $\Omega_E = \Omega$ (pure magnetic obstacle problem). As a consequence of Theorems 1 and 2 in [3], for any

given closed and convex feasible electric set $0 \in \mathbf{K}_E \in \mathbf{L}^2(\Omega)$, the pure electric obstacle problem

$$\begin{aligned}
 \text{(PE)} \quad & \left\{ \begin{aligned}
 & \int_{\Omega} \epsilon \partial_t \mathbf{E}(t) \cdot (\mathbf{v} - \mathbf{E}(t)) - \mathbf{H}(t) \cdot \mathbf{curl}(\mathbf{v} - \mathbf{E}(t)) \, dx \geq \int_{\Omega} \mathbf{f}(t) \cdot (\mathbf{v} - \mathbf{E}(t)) \, dx \\
 & \text{for all } \mathbf{v} \in \mathbf{H}_0(\mathbf{curl}) \cap \mathbf{K}_E \text{ and a.e. } t \in (0, T) \\
 & \mu \partial_t \mathbf{H}(t) + \mathbf{curl} \mathbf{E}(t) = 0 \text{ for a.e. } t \in (0, T) \\
 & \mathbf{E}(t) \in \mathbf{K}_E \text{ for all } t \in [0, T] \\
 & (\mathbf{E}, \mathbf{H})(0) = (\mathbf{E}_0, \mathbf{H}_0)
 \end{aligned} \right.
 \end{aligned}$$

admits a unique solution

$$(\mathbf{E}, \mathbf{H}) \in L^\infty((0, T), \mathbf{H}_0(\mathbf{curl}) \times \mathbf{L}^2(\Omega)) \cap W^{1,\infty}((0, T), \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega)).$$

We note that (PE) preserves the Faraday law but modifies the Maxwell-Ampère equation $\epsilon \partial_t \mathbf{E} - \mathbf{curl} \mathbf{H} = \mathbf{f}$ into a variational inequality of the first kind. Similarly, for any given closed and convex feasible magnetic set $0 \in \mathbf{K}_H \in \mathbf{L}^2(\Omega)$, the pure magnetic obstacle problem

$$\begin{aligned}
 \text{(PH)} \quad & \left\{ \begin{aligned}
 & \int_{\Omega} \mu \partial_t \mathbf{H}(t) \cdot (\mathbf{w} - \mathbf{H}(t)) + \mathbf{E}(t) \cdot \mathbf{curl}(\mathbf{w} - \mathbf{H}(t)) \, dx \geq 0 \\
 & \text{for all } \mathbf{w} \in \mathbf{H}(\mathbf{curl}) \cap \mathbf{K}_H \text{ and a.e. } t \in (0, T) \\
 & \epsilon \partial_t \mathbf{E}(t) - \mathbf{curl} \mathbf{H}(t) = \mathbf{f}(t) \text{ for a.e. } t \in (0, T) \\
 & \mathbf{H}(t) \in \mathbf{K}_H \text{ for all } t \in [0, T] \\
 & (\mathbf{E}, \mathbf{H})(0) = (\mathbf{E}_0, \mathbf{H}_0)
 \end{aligned} \right.
 \end{aligned}$$

admits a unique solution

$$(\mathbf{E}, \mathbf{H}) \in L^\infty((0, T), \mathbf{L}^2(\Omega) \times \mathbf{H}(\mathbf{curl})) \cap W^{1,\infty}((0, T), \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega)).$$

Differently from (PE), the magnetic shielding case (PH) preserves the Maxwell-Ampère equation and modifies the Faraday law by a variational inequality of the first kind.

The well-posedness results for (1), (PE), and (PH) serve as a basis for further investigations, including

- finite element analysis
- shape optimal design
- ferromagnetic shielding

which have been the subject of our ongoing research.

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Constrained Exact Boundary Controllability for a System of Semilinear Hyperbolic PDEs

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(joint work with Martin Gugat, Jens Habermann, and Michael Hintermüller)

Motivated by the operation of a gas network, we investigate the exact boundary controllability of a semilinear model of gas flow in 1D with pointwise constraints on the pressure and Mach number. While there exists a large body of work in the study of existence of solution and exact controllability for both semilinear and quasilinear systems, see for instance [3] and [4], our focus is the case where the solutions and controls are continuous and constrained.

