NUMERICAL SOLUTION OF OPTIMAL CONTROL AND INVERSE PROBLEMS IN NON-REFLEXIVE BANACH SPACES

CUMULATIVE HABILITATION THESIS

Christian Clason

December 2012

Institute for Mathematics and Scientific Computing
Karl-Franzens-Universität Graz

CONTENTS

V   APPLICATIONS IN BIOMEDICAL IMAGING

PREFACE

Historically, variational problems such as those arising in optimal control and inverse problems were predominantly posed in Hilbert spaces. Although this is indeed the correct setting for many physical models (e.g., those involving energy terms), it is just as often simply due to convenience and numerical tractability, and a Banach space setting would be more natural. In addition, interest in total variation minimization, sparsity constraints and bang-bang control have lead to significant progress in the analysis of such problems over the last decade. Numerical approaches, on the other hand, still tend to focus on either finite-dimensional (e.g., discretized) problems or those set in reflexive Banach spaces such as L^p, $1 < p < \infty$, due to their better differentiability properties. Hence, the motivation for this work, and its main contribution, is the development of efficient numerical algorithms for optimization problems in non-reflexive Banach spaces such as L^1 and L^∞. The main difficulty to overcome, apart from the non-standard functional-analytic setting, is the non-differentiability inherent in their formulation.

The problems treated here can be grouped as follows.

- *Optimal control problems in measure spaces.* These arise from control problems with sparsity constraints, which in finite dimensions can be enforced by ℓ^1 penalties. The corresponding infinite-dimensional problem, however, is not well-posed in L^1 due to the lack of weak compactness, and needs to be considered in spaces of Radon measures. Included here are also control problems in the space of functions of bounded variation (i.e., whose distributional gradient is a Radon measure), which can be used to promote piecewise constant controls.

- *Optimal control problems with L^∞ functionals.* The works in this group are concerned with problems with either tracking terms in L^∞, which correspond to minimizing the worst-case deviation from the target, or control costs in L^∞, which lead to bang-bang controls.

- *Inverse problems with nonsmooth discrepancy terms.* The standard L^2 data fitting term is statistically motivated by the assumption of Gaussian noise. For non-Gaussian noise, however, other data fitting terms turn out to be more appropriate. For impulsive noise (e.g., salt-and-pepper noise in digital imaging), L^1 fitting is more robust. Uniform noise (e.g., quantization errors) leads to L^∞ fitting.

- *Applications in biomedical imaging.* This group contains two examples from interdisciplinary cooperations where the non-reflexive Banach spaces considered above occur in applications. The first example demonstrates that the Radon measure space setting can be used to solve the problem of optimal placement of discrete light sources for the homogeneous illumination of tissue in optical tomography. The second example addresses an inverse problem in image reconstruction in magnetic resonance imaging using penalities of total variation-type.

For the numerical solution, Newton-type methods in function space are preferred due to their superlinear convergence and mesh independence. To apply these in spite of the lack of differentiability of the problems, a common approach is followed:

1. Using convex analysis (in particular, Fenchel duality) or a relaxation technique (or both), the original problem is transformed into a differentiable problem subject to pointwise constraints. Standard techniques (e.g, Maurer–Zowe-type conditions) then allow derivation of first order optimality conditions.

2. Due to the nonsmoothness of the original problem, these optimality systems are typically not sufficiently smooth to be solved by a Newton-type method. We therefore introduce a family of approximations that are amenable to such methods while avoiding unnecessary smoothing.

3. The resulting regularized optimality conditions lead to semismooth operator equations in function spaces, which can be solved using a semismooth Newton method. To deal with the local convergence of Newton-type methods, the Newton method is combined with a continuation strategy in the regularization parameter. In practice, this results in a globalization effect.

This thesis is organized as follows. Part I contains a summary of the submitted papers. It begins with a chapter collecting common background on partial differential equations with measure data, convex analysis, and semismooth Newton methods; the following chapters then summarize in turn the precise setting and the main results for each of the above groups. The purpose, besides introducing a consistent notation and terminology, is to motivate the appearing concepts and to illustrate their connections. Hence, some derivations and calculations are sketched, while formal statements of theorems and proofs are omitted; the reader is instead referred to the cited literature and to the full discussions in the corresponding chapters of the remaining parts. It should be pointed out that achieving a consistent notation and terminology in this part requires deviating, at times significantly, from that used in the original papers which make up Parts II–V of the thesis.

ACKNOWLEDGMENTS

Graz, September 2012

LIST OF PUBLICATIONS

This thesis consists of the following publications (in chronological order of submission), which have been retypeset from the original sources. Besides unifying the layout and the bibliography and correcting typos, no changes have been made.

C. Clason and K. Kunisch (2011). *A duality-based approach to elliptic control problems in non-reflexive Banach spaces*. ESAIM: Control, Optimisation and Calculus of Variations 17.1, pp. 243–266. DOI: 10.1051/cocv/2010003.

C. Clason, B. Jin, and K. Kunisch (2010). *A semismooth Newton method for L^1 data fitting with automatic choice of regularization parameters and noise calibration*. SIAM Journal on Imaging Sciences 3.2, pp. 199–231. DOI: 10.1137/090758003.

C. Clason, K. Ito, and K. Kunisch (2010). *Minimal invasion: An optimal L^∞ state constraint problem*. ESAIM: Math. Model. Numer. Anal. 45.3, pp. 505–522. DOI: 10.1051/m2an/2010064.

C. Clason and B. Jin (2012). *A semismooth Newton method for nonlinear parameter identification problems with impulsive noise*. SIAM Journal on Imaging Sciences 5, pp. 505–536. DOI: 10.1137/110826187.

F. Knoll, C. Clason, K. Bredies, M. Uecker, and R. Stollberger (2012). *Parallel imaging with nonlinear reconstruction using variational penalties*. Magnetic Resonance in Medicine 67.1, pp. 34–41. DOI: 10.1002/mrm.22964.

C. Clason, K. Ito, and K. Kunisch (2012). *A minimum effort optimal control problem for elliptic PDEs*. ESAIM: Mathematical Modelling and Numerical Analysis 46.4, pp. 911–927. DOI: 10.1051/m2an/2011074.

C. Clason and K. Kunisch (2012). *A measure space approach to optimal source placement*. Computational Optimization and Applications 53.1, pp. 155–171. DOI: 10.1007/s10589-011-9444-9.

E. Casas, C. Clason, and K. Kunisch (2012b). *Approximation of elliptic control problems in measure spaces with sparse solutions*. SIAM Journal on Control and Optimization 50.4, pp. 1735–1752. DOI: 10.1137/110843216.

C. Clason (2012). *L^∞ fitting for inverse problems with uniform noise*. Inverse Problems 28, p. 104007. DOI: 10.1088/0266-5611/28/10/104007.

E. Casas, C. Clason, and K. Kunisch (2012a). *Parabolic control problems in measure spaces with sparse solutions*. SIAM Journal on Control and Optimization. To appear.

P. Brunner, C. Clason, M. Freiberger, and H. Scharfetter (2012). *A deterministic approach to the adapted optode placement for illumination of highly scattering tissue*. Biomedical Optics Express 3.7, pp. 1732–1743. DOI: 10.1364/BOE.3.001732.

In addition, the following publications were written after the completion of the author's PhD degree in 2006.

C. Clason, B. Kaltenbacher, and S. Veljović (2009). *Boundary optimal control of the Westervelt and the Kuznetsov equation*. Journal of Mathematical Analysis and Applications 356.2, pp. 738–751. DOI: 10.1016/j.jmaa.2009.03.043.

S. Keeling, C. Clason, M. Hintermüller, F. Knoll, A. Laurain, and G. von Winckel (2012). *An image space approach to Cartesian based parallel MR imaging with total variation regularization*. Medical Image Analysis 16.1, pp. 189–200. DOI: 10.1016/j.media.2011.07.002.

F. Bauer and C. Clason (2011). *On theoretical limits in parallel magnetic resonance imaging*. International Journal of Tomography & Statistics 18.F11, pp. 10–23.

C. Clason and P. Hepperger (2009). *A forward approach to numerical data assimilation*. SIAM Journal on Scientific Computing 31.4, pp. 3090–3115. DOI: 10.1137/090746240.

F. Knoll, C. Clason, C. Diwoky, and R. Stollberger (2011). *Adapted random sampling patterns for accelerated MRI*. Magnetic Resonance Materials in Physics, Biology and Medicine (MAGMA) 24.1, pp. 43–50. DOI: 10.1007/s10334-010-0234-7.

M. Freiberger, C. Clason, and H. Scharfetter (2010a). *Adaptation and focusing of optode configurations for fluorescence optical tomography by experimental design methods*. Journal of Biomedical Optics 15.1, 016024, p. 016024. DOI: 10.1117/1.3316405.

F. Knoll, M. Unger, C. Clason, C. Diwoky, T. Pock, and R. Stollberger (2010). *Fast reduction of undersampling artifacts in radial MR angiography with 3D total variation on graphics hardware*. Magnetic Resonance Materials in Physics, Biology and Medicine (MAGMA) 23.2, pp. 103–114. DOI: 10.1007/s10334-010-0207-x.

C. Clason and G. von Winckel (2010). *On a bilinear optimization problem in parallel magnetic resonance imaging*. Applied Mathematics and Computation 216.4, pp. 1443–1452. DOI: 10.1016/j.amc.2010.02.047.

C. Clason, B. Jin, and K. Kunisch (2010). *A duality-based splitting method for ℓ^1–TV image restoration with automatic regularization parameter choice*. SIAM Journal on Scientific Computing 32.3, pp. 1484–1505. DOI: 10.1137/090768217.

