P 1 Sparse controls (K. Kunisch, B. Vexler) $\rightarrow$ AO, NS

The focus in this project lies on the development of sparsity concepts in the context of optimal control and inverse (control-in-the-coefficients) problems governed by partial differential (PDEs). The interest in this topic is in part application-driven, including optimal actuator and sensor placement. To the other part it lies in the mathematically challenge. Measure-valued formulations and non-smooth structures naturally arise. They require tailored approaches from both the theoretical and algorithmic point of view.

State of the art. In [15], a framework for controls from the space of bounded Borel measures in the context of elliptic equations was introduced, which allows to formulate well-posed problems, where the support of the optimal control can be of measure zero. Based on this framework, further analytical and numerical results for linear elliptic [8], [24], parabolic [9], [14], [23], second order hyperbolic equations [20], as well as for nonlinear PDEs [10, 7] were obtained. Within the previous funding period the project 'Sparse Controls' significantly contributed to these developments (see the progress report for details). Another approach which leads to optimal controls supported on small sets (not of measures zero), is based on L^1 control cost terms with additional pointwise control constraints and/or an L^2 regularization terms. We refer to, e.g., [25, 28, 17, 13].

For the new funding period we proposes *three thesis topics* within this project. In the first one, optimal control problems with BV control costs are investigated. The other two topics belong to optimal experimental design for inverse problems involving PDEs. Here we seek for sparsity of design parameters, describing the optimal location of observers or actuators. These parameters must be chosen such that the modeling problems, which in our cases are inverse problems for PDEs are as 'well-posed' as possible.

With respect to the latter, we recall that inverse problems in general, and parameter estimation problems in particular, are ill-posed or ill-conditioned, and as a consequence small errors in the data can have a large effect on the numerically identified objects. This conditioning, however, depends on observers and estimators whose location is optimized by sparsity techniques. While this topic has received a considerable amount of attention in the case of ordinary differential equation, see e.g. [5, 6, 22], it has only recently attracted attention in the context of PDEs, see [1, 2, 3, 4].

First thesis project: *Sparse control with respect to a differential operator* to be supervised by Karl Kunisch. Here we focus on control costs which involve the semi-norm of first order spatial and/or temporal differential operators. Their use penalizes (directional) jumps and favors piecewise constant controls. This approach can be used to optimize for values $\bar{u}_j$ of piecewise constant control regimes. This can be desirable for technological applications, but is also of interest in its own right. As a starting point we consider

$$\begin{aligned} &\text{minimize } \frac{1}{2}\int_0^T\int_\Omega |y-z|^2\,dxdt + \beta\int_0^T\int_\Omega |Du|\,dxdt \\ &\text{subject to } y_t = Ay + Bu, \quad u \in K, \end{aligned} \tag{1}$$

together with initial and boundary conditions, and $\beta > 0$. Here $\int_0^T \int_\Omega |Du|\, dxdt$ denotes the BV semi-norm of the control u, A is an elliptic operator, B the control operator, and K is a convex, not necessarily bounded, set in $L^p((0,T)\times\Omega)$, with $p \geq 1$. The case of separable controls $u(t,x) = u_1(t)u_2(x)$ with one of the two controls u_i in BV and the other one in L^2 (or even in $M(\Omega)$) are equally important and so are the cases $u \in BV(\Omega, L^2(0,T))$ and $u \in L^2([0,T], BV(\Omega))$. But at first, the student must study the existence of solutions to (1), obtain the optimality system for (1), devise a finite element scheme for its approximation and an efficient semi-smooth Newton-type scheme for its numerical realization. This will also require to find a structure preserving regularization technique and to analyze its convergence. – The stationary case associated to (1) was briefly addressed in [15], where optimal solutions obtained numerically possess the expected characteristics with respect to sparsity. – Once the solution to (1) is numerically realized, averaged constant values $\bar{u}_j$ of the optimal controls in flat regions of the optimal controls can be obtained by a clustering algorithm.

These values can be used in a second stage which is given by

$$\begin{aligned} &\text{minimize } \frac{1}{2}\int_0^T \int_\Omega |y-z|^2\, dxdt + \beta \int_0^T \int_\Omega |Du(t,\cdot)|\, dt + \gamma \int_0^T \int_\Omega \Pi_j |u - \bar{u}_j|\, dxdt \\ &\text{subject to } y_t = Ay + Bu, \quad u \in K, \end{aligned} \tag{2}$$

with $\gamma > 0$. This formulation enhances the optimal controls to only take the predefined values $\bar{u}_j$, with few jumps between them. Problem (2) is related to the multibang formulation in [16], but differs due to the appearance of the BV-term. The latter also has an influence on the range of γ-values for which pure switching is expected.

Concerning FE approximations of variational problems in BV with P^0 and P^1 elements, we refer to [12] and [21], which consider this problem in the context of BV-regularized image reconstruction. In [12] it was pointed out that for the approximation with piecewise constant functions, the choice of the triangulation and the norm on $\mathbb{R}^n$ within the BV norm are of special importance.