Since the length L of a pipeline is much larger than its diameter D , only one spatial dimension is considered. We assume that the isothermal Euler equations (see for example [2]) govern the evolution of the flow through a pipe:

$$\begin{cases} \rho_t + q_x = 0, \\ q_t + \left(p + \frac{q^2}{\rho}\right)_x = -\frac{1}{2}\theta \frac{q|q|}{\rho} - \rho g s_{\text{slope}}, \end{cases}$$

where $\rho > 0$ denotes the gas density, $p > 0$ the pressure and q the mass flux. The friction coefficient is denoted by $\lambda_{\text{fric}} \geq 0$ and the slope by $\varphi \in (-\infty, \infty)$. Define $s_{\text{slope}} = \sin(\varphi)$ and $\theta = \frac{\lambda_{\text{fric}}}{D}$. Let g denote the gravitational constant. The gas is supposed to be ideal, satisfying the state equation $p = R_s T_{\text{emp}} \rho$ where R_s is the specific gas constant and T_{emp} is the temperature. The velocity of the gas is given by $v = \frac{q}{\rho}$ and the sound speed $c = \sqrt{R_s T_{\text{emp}}}$ is taken to be constant. For the Mach number M this yields $M = \frac{v}{c} = c \frac{q}{p}$. When $|M| < 1$ the flow is said to be *subsonic*. From this quasilinear system, one can derive the semilinear model:

$$\begin{cases} p_t + c^2 q_x = 0 \\ q_t + p_x = -\frac{1}{2}\theta c^2 \frac{q|q|}{p} - g s_{\text{slope}} \frac{p}{c^2}. \end{cases}$$

First, we recall how in the regime of high pressures and slow subsonic flows, the semilinear system can be a valid approximation of the quasilinear one. This regime of low Mach number is typical in the operation of gas networks to reduce noise and internal corrosion.

The constraints we consider are as follows: given $0 < \underline{p} < \bar{p}$ and $0 < \lambda < 1$, the following relations must hold in a pointwise sense:

$$\underline{p} \leq p \leq \bar{p} \quad \text{and} \quad |M| \leq \lambda.$$

Finally, we assume that we have Dirichlet boundary controls.

The subsequent analysis is performed on the semilinear system in diagonal form. To this end, we introduce the RIEMANN invariants R_+ and R_- :

$$R_{\pm} = \pm p + M p = (\pm 1 + M) p.$$

The characteristic curves are straight lines. The physical variables can be expressed in terms of the RIEMANN invariants as

$$p = \frac{R_+ - R_-}{2}, \quad M = \frac{R_+ + R_-}{R_+ - R_-}, \quad q = \frac{1}{2c}(R_+ + R_-).$$

The system in diagonal form reads

$$(R_{\pm})_t \pm c(R_{\pm})_x = -\frac{1}{4}\theta c F(R_+, R_-) - g_{slope} \frac{1}{c} \frac{R_+ - R_-}{2},$$

where $F(R_+, R_-) = (R_+ + R_-) \left| \frac{R_+ + R_-}{R_+ - R_-} \right|$. The pressure and Mach number constraints can be expressed in terms of the RIEMANN invariants as

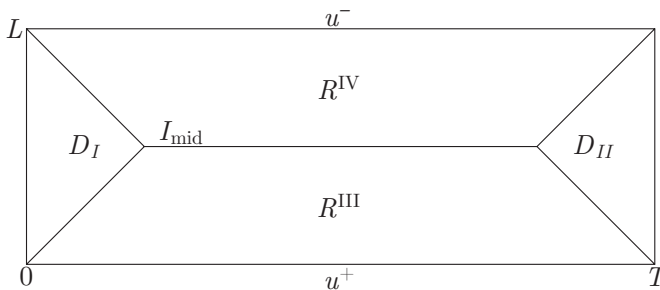
$$\begin{aligned} 2p &\leq R_+ - R_- \leq 2\bar{p}, \\ (1 + \lambda)R_+ + (1 - \lambda)R_- &\geq 0, \\ (1 - \lambda)R_+ + (1 + \lambda)R_- &\leq 0. \end{aligned}$$

whenever $p > 0$. Note that in this case, it is easy to see that $|M| < 1$ implies that $R_+ > 0$ and $R_- < 0$.

The existence of continuous solutions of the semilinear model fulfilling the point-wise constraints over a certain time horizon is established. The conditions are all numerically ascertainable and are of two types. On one hand, the RIEMANN invariants on the initial state and the boundary must satisfy some inequalities similar to the pressure and Mach number constraints. On the other hand, the following inequality, involving the physical characteristics of the pipe and gas, must hold:

$$\frac{\theta\lambda\sqrt{5}}{2} + \frac{g|slope|}{c^2} \leq \frac{1}{L}.$$

Then, the question of exact constrained controllability is tackled. We proceed with the following strategy. The rectangle $[0, T] \times [0, L]$ is partitioned into 4 domains: the triangles D_I, D_{II} and the parallelograms R^{III}, R^{IV} , as shown on the diagram below.