M. Freiberger, C. Clason, and H. Scharfetter (2010b). *Total variation regularization for nonlinear fluorescence tomography with an augmented Lagrangian splitting approach*. Applied Optics 49.19. Selected for Virtual Journal for Biomedical Optics, Volume 5, Issue 11, pp. 3741–3747. DOI: 10.1364/AO.49.003741.

C. Clason and G. von Winckel (2012). *A general spectral method for the numerical simulation of one-dimensional interacting fermions*. Computer Physics Communications 183.2. Code published in *CPC Program Library* as AEKO_v1_1, pp. 405–417. DOI: 10.1016/j.cpc.2011.10.005.

C. Clason and B. Kaltenbacher (2013). *On the use of state constraints in optimal control of singular PDEs*. Systems & Control Letters 62.1, pp. 48–54. DOI: 10.1016/j.sysconle.2012.10.006.

A complete and up-to-date list of publications, including preprints and – where applicable – Matlab and Python code, can be found online at

http://www.uni-graz.at/~clason/publications.html.

Part I

SUMMARY

BACKGROUND

The purpose of this chapter is to collect the definitions and results on measure spaces, convex analysis and semismooth Newton methods that form the common basis for the results described in the remaining chapters, and to motivate the approach followed there.

1.1 MEASURE SPACES

We begin by giving some elementary definitions of dual spaces and operators, which serve to fix a common notation. In particular, we define spaces of Radon measures as dual spaces of continuous functions and discuss the well-posedness of partial differential equations with measures on the right hand side.

1.1.1 WEAK TOPOLOGIES

For a normed vector space V, we denote by V^* the topological dual of V. Note that this definition depends on the choice of the topology, specified via the *duality pairing* $\langle \cdot, \cdot \rangle_{V,V^*}$ between V and V^* (i.e., $(V, V^*, \langle \cdot, \cdot \rangle_{V,V^*})$ is a *dual pair*; see, e.g., [Werner 2011, Chapter VIII.3]). This fact that will play an important role in this work. The topological dual V^* is always a Banach space if equipped with the norm

$$\|v^*\|_{V^*} = \sup \left\{ \langle v, v^* \rangle_{V,V^*} : v \in V, \|v\|_V \leqslant 1 \right\}.$$

For non-reflexive spaces, two different topologies are of particular relevance.

(i) The *weak topology* corresponds to the duality pairing between V and V^* defined by

$$\langle v, v^* \rangle_{V,V^*} := v^*(v)$$

for all $v \in V$ and $v^* \in V^*$. In this case, V^* can be identified via the Hahn–Banach theorem with the space of all continuous linear forms on V, and the topological dual

coincides with the standard definitions. For example, the weak topological dual of $L^1(\Omega)$ can be identified with $L^\infty(\Omega)$, with the duality pairing reducing to

$$\langle v, v^* \rangle_{L^1, L^\infty} = \int_\Omega v(x) v^*(x) \, dx,$$

see, e.g., [Brezis 2010, Theorem 4.14]. If not specified otherwise, the topological dual is to be understood with respect to the weak topology.

(ii) If V^* is the weak topological dual of V, the duality pairing between V^* and V is defined by

$$\langle v^*, v \rangle_{V^*, V} := v^*(v)$$

for all $v^* \in V^*$ and $v \in V$. This allows identifying the *weak-⋆ topological dual* (or *predual*) of V^* with V (i.e, the weak-⋆ dual of $L^\infty(\Omega)$ is $L^1(\Omega)$).

(For reflexive Banach spaces, of course, both notions coincide.)

For a linear operator $A : X \to Y$ between the normed vector spaces X and Y, we call $A^* : Y^* \to X^*$ the *adjoint operator* to A if

$$\langle x, A^* y^* \rangle_{X, X^*} = \langle Ax, y^* \rangle_{Y, Y^*}$$

for all $x \in X$ and $y^* \in Y^*$. If the duality is taken with respect to the weak topology, this coincides again with the standard definition. On the other hand, if there exists $B : Y \to X$ such that $B^* = A$ with respect to the weak topology, we can identify the *weak-⋆ adjoint* (or *preadjoint*) A^* of an operator $A : X^* \to Y^*$ with B, since

$$\langle x^*, By \rangle_{X^*, X} = \langle Ax^*, y \rangle_{Y^*, Y}$$

for all $x^* \in X^*$ and $y \in Y$.

1.1.2 SPACE OF RADON MEASURES

Let $\mathcal{M}(X)$ denote the vector space of all bounded Borel measures on $X \subset \mathbb{R}^n$, that is of all bounded σ-additive set functions $\mu : \mathcal{B}(X) \to \mathbb{R}$ defined on the Borel algebra $\mathcal{B}(X)$ satisfying $\mu(\emptyset) = 0$. The *total variation* of $\mu \in \mathcal{M}(X)$ is defined for all $B \in \mathcal{B}(\Omega)$ as

$$|\mu|(B) := \sup \left\{ \sum_{i=0}^\infty |\mu(B_i)| : \bigcup_{i=0}^\infty B_i = B \right\},$$

where the supremum is taken over all partitions of B. We recall that every Radon measure μ has a unique *Jordan decomposition* $\mu = \mu^+ - \mu^-$ into two positive measures (i.e., $\mu^+(B), \mu^-(B) \geqslant 0$ for all Borel sets B). The *support* $\mathrm{supp}(\mu)$ of a Radon measure μ is defined as the complement of the union of all open null sets with respect to μ.

By the Riesz representation theorem, $\mathcal{M}(X)$ can be identified with the dual of spaces of continuous functions on X, endowed with the norm $\|v\|_C = \sup_{x \in X} |v(x)|$. Based on the boundary behavior of the continuous functions, we discern three cases.

(i) Let $C_0(\Omega)$ be the completion of the space of all continuous functions with compact support in the simply connected domain $\Omega \subset \mathbb{R}^n$ with respect to the norm $\|v\|_C$, i.e, the space of all functions vanishing on the boundary $\partial\Omega$ (or at infinity if Ω is unbounded). In this case, we set $X = \Omega$ and have from [Elstrodt 2005, Satz VIII.2.26] that the weak topological dual of $C_0(\Omega)$ can be isometrically identified with $\mathcal{M}(\Omega)$.

(ii) If Ω is bounded, $\overline{\Omega}$ is compact, and we can identify $\mathcal{M}(\overline{\Omega})$ with the weak topological dual of the space $C(\overline{\Omega})$ of continuous functions that can be continuously extended to the boundary of Ω; see, e.g., [Dunford and Schwartz 1988, Theorem IV.6.3].

(iii) If the functions vanish only on an open part Γ of the boundary, we set $X = \overline{\Omega} \setminus \Gamma$. Then, X is compact, and we can apply the same argument as in case (ii) to deduce that the weak topological dual of $C_\Gamma(\overline{\Omega}) := \{v \in C(\overline{\Omega}) : v|_\Gamma = 0\}$ can be identified with the space $\mathcal{M}_\Gamma(\overline{\Omega}) := \{\mu \in \mathcal{M}(\overline{\Omega}) : \mu(\Gamma) = 0\}$.

For the sake of presentation, we will restrict the discussion to the first case; however, all results hold for the other two cases as well (with obvious modifications regarding the boundary behavior). The Riesz representation theorem leads to the equivalent characterization

$$(1.1.1) \qquad \|\mu\|_{\mathcal{M}} = \sup \left\{ \int_\Omega v \, d\mu : v \in C_0(\Omega), \|v\|_{C_0} \leqslant 1 \right\}.$$

In particular, this makes $\mathcal{M}(\Omega)$ a Banach space. For the purposes of dual pairings, we will always equip $\mathcal{M}(\Omega)$ with the weak-$\star$ topology, with respect to which $\|\cdot\|_{\mathcal{M}}$ is lower semicontinuous.

With the formalism of section 1.1.1, this allows identifying the weak-$\star$ dual of $\mathcal{M}(\Omega)$ with $C_0(\Omega)$, corresponding to the duality pairing

$$\langle \mu, v \rangle_{\mathcal{M}, C} = \int_\Omega v \, d\mu.$$

Note that (1.1.1) allows us to isometrically identify $L^1(\Omega)$ with a subspace of $\mathcal{M}(\Omega)$, such that $\|u\|_{\mathcal{M}} = \|u\|_{L^1}$ for all $u \in L^1(\Omega)$; see, e.g., [Brezis 2010, Chapter 4.5.3]. In addition, the Rellich–Kondrachov theorem yields that $W_0^{1,q}(\Omega) \hookrightarrow C_0(\Omega)$ for $q > n$, and this embedding is dense and compact. Hence we have the dense and compact embedding

$$\mathcal{M}(\Omega) \hookrightarrow W_0^{1,q}(\Omega)^* = W^{-1,q'}(\Omega)$$

for $1 < q' < \frac{n}{n-1}$. We will make use of this embedding to show well-posedness of partial differential equations with measure right hand sides.