To be successful with this and the two following thesis topics, the PhD candidates must have and will further develop skills in the following areas: PDEs, convex analysis, calculus of variations, numerical analysis and algorithm development.

Second thesis project: *Optimal sensor placement in the context of optimum experimental design in PDE models* to be supervised by Boris Vexler. For models described by ODEs or DAEs several optimization algorithms for optimal experimental design have been developed, see, e.g., [6]. Much less is known in the context of PDEs, see [2]. The main goal of this project is to propose a framework based on measure-valued sparse control formulations (see the description of the state of the art above) to find the optimal positions of pointwise measurement sensors.

To this end, we will consider elliptic equations abstractly denoted by $A(u,y) = f$ on the domain Ω for the state variable y depending on a finite dimensional parameter $u \in \mathbb{R}^n$ and some data f. The parameter variable u is involved, e.g., in the parametrization of the diffusion, reaction or convection coefficients. For each set of parameters u, the state equation is assumed to possess a unique solution $y = S(u)$ in the space of continuous functions $C_0(\Omega)$.

To estimate the unknown parameters u, we formulate a parameter estimation problem with pointwise measurements, the *lower level problem*:

$$\underset{(u,y)}{\text{minimize}}\ J(u) = \frac{1}{2}\left\langle (y-y_m)^2, \omega \right\rangle_{C_0(\Omega),M(\Omega)}, \quad \text{subject to } A(u,y) = f, \tag{L}$$

where $\omega \geq 0$ is in the space of regular Borel measures $M(\Omega) = C_0(\Omega)^*$. It describes the location of measurement sensors and y_m describes the corresponding measurements. The desired structure of ω is a linear combination of Dirac functionals

$$\omega = \sum_{i=1}^{N} \alpha_i \delta_{x_i}, \quad \alpha_i \geq 0, \tag{3}$$

where the optimal choice of the number N, the positions x_i and the coefficients α_i is not a priori known. Due to measurement errors, the solution to this optimization problem $\bar{u} = \bar{u}(\omega)$ for a fixed experimental design described by ω is only an approximation of the true parameter value. In order to improve the quality of this approximation we will formulate, analyze and solve a *design problem* or *upper level problem*, where the goal is to minimize the size of a confidence region $F(\bar{u}, \omega)$ around the estimated parameter $\bar{u}$.

We refer to, e.g., [6] for possible definitions of F corresponding to different optimality criteria based on the inverse of the Fisher information matrix $C(\bar{u}, \omega) \in \mathbb{R}^{n \times n}$, which is given here as

$$(C(\bar{u}, \omega))_{ij} = \langle S'(\bar{u})(e_i) S'(\bar{u})(e_j), \omega \rangle_{C_0(\Omega),M(\Omega)}.$$

In the above definition of $C(\bar{u}, \omega)$, $S'(\bar{u})(v)$ is the directional derivative of the solution operator S in the direction v and $e_i, e_j \in \mathbb{R}^n$ are unit vectors. To obtain the desired sparse structure of ω, the *design problem* will involve the total variation of the measure ω leading to

$$\underset{\omega \in M(\Omega), \omega \geq 0}{\text{minimize}}\ F(\bar{u}, \omega) + \alpha \|\omega\|_{M(\Omega)} \tag{U$_1$}$$

or

$$\underset{\omega \in M(\Omega), \omega \geq 0}{\text{minimize}}\ F(\bar{u}, \omega), \quad \text{subject to } \|\omega\|_{M(\Omega)} \leq \gamma. \tag{U$_2$}$$

We emphasize, that in the above formulated problems (U_1) and (U_2), the reference parameter $\bar{u}$ is fixed. Within an iterative approach used in the ODE or DAE case, see, e.g., [6], the problems (L) and (U_1) (or (U_2)) are solved in an alternating manner, i.e., the problem (L) is solved for a fixed experiment design ω_0 obtaining a parameter $\bar{u}_0$, then the problem (U_1) is solved with fixed $\bar{u}_0$ providing a new experiment design ω_1, etc. For this procedure, it is assumed, that the measurements y_m can be made available in the support of each iterate ω_k. In practice, this iterative approach involves new experiments (with new measurements) in each iteration.

In the first stage of the proposed project we will analyze problems (U_1) and (U_2) in this fashion, i.e., without back coupling to the problem (L). This means, we take $\bar{u}$ as a fixed solution of (L) for a given set of measurements. Note that the upper level problem (U_1) (or (U_2)) does not explicitly depend on the measurements y_m. For this stage the goals of the project are the following:

(a) to establish a proper function space framework for the optimum experimental design problem and to prove the existence of solutions to (U_1) and (U_2) as well as a relation between them. Uniqueness can in general not be expected, since the functional is convex but in general not strictly convex.

(b) to analyze the sparsity structure of the solution and to describe a set of general assumptions leading to the existence of an optimal design ω consisting of a finite number of Dirac functionals (3),

(c) to develop an appropriate structure-preserving regularization and efficient optimization algorithms based on semi-smooth Newton methods,

(d) to provide and to analyze a suitable finite element discretization including adaptivity.