On the triangles D_I and D_{II} , the existence of bounded continuous solutions follows from the previous result. For R^{III} (resp. R^{IV}), we define the values of R_{\pm} on I_{mid} using a convex combination of the values at the inner vertices of D_I

and D_{II} . The role of time and space is inverted and the evolution of RIEMANN invariants is governed by

$$(R_{\pm})_x \mp c^{-1}(R_{\pm})_t = -\frac{1}{2}\theta F(R_+, R_-) - g_{slope} \frac{R_+ - R_-}{2c^2}.$$

An IVP is then solved to compute the solution on R^{III} and R^{IV} . The existence of a continuous solution satisfying the box constraints is investigated using similar conditions and techniques as for the first result. Finally, the boundary controls are obtained as $u^+ = R_+(\cdot, 0)$ and $u^- = R_-(\cdot, L)$.

Let us now turn our attention to the computation of the boundary control. A triangular grid is built in the following fashion: consider three points (t_i, x_i) , (t_j, x_j) , and (t_k, x_k) , such that (t_k, x_k) is at the intersection of the two characteristics lines starting from (t_i, x_i) and (t_j, x_j) and the resulting triangle is isosceles. For each system, an integration along the characteristics with the midpoint rule is performed. Let R_{\pm}^k , R_{\pm}^i and R_{\pm}^j be the values of the RIEMANN invariants at those points. For the D_I and D_{II} triangles, R_{\pm}^k is the solution of the nonlinear system

$$R_+^k - R_+^i = \frac{\Delta}{2} \left[\frac{1}{4}\theta c (F(R_+^i, R_-^i) + F(R_+^k, R_-^k)) - g_{slope} \frac{R_+^i - R_-^i + R_+^k - R_-^k}{2c} \right]$$

$$R_-^k - R_-^j = \frac{\Delta}{2} \left[\frac{1}{4}\theta c (F(R_+^j, R_-^j) + F(R_+^k, R_-^k)) - g_{slope} \frac{R_+^j - R_-^j + R_+^k - R_-^k}{2c} \right]$$

where Δ is the length of the integration interval. The computation of the solution on R^{III} and R^{IV} involves solving a similar nonlinear system. The solution of those nonlinear systems is computed using Newton's method. Note that the first (resp. second) equation is symmetric in (R^i, R^k) (resp. (R^j, R^k)). This implies that the numerical solution is reversible along the characteristics, and the values at the boundaries can indeed be used as controls.

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Optimal Control of Stochastic Phase-Field Models for Tumor Growth

LUCA SCARPA

(joint work with Carlo Orrieri and Elisabetta Rocca)

We consider a version of a two-phase phase-field model for tumor growth recently introduced in [2], where we have neglected the effects of chemotaxis and active transport. The new feature of the work consists in adding possible stochastic perturbations in both the PDEs ruling the tumor-dynamic and then studying a related optimal control problem in the direction of therapy optimisation. The evolution of the tumor is described by an order parameter φ which represents the local concentration of tumor cells; the interface between the tumor and healthy cells is supposed to be represented by a narrow transition layer separating the pure regions where $\varphi = \pm 1$, with $\varphi = 1$ denoting the tumor phase and $\varphi = -1$ the healthy phase. The second main variable is the concentration of nutrient $\sigma \in [0, 1]$, which is responsible for the growth and decay of the tumoral cells.

We consider here the case of an incipient tumor, i.e., before the development of quiescent cells, when the equation ruling the evolution of the tumor growth process is often given by a Cahn–Hilliard equation for φ coupled with a reaction-diffusion equation for the nutrient σ . As far as the random perturbations are concerned, we directly add an additive noise to the Cahn–Hilliard equation, taking thus into account all the microscopical fluctuation affecting cell-aggregation and modelling a possible background noise. Moreover, we introduce a multiplicative noise in the reaction diffusion equation for the nutrient, with the aim of modelling the effects of angiogenesis: a stochastic forcing of this type is related to the oxygen received by cancerous cells, and may result in enhancing its effectiveness, and therefore its contribution, to the total growth process of the tumor.