For time-dependent measure-valued functions, the situation is slightly more delicate. Associated to the interval $(0, T)$ we define the space $L^2(0, T; C_0(\Omega))$ of measurable functions $z : (0, T) \to C_0(\Omega)$ for which the associated norm given by

$$\|z\|_{L^2(C_0)} := \left(\int_0^T \|z(t)\|_{C_0}^2 \, dt \right)^{1/2}$$

is finite. Due to the fact that $C_0(\Omega)$ is a separable Banach space, $L^2(0, T; C_0(\Omega))$ is also a separable Banach space; see, e.g., [Warga 1972, Theorem I.5.18]. Let $L^2(0, T; \mathcal{M}(\Omega))$ denote the space of weakly measurable functions $u : [0, T] \to \mathcal{M}(\Omega)$ for which the norm

$$\|u\|_{L^2(\mathcal{M})} = \left(\int_0^T \|u(t)\|_{\mathcal{M}}^2 \, dt \right)^{1/2}$$

is finite. This choice makes $L^2(0, T; \mathcal{M}(\Omega))$ a Banach space and guarantees that it can be identified with the weak topological dual of $L^2(0, T; C_0(\Omega))$, where the duality relation is given by

$$\langle z, u \rangle_{L^2(C_0), L^2(\mathcal{M})} = \int_0^T \langle z(t), u(t) \rangle_{C_0, \mathcal{M}} \, dt,$$

with $\langle \cdot, \cdot \rangle_{C_0, \mathcal{M}}$ denoting the duality pairing between $C_0(\Omega)$ and $\mathcal{M}(\Omega)$; see [Edwards 1965, Theorem 8.20.3]. Vice versa, $L^2(0, T; C_0(\Omega))$ can be seen as the weak-$\star$ dual of $L^2(0, T; \mathcal{M}(\Omega))$.

Finally, we recall that $BV(\Omega)$, the space of functions of bounded variation, consists of all $u \in L^1(\Omega)$ for which the distributional gradient Du belongs to $(\mathcal{M}(\Omega))^n$. Furthermore, the mapping $u \mapsto \|u\|_{BV}$,

$$(1.1.2) \quad \|u\|_{BV} := \int_\Omega |Du| \, dx = \sup \left\{ \int_\Omega u(-\operatorname{div} v) \, dx : v \in (C_0^\infty(\Omega))^n, \, \|v\|_{(C_0)^n} \leqslant 1 \right\}$$

(which can be infinite) is lower semicontinuous in the topology of $L^1(\Omega)$, and $u \in L^1(\Omega)$ is in $BV(\Omega)$ if and only if $\|u\|_{BV}$ is finite. In this case $\|\cdot\|_{BV}$ is referred to as the *total variation seminorm*. (If $v \in H^1(\Omega)$, then $\|u\|_{BV} = \int_\Omega |\nabla u| \, dx$.) Endowed with the norm $\|\cdot\|_{L^1} + \|\cdot\|_{BV}$, $BV(\Omega)$ is a (non-reflexive) Banach space; see, e.g., [Attouch, Buttazzo, and Michaille 2006, Chapter 10.1].

1.1.3 PARTIAL DIFFERENTIAL EQUATIONS WITH MEASURE DATA

Measure-valued right hand sides or boundary conditions in partial differential equations have attracted recent interest due to their role in the adjoint equation for optimal control problems with pointwise state constraints (see, e.g., [Casas 1986; Alibert and Raymond 1997]), although measure-valued right hand sides have already been treated in [Stampacchia 1965] in the context of the Green's function of the Dirichlet problem for an elliptic operator with

discontinuous coefficients. Correspondingly, several different solution concepts have been introduced in [Stampacchia 1965; Boccardo and Gallouët 1989; Casas 1986; Alibert and Raymond 1997]. All of these are fundamentally based on a duality technique, and have been shown to coincide; see [Meyer, Panizzi, and Schiela 2011]. Here, we follow [Casas 1986].

We first discuss elliptic problems. Consider the operator

$$Ay = - \sum_{j,k=1}^{n} \partial_j (a_{jk}(x) \partial_k y + d_j(x) y) + \sum_{j=1}^{n} b_j(x) \partial_j y + d(x) y,$$

and for $\mu \in \mathcal{M}(\Omega)$ the abstract Dirichlet problem

$$(1.1.3) \qquad \begin{cases} Ay = \mu, & \text{in } \Omega, \\ y = 0, & \text{on } \partial \Omega. \end{cases}$$

We call $y \in L^1(\Omega)$ a *very weak solution* of (1.1.3) if

$$\int_\Omega y A^* z \, dx = \int_\Omega z \, d\mu \qquad \text{for all } z \in H^2(\Omega) \cap H_0^1(\Omega),$$

where A^* is the (weak) adjoint of A. Here, we shall for simplicity assume that A^* has maximal regularity as an operator from $W_0^{1,q}(\Omega)$ to $W^{-1,q}(\Omega)$ for $q > n$, which is the case if $a_{jk}, b_j \in C^{0,\delta}(\overline{\Omega})$ for some $\delta \in (0,1)$; A is uniformly elliptic; $d_j, d \in L^\infty(\Omega)$; the lower order coefficients are small enough (see, e.g., [Gilbarg and Trudinger 2001, Th. 8.3]); and $\partial \Omega$ is of class $C^{1,1}$, or Ω is a parallelepiped; see, e.g., [Ladyzhenskaya and Ural'tseva 1968, pp. 169–189] and [Troianiello 1987, Th. 2.24]. If not otherwise specified, any elliptic operator A mentioned in the following is assumed to satisfy these requirements. Under these conditions, A^* is an isomorphism from $W_0^{1,q}(\Omega)$ to $W^{-1,q}(\Omega)$, and the closed range theorem together with reflexivity of these spaces implies that A is an isomorphism from $W_0^{1,q'}(\Omega)$ to $W^{-1,q'}(\Omega)$ for $q' < \frac{n}{n-1}$. Hence by the continuous embedding $\mathcal{M}(\Omega) \hookrightarrow W^{-1,q'}(\Omega)$, problem (1.1.3) admits a unique solution $y \in W_0^{1,q'}(\Omega)$ satisfying

$$\|y\|_{W^{1,q'}} \leqslant C \|\mu\|_{\mathcal{M}}$$

for a constant C independent of μ. In this case, y also solves (1.1.3) in the usual weak sense. Note that this approach ensures the existence of a weak-$\star$ adjoint of A, which can be identified with A^*; and similarly for A^{-1} and $(A^*)^{-1}$. Furthermore, the compactness of the embedding $\mathcal{M}(\Omega) \hookrightarrow W^{-1,q'}(\Omega)$ yields that for any sequence μ_k converging weakly-$\star$ in $\mathcal{M}(\Omega)$ to μ, the sequence of corresponding solutions y_k converges strongly in $W_0^{1,q'}(\Omega)$ to y.

If A^* does not enjoy maximal regularity, we still have existence of a solution $y \in W^{1,q'}(\Omega)$ to (1.1.3), but uniqueness in $W^{1,q'}(\Omega)$ requires (one of several equivalent) additional assumptions (such as y being the limit of a sequence of regularized problems or satisfying an integration by parts formula). We refer to [Meyer, Panizzi, and Schiela 2011] for details.

The case of measure-valued boundary data or parabolic equations can be treated in an analogous fashion; see, e.g., [Casas 1993] and [Casas 1997], respectively. Finally, we note that by the chain of continuous embeddings $BV(\Omega) \hookrightarrow L^1(\Omega) \hookrightarrow \mathcal{M}(\Omega)$, we can apply the above results to $\mu \in BV(\Omega)$ as well.

1.2 CONVEX ANALYSIS

The task of finding a minimizer u of a Fréchet differentiable functional J can often be reduced to solving the first order necessary optimality conditions $J'(u) = 0$, which is sometimes referred to as *Fermat's principle*. If J is non-differentiable but convex, as is mostly the case in this work, the convex subdifferential replaces the nonexistant Fréchet derivative, as it satisfies Fermat's principle and allows for a rich calculus – in particular Fenchel duality – that can be used to obtain explicit optimality conditions. The classical reference in the context of this work is [Ekeland and Témam 1999], while [Attouch, Buttazzo, and Michaille 2006, Chapter 9] contains a readable and complete overview. A rigorous and extensive treatment can be found in the excellent textbook [Schirotzek 2007], which we follow here.

1.2.1 CONVEX CONJUGATES

Here and below, let V again be a normed vector space. Recall that a function $f : V \to \bar{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ is called *convex* if

$$f(\lambda v_1 + (1 - \lambda)v_2) \leqslant \lambda f(v_1) + (1 - \lambda)f(v_2)$$

for all $v_1, v_2 \in V$ and $\lambda \in (0, 1)$, and *proper* if f is not identically equal to $+\infty$. For example, the *indicator function* δ_C of a nonempty, convex set $C \subset V$, defined by

$$\delta_C(v) := \begin{cases} 0 & \text{if } v \in C, \\ \infty & \text{otherwise,} \end{cases}$$

is convex and proper. This function will appear frequently in the following.

As we will see, one reason for the usefulness of convex subdifferentials in our context is their connection with the Legendre–Fenchel transform. For a function $f : V \to \bar{\mathbb{R}}$, the *Fenchel conjugate* (or *convex conjugate*) is defined as

$$(1.2.1) \qquad f^* : V^* \to \bar{\mathbb{R}}, \qquad f^*(v^*) = \sup_{v \in V} \langle v, v^* \rangle_{V, V^*} - f(v).$$

The convex conjugate is always convex and lower semicontinuous. If f is convex and proper, then f^* is proper as well; see, e.g., [Schirotzek 2007, Proposition 2.2.3]. We also introduce the *biconjugate* of f, defined as

$$f^{**} : V \to \bar{\mathbb{R}}, \qquad f^{**}(v) = \sup_{v^* \in V^*} \langle v^*, v \rangle_{V^*, V} - f^*(v^*)$$

(i.e., if V^* is the weak dual of V, we take V as the weak-$\star$ dual of V^* (or vice versa) and set $f^{**} = (f^*)^*$). If f is proper, the Fenchel–Moreau–Rockafellar theorem states that $f^{**} = f$ if and only if f is convex and lower semicontinuous; see, e.g., [Schirotzek 2007, Theorem 2.2.4].