In a second stage of the project, we aim at providing a fully coupled formulation leading to a two-level optimization problem. For this consideration we will first assume that the data y_m is known in the whole domain Ω. The corresponding problem will be non convex, and the iterative procedure described above is a fix-point strategy to solve this problem. Based on an appropriate regularization, we will work out a solution algorithm for the coupled problem and compare it to the fix-point strategy. A further direction can include a treatment of the uncertainty in y_m.

Third thesis project: *Optimal actuator placement in the context of inverse problems for PDE models* to be supervised by Karl Kunisch In the context of systems theory for ordinary differential equations, the choice of optimal input parameters has received a considerable amount of attention. We mention the highly noted early work [22], the thesis [5], and selected recent publications [1, 27, 26]. Very little attention has been paid so far to the problem of choosing optimal inputs for inverse problems in the context of PDEs. Here we are only aware of [19]. In all of these contributions the Fisher information matrix, involving the Jacobian of the output with respect to unknown parameters to be identified, plays a central role. In the context of nonlinear inverse problems - which is the case for parameter estimation problems - a choice must be made, where to evaluate the Jacobian. Ideally this would be done at the "optimal" parameters. Since they are unavailable, one typically resorts to educated initial guesses, [19, 22]. We propose to improve this procedure by formulating the optimal input problem as a bilevel optimization problem, while searching for optimal inputs with sparse support.

Let us consider the parameter dependent evolution equation

$$y_t + A(y,u) = f \text{ in } Q = (0,T) \times \Omega, \tag{4}$$

together with initial and boundary conditions, where for fixed $u \in \mathbb{R}^m$, the operator A is strongly elliptic with respect to the state variable y, and the inputs are chosen as $f \in \mathcal{M}(Q)$, the space of regular Borel measures in Q. The choices of directionally sparse inputs $f \in L^2(0,T;\mathcal{M}(\Omega))$, $f \in \mathcal{M}(\Omega; L^2(0,T))$ or $f \in \mathcal{M}(0,T;L(\Omega))$ are of equal importance. The a-priori unknown parameter vector u can stand, e.g., for the coefficient vector of a piecewise constant diffusion or convection coefficient $a = \sum_{i=1}^m u_i \chi_{\Omega_i}$, with χ_{Ω_i} the characteristic functions of a partition of Ω into subdomains Ω_i. Given data y_m, (for the sake of presentation here assumed to be distributed data in Q), the regularized least-squares formulation for the inverse problem of identifying u from y_m is given by

$$\min \frac{1}{2}\int_0^T \int_\Omega \frac{1}{\sigma^2}|y(u) - y_m|^2\,dxdt + \frac{\alpha}{2}\|u\|^2_{\mathbb{R}^m} \quad \text{over } u \in \mathbb{R}^m, \text{ subject to (4)}, \tag{LS}$$

where $\alpha > 0$ and σ^2 denotes the variation of the noise process. The conditioning of this inverse problem significantly depends on the choice of the input (forcing function) f.

For this purpose we introduce a sensitivity functional $\mathcal{F}(u, f)$, which typically involves the determinant, the trace, or the largest eigenvalue, of the inverse of the Fischer information matrix C, the latter implying that the maximal diameter of the asymptotic confidence ellipsoid of u is minimized, see e.g. [3, 4]. Here $C \in \mathbb{R}^{m\times m}$ is given by

$$C_{i,j} = \int_Q \frac{1}{\sigma^2} y_f'(\bar{u})(e_i)\, y_f'(\bar{u})(e_j)\, dxdt,$$

where $y_f'(\bar{u})(e_i)$ denotes the Fréchet derivative of the solution to (4) with respect to u at a reference parameter $\bar{u}$ in direction of the unit vector e_i. The subscript f emphasizes the dependence of the solution y on the forcing function f. Now we are prepared to formulate the optimal sparse input problem: for $\beta > 0$ solve

$$\min \mathcal{F}(\bar{u}, f) + \beta \|f\|_{\mathcal{M}(Q)} \text{ over } f \in \mathcal{M}(Q). \tag{OPT-IN}$$

The PhD student will first investigate (OPT-IN) for a fixed $\bar{u}$. If data y_m are available corresponding to a reference value of f then $\bar{u}$ can be chosen as a solution to (LS). The optimality conditions for (OPT-IN) will be derived and the desired sparsity structure of the solutions will be analyzed. Concerning diffusion equations with measure-valued forcing functions, the student can rely, in part, on recent results in [23, 11]. Subsequently a numerical scheme for solving (OPT-IN) must be developed and tested.

Subsequently, observing the fact that $\bar{u}$ is not available in general, a *bilevel optimization problem* will be investigated, consisting of the upper-level problem (OPT-IN) with $\bar{u}$ replaced by u and the lower level problem (LS). Here we assume availability of data y_m which correspond to different input parameters f. The bilevel problem will be investigated with respect to existence, first order necessary conditions, and the categorization of the resulting complementarity conditions [18]. Finally, first steps towards solving the bilevel problem numerically will be taken.

The proposed third project shares certain common technical aspects with the second project, but they are also sufficiently different: stationary/evolutionary, sparsity/directional sparsity, design parameters enter into output/input space.

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