We study the following stochastic Cahn-Hilliard-reaction-diffusion model:

$$\begin{aligned}
 (1) \quad & d\varphi - \Delta\mu \, dt = (\mathcal{P}\sigma - a - \alpha u)h(\varphi) \, dt + G \, dW_1 && \text{in } (0, T) \times D, \\
 (2) \quad & \mu = -\Delta\varphi + \psi'(\varphi) && \text{in } (0, T) \times D, \\
 (3) \quad & d\sigma - \Delta\sigma \, dt + c\sigma h(\varphi) \, dt + b(\sigma - w) \, dt = \mathcal{H}(\sigma) \, dW_2 && \text{in } (0, T) \times D, \\
 (4) \quad & \partial_{\mathbf{n}}\varphi = \partial_{\mathbf{n}}\mu = \partial_{\mathbf{n}}\sigma = 0 && \text{in } (0, T) \times \partial D, \\
 (5) \quad & \varphi(0) = \varphi_0, \quad \sigma(0) = \sigma_0 && \text{in } D.
 \end{aligned}$$

Here, $D \subset \mathbb{R}^3$ is a smooth bounded domain with smooth boundary, $T > 0$ is a fixed final time, W_1, W_2 are independent cylindrical Wiener processes on separable Hilbert spaces U_1 and U_2 , respectively, defined on a stochastic basis $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \in [0, T]}, \mathbb{P})$, G is a stochastically integrable operator with respect to W_1 and \mathcal{H} is a suitable Lipschitz-type operator.

The parameters $\mathcal{P}, a, \alpha, c, b$ are assumed to be strictly positive constants, and denote, respectively, the tumor proliferation rate, the apoptosis rate, the effectiveness rate of the cytotoxic drugs, the nutrient consumption rate, and the nutrient supply rate. The function h is assumed to be monotone increasing, nonnegative in the “physical” interval $[-1, 1]$, and normalized so that $h(-1) = 0$ and $h(1) = 1$.

The term $\mathcal{P}sh(\varphi)$ models the proliferation of tumor cells, which is proportional to the concentration of the nutrient, the term $ah(\varphi)$ describes the apoptosis (or death) of tumor cells, and $csh(\varphi)$ represents the consumption of the nutrient by the tumor cells, which is higher if more tumor cells are present. The control variables are u in (1) and w in (3), which can be interpreted as a therapy distribution (chemotherapy and antiangiogenic therapy, respectively, for example) entering the system, either via the mass balance equation or the nutrient. Finally, ψ' stands for the derivative of a double-well potential ψ , with the typical choice being

$$\psi(r) = \frac{1}{4}(r^2 - 1)^2, \quad r \in \mathbb{R}.$$

We are interested in the study of the following optimal control problem:

(CP): *Minimize the cost functional*

$$\begin{aligned} J(\varphi, u, w) := & \frac{\beta_1}{2} \mathbb{E} \int_Q |\varphi - \varphi_Q|^2 + \frac{\beta_2}{2} \mathbb{E} \int_D |\varphi(T) - \varphi_T|^2 + \frac{\beta_3}{2} \mathbb{E} \int_D (\varphi(T) + 1) \\ & + \frac{\beta_4}{2} \mathbb{E} \int_Q |u|^2 + \frac{\beta_5}{2} \mathbb{E} \int_Q |w|^2, \end{aligned}$$

subject to the control constraint $(u, w) \in \mathcal{U}$ and the system (1)–(5), where

$$\begin{aligned} \mathcal{U} := & \left\{ (u, w) \in L^2(\Omega; L^2(0, T; H))^2 \text{ progressively measurable:} \right. \\ & \left. 0 \leq u, w \leq 1 \text{ a.e. in } \Omega \times (0, T) \times D \right\}. \end{aligned}$$

The function φ_Q indicate some desired evolution for the tumor cells and φ_T stands for a desired final distribution of tumor cells (for example suitable for surgery). The first two terms of J are of standard tracking type, while the third term of J measures the size of the tumor at the end of the treatment. The fourth and fifth terms penalize large concentrations of the cytotoxic drugs through integral over the full space-time domain of the squared nutrient and drug concentrations.