We give a few relevant examples; see [Schirotzek 2007, Examples 2.2.2, 2.2.5, and 2.2.6].

(i) Let $V = L^2(\Omega)$ and $f(v) = \frac{1}{2} \|v\|_{L^2}^2$. We identify V^* with V (i.e., the duality pairing is the inner product in $L^2(\Omega)$). Then, the function to be maximized in (1.2.1) is strictly concave and differentiable, so that the supremum is attained if and only if $v^* = f'(v) = v$. Inserting this into the definition and simplifying, we obtain

$$f^* : L^2(\Omega) \to \mathbb{R}, \qquad f^*(v^*) = \frac{1}{2} \|v^*\|_{L^2}^2 .$$

(ii) Let V be a normed vector space and $f(v) = \delta_{B_V}(v)$, where B_V is the unit ball with respect to the norm $\|\cdot\|_V$. We take V^* as the weak (or weak-$\star$) dual of V and compute $f^*(v^*)$ for $v^* \in V^*$:

$$\delta_{B_V}^*(v^*) = \sup_{v \in V} \langle v, v^* \rangle_{V,V^*} - \delta_{B_V}(v) = \sup_{\|v\|_V \leqslant 1} \langle v, v^* \rangle_{V,V^*} = \|v^*\|_{V^*} .$$

(iii) Let V be as above, V^* its weak topological dual and $f(v) = \|v\|_v$. We compute $f^*(v^*)$ for given $v^* \in V^*$ by discerning two cases:

a) $\|v^*\|_{V^*} \leqslant 1$. In this case, $\langle v, v^* \rangle_{V,V^*} \leqslant \|v\|_V \|v^*\|_{V^*} \leqslant \|v\|_V$ for all $v \in V$ and $\langle 0, v^* \rangle_{V,V^*} = 0 = \|0\|_V$. Hence,

$$f^*(v^*) = \sup_{v \in V} \langle v, v^* \rangle_{V,V^*} - \|v\|_V = 0.$$

b) $\|v^*\|_{V^*} > 1$. Then by the definition of the dual norm, there exists a $v_0 \in V$ with $\langle v_0, v^* \rangle_{V,V^*} > \|v_0\|_V$. Taking $\rho \to \infty$ in

$$0 < \rho \left(\langle v_0, v^* \rangle_{V,V^*} - \|v_0\|_V \right) = \langle \rho v_0, v^* \rangle_{V,V^*} - \|\rho v_0\|_V \leqslant f^*(v^*)$$

yields $f^*(v^*) = +\infty$.

We conclude that $f^* = \delta_{B_{V^*}}$.

If we take the dual with respect to the weak-$\star$ topology between V^* and V, this result also follows directly from the Fenchel–Moreau–Rockafellar theorem and example (ii) by noting that

$$\delta_{B_V}(v) = \delta_{B_V}^{**}(v) = \sup_{v^* \in V^*} \langle v, v^* \rangle_{V,V^*} - \delta_{B_V}^*(v^*)$$

$$= \sup_{v^* \in V^*} \langle v^*, v \rangle_{V^*,V} - \|v^*\|_{V^*} = f^*(v)$$

for all $v \in V$.

Furthermore, straightforward calculation yields the following useful transformation rules; see, e.g., [Ekeland and Témam 1999, page 17]. For $f : V \to \bar{\mathbb{R}}$, we have for all $\alpha \in \mathbb{R}$ and $a \in V$ that

$$(1.2.2) \qquad (\alpha f(\cdot))^*(v^*) = \alpha f^*(\alpha^{-1} v^*),$$

$$(1.2.3) \qquad f(\cdot - a)^*(v^*) = f^*(v^*) + \langle a, v^* \rangle_{V,V^*}.$$

In particular, the above yields for every $\alpha > 0$

$$(1.2.4) \qquad (\alpha \|\cdot\|_{L^1})^*(v^*) = \delta_{B_{L^\infty}}(\alpha^{-1} v^*) = \begin{cases} 0 & \text{if } |v^*(x)| \leqslant \alpha \text{ for almost all } x \in \Omega, \\ \infty & \text{otherwise.} \end{cases}$$

On the other hand, applying the same to $V^* = \mathcal{M}(\Omega)$ and its weak-$\star$ dual $V = C_0(\Omega)$, we obtain

$$(1.2.5) \qquad (\alpha \|\cdot\|_{\mathcal{M}})^*(v) = \delta_{B_{C_0}}(\alpha^{-1} v) = \begin{cases} 0 & \text{if } |v(x)| \leqslant \alpha \text{ for all } x \in \Omega, \\ \infty & \text{otherwise.} \end{cases}$$

We will make use of this duality to pass from problems involving these nonsmooth norms to smooth problems with pointwise constraints.

1.2.2 CONVEX SUBDIFFERENTIALS

Let $f : V \to \bar{\mathbb{R}}$ be convex and proper, and let $\bar{v} \in V$ with $f(\bar{v}) < \infty$. The set

$$(1.2.6) \qquad \partial f(\bar{v}) := \{v^* \in V^* : \langle v - \bar{v}, v^* \rangle_{V,V^*} \leqslant f(v) - f(\bar{v}) \text{ for all } v \in V\}$$

is called *subdifferential* of f at $\bar{v}$. Every $v^* \in \partial f(\bar{v})$ is called *subgradient* of f at $\bar{v}$. From the definition (1.2.6), we immediately obtain Fermat's principle for convex functions: The point $\bar{v}$ is a minimizer of f if and only if $f(\bar{v}) \leqslant f(v)$ for all $v \in V$, which is equivalent to $0 \in \partial f(\bar{v})$.

The convex subdifferential satisfies the following sum rule. Let $f_1, f_2 : V \to \bar{\mathbb{R}}$ be convex and proper. If there exists a point $\bar{v} \in V$ such that $f_1(\bar{v}), f_2(\bar{v}) < \infty$ and f_2 is continuous at $\bar{v}$, then

$$(1.2.7) \qquad \partial(f_1 + f_2)(v) = \partial f_1(v) + \partial f_2(v)$$

for all $v \in V$ for which f_1 and f_2 are finite; see, e.g, [Schirotzek 2007, Proposition 4.5.1]. Further calculus rules can be obtained by relating the convex subdifferential to other derivatives. If f is convex, proper, and Gâteaux differentiable, then $\partial f(v) = \{f'(v)\}$; see, e.g., [Schirotzek 2007, Proposition 4.1.8]. On the other hand, any convex and proper function that is bounded from above is locally Lipschitz, and in this case the convex subdifferential coincides with the generalized gradient of Clarke; see, e.g., [Schirotzek 2007, Proposition 7.3.9]. In particular, we can apply the sum and chain rules for the generalized gradient; see [Clarke 1990, Theorems 2.3.3 and 2.3.10].

The usefulness of the convex subdifferential now lies in the fact that it can often be characterized explicitly. To give an example, we return to the indicator function of a convex set C. For $\bar{v} \in C$, we have

$$v^* \in \partial\delta_C(\bar{v}) \Leftrightarrow \langle v - \bar{v}, v^* \rangle_{V,V^*} \leqslant \delta_C(v) \qquad \text{for all } v \in V$$
$$\Leftrightarrow \langle v - \bar{v}, v^* \rangle_{V,V^*} \leqslant 0 \qquad \text{for all } v \in C,$$

since the condition is trivially satisfied for all $v \notin C$. In other words, the subdifferential of the indicator function of a convex set is its normal cone. Of particular importance for us will be the case when the set C_α for $\alpha > 0$ is given by pointwise constraints,

$$C_\alpha = \{v \in C_0(\Omega) : -\alpha \leqslant v(x) \leqslant \alpha \quad \text{for all } x \in \Omega\},$$

where we can give a pointwise characterization of the subdifferential. By separate pointwise inspection of the

- *positive active set*: $x \in \mathcal{A}^+ := \{x \in \Omega : \bar{v}(x) = \alpha\}$,

- *negative active set*: $x \in \mathcal{A}^- := \{x \in \Omega : \bar{v}(x) = -\alpha\}$,

- *inactive set*: $x \in \mathcal{I} := \{x \in \Omega : |\bar{v}(x)| < \alpha\}$,

we obtain the equivalent *complementarity conditions* for $v^* \in \partial\delta_{C_\alpha}(\bar{v}) \subset \mathcal{M}(\Omega)$:

$$v^*(\mathcal{A}^+) \leqslant 0, \qquad v^*(\mathcal{A}^-) \geqslant 0, \qquad v^*(\mathcal{I}) = 0.$$

If v^* is sufficiently regular (e.g., $v^* \in L^2(\Omega)$ or V is finite-dimensional), the complementarity conditions can equivalently be expressed for any $\gamma > 0$ as

$$(1.2.8) \qquad v^* + \max(0, -v^* + \gamma(\bar{v} - \alpha)) + \min(0, -v^* + \gamma(\bar{v} + \alpha)) = 0,$$

where max and min are taken pointwise almost everywhere in Ω (or componentwise in finite dimensions); this can again be seen by pointwise inspection. Optimality systems involving equation (1.2.8) can then be solved by Newton-type methods, and the regularity requirement is one reason why we will need to introduce approximations.

Another relevant example is the subdifferential of the norm of V. It is straightforward to verify using the definition of the subdifferential and the dual norm that

$$\partial(\|\cdot\|_V)(v) = \begin{cases} \{v^* \in V^* : \langle v, v^* \rangle_{V,V^*} = \|v\|_V \text{ and } \|v^*\|_{V^*} = 1\} & \text{if } v \neq 0, \\ B_{V^*} & \text{if } v = 0, \end{cases}$$

see [Schirotzek 2007, Proposition 4.6.2]. For $V = L^1(\Omega)$, we can use pointwise inspection to explicitly compute $v^* \in L^\infty(\Omega)$ for given v to obtain

$$(1.2.9) \qquad \partial(\|\cdot\|_{L^1})(v) = \text{sign}(v) := \begin{cases} 1 & \text{if } v(x) > 0, \\ -1 & \text{if } v(x) < 0, \\ t \in [-1, 1] & \text{if } v(x) = 0 \end{cases}$$

Since the multi-valued sign is not differentiable even in a generalized sense, we again need to consider an approximation before we can apply a Newton-type method.

1.2.3 FENCHEL DUALITY

We now discuss the relation between the Fenchel conjugate and the subdifferential of convex functions. Let f be a proper and convex function f. Then we immediately obtain from the definitions of the conjugate and the subdifferential that for all $v \in V$ with $f(v) < \infty$ and all $v^* \in V^*$ the *Fenchel–Young inequality*

$$(1.2.10) \qquad \langle v, v^* \rangle_{V,V^*} \leqslant f(v) + f^*(v^*),$$

is satisfied, where equality holds (and thus the supremum in (1.2.1) is attained) if and only if $v^* \in \partial f(v)$. Hence, inserting in turn arbitrary $w^* \in V^*$ and $v^* \in \partial f(v)$ into (1.2.10) and subtracting yields

$$\langle v, w^* - v^* \rangle_{V,V^*} \leqslant (f(v) + f^*(w^*)) - (f(v) + f^*(v^*)) = f^*(w^*) - f^*(v^*)$$

for every $w^* \in V^*$, i.e., $v \in \partial f^*(v^*)$. If f is in addition lower semicontinuous, we can apply the Fenchel–Moreau–Rockafellar theorem to also obtain the converse, and thus

$$(1.2.11) \qquad v^* \in \partial f(v) \quad \Leftrightarrow \quad v \in \partial f^*(v^*),$$

see [Schirotzek 2007, Proposition 4.4.4]. When combined with (1.2.4) or (1.2.5) and the characterization (1.2.8) or (1.2.9), this relation is the key in deriving useful optimality conditions for problems involving L^1 or measure space norms.

The *Fenchel duality theorem* combines in a particularly elegant way the relation (1.2.11), the sum rule (1.2.7), and a chain rule to obtain existence of and optimality conditions for a solution to a convex optimization problem. Let V and Y be Banach spaces, $\mathcal{F} : V \to \bar{\mathbb{R}}$, $\mathcal{G} : Y \to \bar{\mathbb{R}}$ be convex, proper, lower semicontinuous functions and $\Lambda : V \to Y$ be a continuous linear operator. If there exists a $v_0 \in V$ such that $\mathcal{F}(v_0) < \infty$, $\mathcal{G}(\Lambda v_0) < \infty$, and $\mathcal{G}$ is continuous at Λv_0, then

$$(1.2.12) \qquad \inf_{v \in V} \mathcal{F}(v) + \mathcal{G}(\Lambda v) = \sup_{q \in Y^*} -\mathcal{F}^*(\Lambda^* q) - \mathcal{G}^*(-q),$$

and the optimization problem on the right hand side (referred to as the *dual problem*) has at least one solution; see, e.g., [Ekeland and Témam 1999, Theorem III.4.1]. (Existence of a solution to the problem on the left hand side – the *primal problem* – follows directly from the assumptions on $\mathcal{F}$, $\mathcal{G}$, and Λ by standard arguments.) Furthermore, the equality in (1.2.12) is attained at $(\bar{v}, \bar{q})$ if and only if the *extremality relations*

$$(1.2.13) \qquad \begin{cases} \Lambda^* \bar{q} \in \partial \mathcal{F}(\bar{v}), \\ -\bar{q} \in \partial \mathcal{G}(\Lambda \bar{v}), \end{cases}$$

hold; see, e.g., [Ekeland and Témam 1999, Proposition III.4.1]. Depending on the context, one or both of these relations can be reformulated in terms of $\mathcal{F}^*$ and $\mathcal{G}^*$ using the equivalence (1.2.11). The conditions and consequences of the Fenchel duality theorem should be compared with classical regular point conditions (e.g., [Maurer and Zowe 1979; Ito and Kunisch 2008]) for the existence of Lagrange multipliers in constrained optimization.

1.3 SEMISMOOTH NEWTON METHODS

It remains to formulate a numerical method that can solve nonsmooth equations of the form (1.2.8) in an efficient manner. Just as the convex subdifferential proved to be suitable replacement for the Fréchet derivative in the context of optimality conditions, we need to consider a generalized derivative that can replace the Fréchet derivative in a Newton-type method and still allow superlinear convergence. In addition, it needs to provide a sufficiently rich calculus and the possibility for explicit characterization to be implementable in a numerical algorithm. These requirements lead to semismooth Newton methods. This section gives a brief overview of the theory in finite and infinite dimensions; for details and proofs, the reader is referred to the expositions in [Ito and Kunisch 2008; Ulbrich 2011; Schiela 2008].

To motivate the definitions, it will be instructive to first consider the convergence of an abstract generalized Newton method. Let Banach spaces X, Y, a mapping $F : X \to Y$, and $x^* \in X$ with $F(x^*) = 0$ be given. A generalized Newton method to compute an approximation of x^* can be described as follows:

1: Choose $x^0 \in X$
2: **for** $k = 0, 1, \ldots$ **do**
3:      Choose an invertible linear operator $M_k \in \mathcal{L}(X, Y)$
4:      Set $x^{k+1} = x^k - M_k^{-1} F(x^k)$
5: **end for**

We can now ask ourselves when convergence of the iterates $x^k \to x^*$ holds, and in particular when it is *superlinear*, i.e.,

$$(1.3.1) \qquad \lim_{k \to \infty} \frac{\left\| x^{k+1} - x^* \right\|_X}{\left\| x^k - x^* \right\|_X} = 0.$$

Set $M(x^k) := M_k$ and $d^k = x^k - x^*$. Then we can use the definition of the Newton step and the fact that $F(x^*) = 0$ to obtain

$$\begin{aligned}
\left\| x^{k+1} - x^* \right\|_X &= \left\| x^k - M(x_k)^{-1} F(x^k) - x^* \right\|_X \\
&= \left\| M(x_k)^{-1} \left[F(x^k) - F(x^*) - M(x_k)(x^k - x^*) \right] \right\|_X \\
&= \left\| M(x_k)^{-1} \left[F(x^k) - F(x^*) - M(x_k) d^k \right] \right\|_X \\
&\leqslant \left\| M(x_k)^{-1} \right\|_{\mathcal{L}(Y,X)} \left\| F(x^* + d^k) - F(x^*) - M(x^k) d^k \right\|_Y
\end{aligned}$$

Hence, (1.3.1) holds if both a

- *uniform regularity condition*: there exists a $C > 0$ such that

$$\left\| M(x_k)^{-1} \right\|_{\mathcal{L}(Y,X)} \leqslant C$$

for all k, and an

- *approximation condition*:

$$\lim_{\|d^k\|_X \to 0} \frac{\left\| F(x^* + d^k) - F(x^*) - M(x^* + d^k)d^k \right\|_Y}{\|d^k\|_X} = 0,$$

hold. In this case, there exists a neighborhood $N(x^*)$ of x^* such that

$$\left\| x^{k+1} - x^* \right\|_X < \frac{1}{2} \left\| x^k - x^* \right\|_X$$

for an $x^k \in N(x^*)$, which by induction implies $d^k \to 0$ and hence the desired (local) superlinear convergence.

If F is continuously Fréchet differentiable, the approximation condition holds by definition for the Fréchet derivative $M_k = F'(x^k)$, and we arrive at the classical Newton method. For nonsmooth F, we simply take a linear operator which satisfies the uniform regularity and approximation conditions. Naturally, the choice $M_k \in \partial F(x^k)$ for an appropriate subdifferential suggests itself.

1.3.1 SEMISMOOTH NEWTON METHODS IN FINITE DIMENSIONS

If X and Y are finite-dimensional, an appropriate choice is the Clarke subdifferential. Recall that by Rademacher's theorem, every Lipschitz function $f : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable almost everywhere; see, e.g. [Ziemer 1989, Theorem 2.2.1]. We can then define the *Clarke subdifferential* at $x \in \mathbb{R}^n$ as

$$\partial_C f(x) = \mathrm{co} \left\{ \lim_{n \to \infty} f'(x_n) : \{x_n\}_{n \in \mathbb{N}} \text{ with } x_n \to x, \ f \text{ differentiable at } x_n \right\},$$

where co denotes the convex hull. To use an element of the Clarke subdifferential as linear operator in our Newton method, we need to ensure in particular that the approximation condition holds. In fact, we will require a slightly stronger condition. A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is called *semismooth* at $x \in \mathbb{R}^n$ if

(i) f is Lipschitz continuous near x,

(ii) f is directionally differentiable at x,

(iii) $\displaystyle \lim_{\|h\| \to 0} \sup_{M \in \partial_C f(x+h)} \frac{\|F(x+h) - F(x) - Mh\|}{\|h\|} = 0.$

Note that we take the subgradient not in the linearization point but in a neighborhood, so we avoid evaluating $\partial_C f$ at the points where f is not differentiable. This definition is equivalent to the original one of [Mifflin 1977] (for real-valued functions) and [Qi and Sun 1993] (for vector-valued functions); see [Ulbrich 2011, Proposition 2.7].