The first result that we obtain concerns existence–uniqueness of solutions to the state system (1)–(5), and continuous dependence with respect to the controls. This allows to properly define the control-to-state map $S : (u, w) \mapsto \varphi$ and to rewrite the optimisation problem in a reduced form as

$$\min_{(u, w) \in \mathcal{U}} J(S(u, w), u, w).$$

The second issue that we analyse is existence of optimal controls: the idea is to use the direct method of calculus of variations. However, the lack of compactness in the probability space prevents from arguing straightforwardly as in the deterministic case: through stochastic compactness methods à la Gyöngy–Krylov, one is only able to restore strong compactness on an enlarged probability space. Since optimal controls are not generally unique, in the stochastic case one can only show existence of so-called relaxed optimal controls, meaning that the optimality condition has to be intended in distribution.

The third point that we investigate is the differentiability of the control-to-state map S and the analysis of the linearised system, which is formally obtained by

differentiating (1)–(5) with respect to the controls. We show that S is Gâteaux-differentiable with respect to suitable weak topologies, and that a first version of necessary conditions for optimality can be written in terms of a classical nonnegativity condition on $D(J \circ S)$.

Eventually, we characterise the derivative of S through the analysis of the adjoint system, and refine the first order conditions for optimality by employing the intrinsic adjoint variables only. The adjoint system is a backward-in-time system of SPDEs, and requires then the introduction of two additional variables in the spirit of martingale representation theorems: this reads

$$\begin{aligned} -d\pi - \Delta\tilde{\pi} dt + \psi''(\varphi)\tilde{\pi} dt &= h'(\varphi)(\mathcal{P}\sigma - a - \alpha u)\pi dt \\ &\quad - ch'(\varphi)\sigma\rho dt + \beta_1(\varphi - \varphi_Q) dt - \xi dW_1, \\ -d\rho - \Delta\rho dt + ch(\varphi)\rho dt + b\rho dt &= \mathcal{P}h(\varphi)\pi dt - \theta dW_2, \end{aligned}$$

where $\tilde{\pi} = -\Delta\pi$, complemented with homogeneous Neumann boundary conditions for π , $\tilde{\pi}$ and ρ , and with final conditions

$$\pi(T) = \beta_2(\varphi(T) - \varphi_T) + \frac{\beta_3}{2}, \quad \rho(T) = 0.$$

Due to the nonlinear nature of the problem and the backward setting, one is not able to tackle the stochastic adjoint system directly. To overcome this difficulty, we employ a duality argument: at a suitable approximate level, we show that a generalised version of the linearised system satisfies a duality relation with the corresponding approximation of the adjoint system. Consequently, showing uniform estimates on the linearised system with respect to arbitrary forcing terms allows us to transfer such uniform estimates on the adjoint system. This idea is very powerful and crucial in this situation, as it allows to prove uniform bounds on the adjoint system exclusively by duality, without tackling it directly. Our main and final result is then the well-posedness and the adjoint system in a suitable weak sense, and the final version of first-order conditions for optimality.

Theorem 1. *Let $(\bar{u}, \bar{w}) \in \mathcal{U}$ be an optimal control. Then it holds that*

$$\mathbb{E} \int_Q (\beta_4 \bar{u} - \alpha h(\bar{\varphi})\pi)(u - \bar{u}) + \mathbb{E} \int_Q (\beta_5 \bar{w} + b\rho)(w - \bar{w}) \geq 0 \quad \forall (u, w) \in \mathcal{U}.$$

The presence of stochastic perturbations is widely recognised as an essential feature of models for tumor growth. Further questions to be investigated concern, for example, optimisation of treatment time - which amounts to studying a related stochastic optimal stopping problem - and performing numerical simulations.

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A Variational Inequality for the Derivative of the Scalar Play Operator

MARTIN BROKATE

(joint work with Pavel Krejčí)

This contribution is based on the results obtained in [2].

The scalar stop operator \mathcal{S}_r arises as the solution operator $(u, z_0) \mapsto z$ of the rate-independent evolution variational inequality

$$(1a) \quad (\dot{u}(t) - \dot{z}(t))(z(t) - \zeta) \geq 0 \quad \forall \zeta \in Z, \quad \text{for a.e. } t \in (a, b),$$

$$(1b) \quad z(t) \in Z \quad \forall t \in [a, b], \quad z(a) = z_0,$$

with $Z = [-r, r]$, $r > 0$, $z_0 \in [-r, r]$. Its twin, the scalar play operator \mathcal{P}_r , is given by

$$\mathcal{P}_r[u; z_0] = u - \mathcal{S}_r[u; z_0].$$

The operators \mathcal{S}_r and \mathcal{P}_r are well-defined on $W^{1,1}(a, b) \times Z$ with values in $W^{1,1}(a, b)$ and can be extended to Lipschitz continuous operators from $C[a, b] \times Z$ to $C[a, b]$. They are not differentiable in the classical sense.