For a locally Lipschitz continuous function, this leads to the *semismooth Newton method*

1: Choose $x^0 \in X$
2: **for** $k = 0, 1, \dots$ **do**
3:    Choose $M_k \in \partial_C f(x^k)$
4:    Set $x^{k+1} = x^k - M_k^{-1} f(x^k)$
5: **end for**

If f is semismooth at x^* with $f(x^*) = 0$ and all M_k satisfy the uniform regularity condition, this iteration converges (locally) superlinearly to x^*; see, e.g., [Ulbrich 2011, Proposition 2.12]. (In fact, condition (iii) of the definition is sufficient.) A similar abstract framework for the superlinear convergence of Newton methods was proposed in [Kummer 1988].

We close this section with some relevant examples. Clearly, if f is continuously differentiable at x, then f is semismooth at x with $\partial_C f(x) = \{f'(x)\}$. This can be extended to continuous piecewise differentiable functions. Let $f_1, \dots, f_N \in C^1(\mathbb{R}^n; \mathbb{R}^m)$ be given. A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is called *piecewise differentiable* if

$$f(x) \in \{f_1(x), \dots, f_N(x)\} \quad \text{for all } x \in \mathbb{R}^n.$$

Then, f is semismooth, and

$$\partial_C f(x) = \operatorname{co}\{f_i'(x) : f(x) = f_i(x) \text{ and } x \in \operatorname{cl} \operatorname{int}\{y : f(y) = f_i(y)\}\};$$

see, e.g., [Ulbrich 2011, Proposition 2.26]. This means that we can differentiate piecewise, and where pieces overlap, take the convex hull of all possible values at x excluding those that are only attained on a null set containing x. As a concrete example, the function $f : \mathbb{R} \to \mathbb{R}$, $f(x) = \max(0, x)$ is semismooth, and

$$\partial_C f(x) = \begin{cases} \{0\} & \text{if } x < 0, \\ \{1\} & \text{if } x > 0, \\ [0, 1] & \text{if } x = 0. \end{cases}$$

Finally, a vector-valued function is semismooth if and only if all its component functions are semismooth; see [Ulbrich 2011, Proposition 2.10]. This implies semismoothness of (1.2.8) in finite dimensions.

1.3.2 SEMISMOOTH NEWTON METHODS IN INFINITE DIMENSIONS

In infinite dimensions, Rademacher's theorem is not available, and thus the construction above cannot be carried out. Instead of starting from Lipschitz continuous functions, we

directly demand the approximation condition to hold. We call $F : X \to Y$ *Newton differentiable* at $u \in X$ if there exists a neighborhood $N(u)$ and a mapping $G : N(u) \to \mathcal{L}(X, Y)$ with

$$(1.3.2) \qquad \lim_{\|h\|_X \to 0} \frac{\|F(u+h) - F(u) - G(u+h)h\|_Y}{\|h\|_X} = 0.$$

Any $D_N F \in \{G(s) : s \in N(u)\}$ is then a *Newton derivative* at u. Note that Newton derivatives are in general not unique, and need not be elements of any generalized subdifferential. If F is Newton differentiable at u and

$$\lim_{t \to 0^+} G(u + th)h$$

exists uniformly in $\|h\|_X = 1$, then F is called *semismooth* at u. This approach to semismoothness in Banach spaces was proposed in [Hintermüller, Ito, and Kunisch 2002], based on the similar (but stronger) notion of slant differentiability introduced in [Chen, Nashed, and Qi 2000]. Related approaches to nonsmooth Newton methods in Banach spaces based on set-valued generalized derivatives were treated in [Kummer 2000] and [Ulbrich 2002]. The exposition here is adapted from [Ito and Kunisch 2008].

For Newton differentiable F, this definition leads to the semismooth Newton method

1: Choose $u^0 \in X$
2: **for** $k = 0, 1, \dots$ **do**
3:     Choose Newton derivative $D_N F(u^k)$
4:     Set $u^{k+1} = u^k - D_N F(u^k)^{-1} F(u^k)$
5: **end for**

If F is Newton differentiable (in particular, if F is semismooth) at u^* with $F(u^*) = 0$ and all $D_N F(u) \in \{G(u) : u \in N(u^*)\}$ satisfy the uniform regularity condition $\|D_N F(u)\|_{\mathcal{L}(Y,X)} \leqslant C$, this iteration converges (locally) superlinearly to u^*; see, e.g., [Ito and Kunisch 2008, Theorem 8.16].

If we wish to apply a semismooth Newton method to a concrete function F such as the one in (1.2.8), we need to decide whether it is semismooth and give an explicit and computable Newton derivative. Clearly, if F is continuously Fréchet differentiable near u, then F is semismooth at u, and its Fréchet derivative $F'(u)$ is a Newton derivative (albeit not the only one). However, this cannot be extended directly to "piecewise differentiable" functions such as the pointwise max operator acting on functions in $L^p(\Omega)$. It is instructive to consider a concrete example. Take $F : L^p(\Omega) \to L^p(\Omega)$, $F(u) = \max(0, u)$. A candidate for its Newton derivative is defined by its action on $h \in L^p(\Omega)$ as

$$[G(u)h](x) = \begin{cases} 0 & u(x) < 0 \\ h(x) & u(x) > 0 \\ \delta\, h(x) & u(x) = 0 \end{cases}$$

for almost all $x \in \Omega$ and arbitrary $\delta \in \mathbb{R}$. (Since the Newton derivative coincides with the Fréchet derivative where F is continuously differentiable, we only have the freedom to choose

its value where $u(x) = 0$.) To show that the approximation condition (1.3.2) is violated at $u(x) = -|x|$ on $\Omega = (-1, 1)$ for any $1 \leqslant p < \infty$, we take the sequence

$$h_n(x) = \begin{cases} \frac{1}{n} & \text{if } |x| < \frac{1}{n}, \\ 0 & \text{otherwise,} \end{cases}$$

with $\|h_n\|_{L^p}^p = \frac{2}{n^{p+1}}$. Then, since $[F(u)](x) = \max(0, -|x|) = 0$ almost everywhere, we have

$$[F(u + h_n) - F(u) - G(u + h_n)h_n](x) = \begin{cases} -|x| & \text{if } |x| < \frac{1}{n}, \\ 0 & \text{if } |x| > \frac{1}{n}, \\ -\frac{\delta}{n} & \text{if } |x| = \frac{1}{n} \end{cases}$$

and thus

$$\|F(u + h_n) - F(u) - G(u + h_n)h_n\|_{L^p}^p = \int_{-\frac{1}{n}}^{\frac{1}{n}} |x|^p \, dx = \frac{2}{p+1}\left(\frac{1}{n}\right)^{p+1}.$$

This implies

$$\lim_{n \to \infty} \frac{\|F(u + h_n) - F(u) - G(u + h_n)h_n\|_{L^p}}{\|h_n\|_{L^p}} = \left(\frac{1}{p+1}\right)^{\frac{1}{p}} \neq 0$$

and hence that F is not semismooth from $L^p(\Omega)$ to $L^p(\Omega)$. A similar example can be constructed for $p = \infty$; see, e.g., [Ito and Kunisch 2008, Example 8.14].

On the other hand, if we consider $F : L^q(\Omega) \to L^p(\Omega)$ with $q > p$, the terms involving n^{-1} do not cancel and the approximation condition holds (at least for this choice of h_n). In fact, for arbitrary $h \in L^q(\Omega)$ one can use Hölder's inequality to create a term involving the Lebesgue measure of the support of the set where the "wrong" linearization is taken (i.e., where $\max(u(x) + h(x)) \neq \max(u(x)) + G(u(x) + h(x))h(x)$), which can be shown to go to zero as $h \to 0$; see [Hintermüller, Ito, and Kunisch 2002, Proposition 4.1]. Semismoothness in function spaces hence fundamentally requires a *norm gap*, which is another reason why approximation may be necessary to apply a semismooth Newton method to equations of type (1.2.8).

The above holds for any pointwise defined operator. If $\psi : \mathbb{R} \to \mathbb{R}$ is semismooth, the corresponding *Nemytskii operator* $\Psi : L^q(\Omega) \to L^p(\Omega)$, defined pointwise almost everywhere as

$$[\Psi(u)](x) := \psi(u(x)),$$

is semismooth if and only if $1 \leqslant p < q \leqslant \infty$, and a Newton derivative of Ψ at x, acting on h, can be taken as

$$[D_N(\Psi(u))h](x) \in \partial_C(\psi(u(x)))h(x).$$

This connection was first investigated systematically in [Ulbrich 2002]; an alternative approach which parallels the theory of Fréchet differentiability is followed in [Schiela 2008]. In particular, $F(u) = \max(0, u)$ is semismooth from $L^q(\Omega)$ to $L^p(\Omega)$ for any $q > p$, with Newton derivative

$$[D_N F(u)h](x) = \begin{cases} 0 & u(x) \leqslant 0 \\ h(x) & u(x) > 0. \end{cases}$$

This can be conveniently expressed with the help of the *characteristic function* $\chi_{\mathcal{A}}$ of the *active set* $\mathcal{A} := \{x \in \Omega : u(x) > 0\}$ (i.e., the function taking the value 1 at $x \in \mathcal{A}$ and 0 otherwise) as $D_N F(u) = \chi_{\mathcal{A}}$.

There is a useful calculus for Newton derivatives. It is straightforward to verify that the sum of two semismooth functions F_1 and F_2 is semismooth, and

$$D_N(F_1 + F_2)(u) := D_N F_1(u) + D_N F_2(u)$$

is a Newton derivative for any choice of Newton derivatives $D_N F_1$ and $D_N F_2$. We also have a chain rule: If $F : X \to Y$ is continuously Fréchet differentiable at $u \in X$ and $G : Y \to Z$ is Newton differentiable at $F(u)$, then $H := G \circ F$ is Newton differentiable at u with Newton derivative

$$D_N H(u + h) = D_N G(F(u + h))F'(u + h)$$

for any $h \in X$ sufficiently small; see [Ito and Kunisch 2008, Lemma 8.15].

A final remark. Although numerical computation almost always involves finite-dimensional problems, there is a practical reason for studying Newton methods in function spaces (besides the uniform framework and the frequently tidier notation this allows): If semismoothness and the uniform regularity condition can be verified for an infinite-dimensional problem, the respective property holds uniformly for any (conforming) discretization. In practice, this is reflected in the observation that the number of Newton iterations required to achieve a given tolerance does not increase with the fineness of the discretization. This property, called *mesh independence*, has been verified for semismooth Newton methods in [Hintermüller and Ulbrich 2004].

OPTIMAL CONTROL WITH MEASURES

This chapter is concerned with optimal control problems for elliptic and parabolic equations, where the controls are sought in spaces of Radon measures instead of the usual Lebesgue or Sobolev spaces. This setting is not a generalization for its own sake, but rather motivated by applications: In finite dimensional optimization, it has frequently been observed that minimizing ℓ^1-norms promotes solutions that are *sparser* than their ℓ^2-norm counterparts, i.e., that have fewer non-zero entries. This would also be desirable in the context of optimal control of partial differential equations, e.g., for the optimal placement of discrete actuators. These could be modeled as a distributed "control field", where a L^1 penalty would favor *sparse*, i.e., strongly localized controls, denoting both location and strength of the actuators; see [Stadler 2009]. Penalties of L^1 type would also be relevant in settings where the control cost is a linear function of its magnitude, e.g., representing fuel costs; see [Vossen and Maurer 2006]. However, optimal control problems in $L^1(\Omega)$ are not well-posed, since boundedness in $L^1(\Omega)$ is not sufficient for the existence of a weakly convergent subsequence. One possibility is to add additional L^2 penalties or L^∞ bounds on the control, in which case the existence of minimizers can be deduced from the Dunford–Pettis theorem; see, e.g., [Edwards 1965, Theorem 4.21.2]. This approach is followed in [Stadler 2009; Wachsmuth and Wachsmuth 2011a; Wachsmuth and Wachsmuth 2011b; Casas, Herzog, and Wachsmuth 2012]. On the other hand, we can identify $L^1(\Omega)$ with a subspace of $\mathcal{M}(\Omega)$ to obtain existence of a weak-$\star$ convergent subsequence in the latter. In this sense, the space $\mathcal{M}(\Omega)$ of Radon measures is the proper analogue of ℓ^1 for infinite-dimensional optimal control problems with sparsity constraints. A framework for the numerical solution of such problems is presented in section 2.1 for elliptic problems; its extension to parabolic problems is the topic of section 2.2.

In a similar fashion, total variation penalties favor piecewise constant controls and for that reason have attracted great interest in signal and image processing. In the context of optimal control problems, this would be relevant when the cost is proportional to changes in the control. Here, the proper setting in infinite dimensions is the space $BV(\Omega)$ of functions of bounded variation. The corresponding approach for elliptic problems is discussed in section 2.3.

18

2.1 ELLIPTIC PROBLEMS WITH RADON MEASURES

The challenge in the numerical solution of optimal control problems with measures arises from the non-reflexivity of the space $\mathcal{M}(\Omega)$ and the non-differentiability of its norm. However, a combination of Fenchel duality and Moreau–Yosida regularization allows approximating the optimal measure-space controls by a family of more regular controls that can be computed using a semismooth Newton method. The next section introduces this framework. Section 2.1.2 discusses the modifications necessary for restricted control and observation. An alternative to regularization is to consider a conforming discretization of the measure space, which is presented in section 2.1.3.

2.1.1 DUALITY-BASED FRAMEWORK

We consider the optimal control problem

$$(2.1.1) \qquad \begin{cases} \displaystyle\min_{u \in \mathcal{M}(\Omega)} \frac{1}{2} \|y - z\|_{L^2}^2 + \alpha \|u\|_{\mathcal{M}} \\[2mm] \text{s.t.} \quad Ay = u. \end{cases}$$

where $\Omega \subset \mathbb{R}^n$, $n \in \{2, 3\}$, is a simply connected bounded domain with Lipschitz boundary $\partial\Omega$, and $\alpha > 0$ and $z \in L^2(\Omega)$ are given. Here, A is a linear second order elliptic differential operator taking homogeneous Dirichlet boundary conditions such that $\|A \cdot\|_{L^2}$ and $\|A^* \cdot\|_{L^2}$ are equivalent norms on

$$\mathcal{W} := H^2(\Omega) \cap H_0^1(\Omega) \hookrightarrow C_0(\Omega).$$

This is a slightly more restrictive assumption than maximal regularity for $p > n$, which can be relaxed; see sections 1.1.3 and 2.1.2. The main motivation for this restriction is to work with a standard Hilbert space for the dual problem; this will be particularly convenient when applying the framework to controls of bounded variation; see section 2.3.

Under this assumption, the equality constraint in (2.1.1) is well-posed, and the existence of a unique solution $\bar{u} \in \mathcal{M}(\Omega)$ follows from standard arguments; see Theorem 7.2.2.

To apply Fenchel duality, we take $C_0(\Omega)$ as the weak-$\star$ dual of $\mathcal{M}(\Omega)$ and set

$$\mathcal{F} : \mathcal{M}(\Omega) \to \mathbb{R}, \qquad \mathcal{F}(v) = \alpha \|v\|_{\mathcal{M}},$$

$$\mathcal{G} : \mathcal{W}^* \to \mathbb{R}, \qquad \mathcal{G}(v) = \frac{1}{2} \left\|A^{-1}v - z\right\|_{L^2}^2,$$

$$\Lambda : \mathcal{M}(\Omega) \to \mathcal{W}^*, \qquad \Lambda v = v,$$

i.e., Λ is the injection corresponding to the embedding $\mathcal{M}(\Omega) \hookrightarrow \mathcal{W}^*$. The conjugate of $\mathcal{G}$ can be directly calculated due to its Fréchet differentiability and the bijectivity of A; the conjugate

of $\mathcal{F}$ is given by (1.2.5). The adjoint Λ^* is the injection corresponding to the embedding $\mathcal{W} \hookrightarrow C_0(\Omega)$. Since $\mathcal{F}$ and $\mathcal{G}$ are convex, proper, and lower semicontinuous, and $\mathcal{G}$ is continuous at, e.g., $v = 0 = \Lambda v$, we can apply the Fenchel duality theorem to deduce that the dual problem

$$
\begin{cases}
\displaystyle \min_{p \in \mathcal{W}} \frac{1}{2} \|A^*p + z\|_{L^2}^2 - \frac{1}{2} \|z\|_{L^2}^2 \\
\text{s.t.} \quad \|p\|_{C_0} \leqslant \alpha,
\end{cases}
$$

has a solution $\bar{p} \in \mathcal{W}$ which is unique by the assumption on A^*. Applying the equivalence (1.2.11) to both extremality relations in (1.2.13) then yields first order (necessary and sufficient) optimality conditions for $\bar{p}$: There exists $\bar{\lambda} := -\bar{u} \in \mathcal{M}(\Omega) \subset \mathcal{W}^*$ such that

(2.1.2)
$$
\begin{cases}
AA^*\bar{p} + Az + \bar{\lambda} = 0, \\
\langle \bar{\lambda}, p - \bar{p} \rangle_{\mathcal{M}, C_0} \leqslant 0,
\end{cases}
$$

holds for all $p \in \mathcal{W}$ with $\|p\|_{C_0} \leqslant \alpha$, where the first equation should be interpreted in the weak sense; see Corollary 7.2.5. From (2.1.2), we can deduce the following structural information for the Jordan decomposition $\bar{u} = \bar{u}^+ - \bar{u}^-$ of the optimal control:

$$
\operatorname{supp}(\bar{u}^+) \subset \{x \in \Omega : \bar{p}(x) = -\alpha\},
$$
$$
\operatorname{supp}(\bar{u}^-) \subset \{x \in \Omega : \bar{p}(x) = \alpha\}.
$$

This can be interpreted as a sparsity property: The optimal control $\bar{u}$ will be nonzero only on sets where the constraint on the dual variable $\bar{p}$ is active, which are typically small; and the larger the penalty α, the smaller the support of the control.