It has been shown in [1] that for $(u, z_0) \in C[a, b] \times Z$ the pointwise directional derivative

$$g(t) = \lim_{\lambda \downarrow 0} \frac{\mathcal{P}_r[u + \lambda h; z_0 + \lambda y_0](t) - \mathcal{P}_r[u; z_0](t)}{\lambda}, \quad t \in [a, b],$$

exists and belongs to $BV[a, b]$ for all directions (h, y_0) with $h \in C[a, b] \times BV[a, b]$ and $y_0 \in \mathbb{R}$. Moreover, g is the directional derivative of \mathcal{P}_r when the latter is viewed as an operator from $C[a, b] \times Z$ to $L^p(a, b)$ with $p \in [1, \infty)$.

Here we prove that g is the unique solution of a certain system of variational inequalities. More precisely, g is the unique solution in $BV[a, b]$ of the system

$$(2a) \quad g(a) = h(a) - \pi'(z_0; y_0),$$

$$(2b) \quad h(t) - g_+(t) \in K(t) \quad \forall t \in [a, b],$$

$$(2c) \quad \int_a^s (h(t) - g_+(t) - v(t)) dg(t) \geq 0 \quad \forall s \in (a, b], v \in G_K[a, s].$$

Moreover, $\text{var}(g) \leq \text{var}(h) + |y_0|$ and $g(t) \in \{g_+(t), g_-(t)\}$ for all $t \in [a, b]$.

We explain the variables and the notation used in (2).

The integral in (2c) is a Kurzweil-Stieltjes integral, see [3]. The expression $\pi'(z_0; y_0)$ stands for the directional derivative of the projection $\pi : \mathbb{R} \rightarrow Z$ at z_0 in the direction y_0 . By g_+ we denote the right limit of g defined by $g_+(b) = g(b)$ and

$$g_+(t) = \lim_{\tau \rightarrow t, \tau > t} g(\tau), \quad a \leq t < b.$$

The left limit g_- is defined analogously. The set $G_K[a, s]$ consists of all regulated functions $v : [a, s] \rightarrow \mathbb{R}$ with $v(t) \in K(t)$ for all $t \in [a, s]$.

The sets $K(t) \subset \mathbb{R}$, $t \in [a, b]$, depend on u by means of the behaviour of the trajectory $\{(w(t), z(t)) : t \in [a, b]\}$ with $w = \mathcal{P}_r[u; z_0]$ and $z = \mathcal{S}_r[u; z_0]$. They are

defined by

$$K(t) = \begin{cases} \mathbb{R}, & t \in A_1, \\ \mathbb{R}_-, & t \in A_2^+, \\ \mathbb{R}_+, & t \in A_2^-, \\ \{0\}, & t \in A_3, \end{cases}$$

where $\mathbb{R}_+ = [0, \infty)$ and $\mathbb{R}_- = (-\infty, 0]$. Here,

$$A_1 = \{t \in [a, b] : |z(t)| < r\},$$

$$A_2^+ = \{t \in [a, b] : z(t) = r, \exists \varepsilon > 0, w = w(t) \text{ on } [t, t + \varepsilon)\},$$

$$A_2^- = \{t \in [a, b] : z(t) = -r, \exists \varepsilon > 0, w = w(t) \text{ on } [t, t + \varepsilon)\},$$

$$A_2 = A_2^+ \cup A_2^-,$$

$$A_3 = \{t \in [a, b] : |z(t)| = r, \exists \varepsilon > 0, w \neq w(t) \text{ on } (t, t + \varepsilon)\}.$$

The definition of A_2^\pm is to be understood as $b \in A_2^\pm$ if $z(b) = \pm r$.

For the proofs, we refer to [2].

This result may be used in various contexts where scalar rate-independent evolutions appear and where generalized derivatives with respect to the forcing function are of interest. This includes in particular optimality conditions and stationarity systems for associated optimal control problems. The result also serves as a stepping stone for the study of directional derivatives in more general situations like

- vector-valued (finite or infinite dimensional) rate-independent evolutions (the interval $[-r, r]$ is replaced by a more general closed convex set Z),
- quasivariational evolution inequalities,
- evolutions including the Preisach operator (which can be represented by a one-parameter family of play operators).

These issues are currently under consideration.

Results of this type may also be of interest for the general class of rate-independent evolutions studied in [4], as the scalar play and stop operators represent one of the simplest cases of the evolutions discussed there.

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