Due to the low regularity $\bar{\lambda} \in \mathcal{W}^*$, we cannot apply a semismooth Newton method directly. We therefore consider for $\gamma > 0$ the family of regularized problems

(2.1.3)
$$
\begin{cases}
\displaystyle \min_{u \in L^2(\Omega)} \frac{1}{2} \|y - z\|_{L^2}^2 + \alpha \|u\|_{L^1} + \frac{1}{2\gamma} \|u\|_{L^2}^2 \\
\text{s.t.} \quad Ay = u,
\end{cases}
$$

which is strictly convex and thus has a unique solution $u_\gamma \in L^2(\Omega)$. Proceeding as above, we now set

$$
\mathcal{F}_\gamma : \mathcal{M}(\Omega) \to \bar{\mathbb{R}}, \qquad \mathcal{F}_\gamma(v) = \alpha \|v\|_{\mathcal{M}} + \frac{1}{2\gamma} \|v\|_{L^2}^2,
$$

which is finite if and only if $v \in L^2(\Omega)$. Direct calculation verifies that the weak-$\star$ Fenchel conjugate $\mathcal{F}_\gamma^* : C_0(\Omega) \to \bar{\mathbb{R}}$ is given by

$$
\mathcal{F}_\gamma^*(v^*) = \frac{\gamma}{2} \|\max(0, v^* - \alpha)\|_{L^2}^2 + \frac{\gamma}{2} \|\min(0, v^* + \alpha)\|_{L^2}^2,
$$

see Remark 7.3.2. The Fenchel duality theorem then yields the existence of a (unique) solution $p_\gamma \in \mathcal{W}$ of the dual problem

$$
\min_{p \in \mathcal{W}} \frac{1}{2} \|A^*p + z\|_{L^2}^2 - \frac{1}{2} \|z\|_{L^2}^2 + \frac{\gamma}{2} \|\max(0, p - \alpha)\|_{L^2}^2 + \frac{\gamma}{2} \|\min(0, p + \alpha)\|_{L^2}^2,
$$

as well as the optimality system

$$(2.1.4) \qquad \begin{cases} AA^*p_\gamma + Az + \lambda_\gamma = 0, \\ \lambda_\gamma = \gamma \max(0, p_\gamma - \alpha)) + \gamma \min(0, p_\gamma + \alpha), \end{cases}$$

where $\lambda_\gamma = -u_\gamma \in L^2(\Omega)$. (The last equation should be compared with (1.2.8); the connection with the Fenchel dual of (2.1.3) justifies calling (2.1.4) a *Moreau–Yosida regularization* of (2.1.2).) As $\gamma \to \infty$, the solutions p_γ converge strongly in $\mathcal{W}$ to $\bar{p}$, while the λ_γ converge weakly-$\star$ in $\mathcal{W}^*$ to $\bar{\lambda}$; see Theorem 7.3.1.

We now consider (2.1.4) as a nonlinear equation $F(p) = 0$ for $F : \mathcal{W} \to \mathcal{W}^*$,

$$(2.1.5) \qquad F(p) := AA^*p + Az + \gamma \max(0, p - \alpha) + \gamma \min(0, p + \alpha),$$

understood in the weak sense. Since $\mathcal{W} \hookrightarrow L^p(\Omega)$ for any $p > 2$, this equation is semismooth with Newton derivative

$$D_N F(p)h = AA^*h + \gamma \chi_{\{x : |p(x)| > \alpha\}} h.$$

By the assumption on A and A^*, the operator AA^* is an isometry from $\mathcal{W}$ to $\mathcal{W}^*$, which implies uniform invertibility of $D_N F(p)$ independently of p. The semismooth Newton method applied to F thus converges locally superlinearly to the solution of (2.1.5). The corresponding control $u_\gamma = -\lambda_\gamma$ can then be obtained from the second equation of (2.1.4). In practice, the basin of convergence shrinks with increasing γ; this can be remedied by computing a sequence of solutions, starting with $\gamma_0 = 1$, and using the solution u_{γ_k} as starting point for the computation of $u_{\gamma_{k+1}}$ with $\gamma_{k+1} > \gamma_k$. We shall refer to this procedure as a *continuation strategy*.

Figure 2.1 shows an example target and the corresponding optimal control u_γ for $A = -\Delta$, $\alpha = 10^{-3}$ and $\gamma = 10^7$, demonstrating the sparsity of the controls. More examples are given in section 7.4.

2.1.2 RESTRICTED CONTROL AND OBSERVATION

The optimal controls obtained from the above approach are strongly localized, and can be used as indicators for the optimal placement of point sources. In practical applications, it is often not possible to place sources in the whole computational domain; similarly, the state may need to be controlled only in a part of the domain. In case of restricted observation, however, the control-to-restricted-state mapping is no longer an isometry, and the above pure (pre)dual approach is no longer applicable. Nevertheless, useful optimality conditions of primal-dual type can still be obtained using Fenchel duality.

We thus consider the problem

$$(2.1.6) \qquad \begin{cases} \displaystyle\min_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2} \|y|_{\omega_o} - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} \\ \qquad \text{s.t.} \quad Ay = \chi_{\omega_c} u, \end{cases}$$

(a) z (b) u_γ
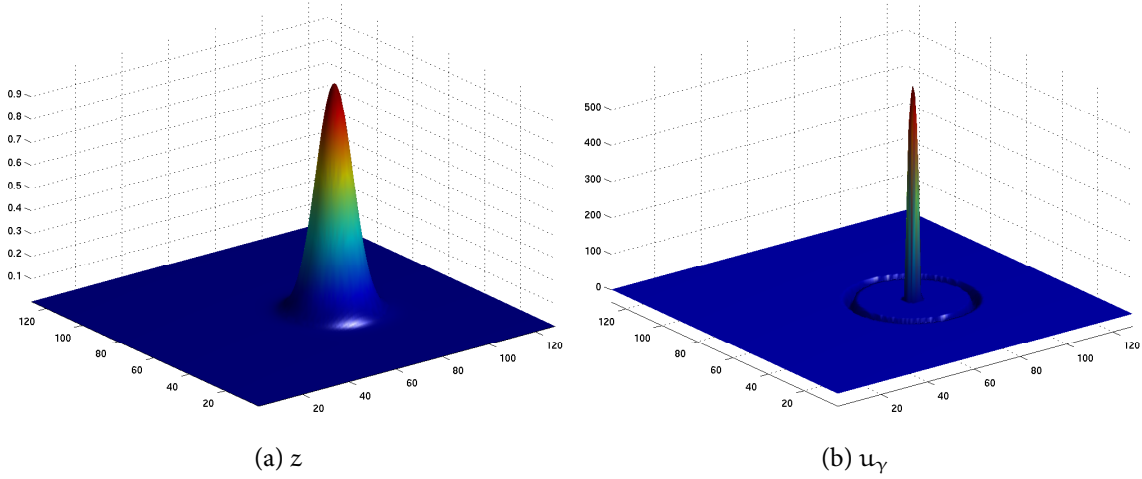
Figure 2.1: Target z and corresponding optimal control u_γ for $\alpha = 10^{-3}, \gamma = 10^7$

where ω_o and ω_c represent the observation and control subdomains of the bounded domain $\Omega \subset \mathbb{R}^n$ with characteristic function χ_{ω_o} and χ_{ω_c}, respectively, and $z \in L^2(\omega_o)$ is given. Furthermore, $\mathcal{M}_\Gamma(\overline{\omega}_c)$ is the topological dual of $C_\Gamma(\overline{\omega}_c) := \{v \in C(\overline{\omega}_c) : v|_{\partial\omega_c \cap \Gamma} = 0\}$, where $\Gamma = \partial\Omega$ and the constraint $v|_{\partial\omega_c \cap \Gamma} = 0$ is dropped if $\partial\omega_c \cap \Gamma = \emptyset$; see section 1.1.2. Under the assumptions of section 1.1.3, the state equation is well-posed and problem (2.1.6) has a solution by standard arguments.

To define the control-to-observation mapping S_ω, we introduce for $q > n$ the canonical restriction operators

$$R_{\omega_o} : W_0^{1,q'}(\Omega) \to W^{1,q'}(\omega_o), \qquad R_{\omega_c} : W_0^{1,q}(\Omega) \to W^{1,q}(\omega_c)$$

and the injections

$$\mathcal{J}_{\omega_o} : W^{1,q'}(\omega_o) \to L^2(\omega_o), \qquad \mathcal{J}_{\omega_c} : W^{1,q}(\omega_c) \to C_\Gamma(\overline{\omega}_c)$$

and set

$$S_\omega : \mathcal{M}_\Gamma(\overline{\omega}_c) \to L^2(\omega_o), \qquad S_\omega(u) = \mathcal{J}_{\omega_o} R_{\omega_o} A^{-1} R_{\omega_c}^* \mathcal{J}_{\omega_c}^* u.$$

By construction, S_ω has the weak-$\star$ adjoint

$$S_\omega^* : L^2(\omega_o) \to C_\Gamma(\overline{\omega}_c), \qquad S_\omega^*(\varphi)) =_{\omega_c} R_{\omega_c}(A^*)^{-1} R_{\omega_o}^* \mathcal{J}_{\omega_o}^* \varphi.$$

We now apply Fenchel duality, this time setting

$$\mathcal{F} : \mathcal{M}_\Gamma(\overline{\omega}_c) \to \mathbb{R}, \qquad \mathcal{F}(v) = \alpha \|v\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)},$$

$$\mathcal{G} : L^2(\omega_o) \to \mathbb{R}, \qquad \mathcal{G}(v) = \frac{1}{2} \|v - z\|_{L^2(\omega_o)}^2,$$

$$\Lambda : \mathcal{M}_\Gamma(\overline{\omega}_c) \to L^2(\omega_o), \qquad \Lambda v = S_\omega v.$$

The Fenchel duality theorem now yields the existence of $\bar{q} \in L^2(\omega_o)$ satisfying

$$
\begin{cases}
-\bar{q} = S_\omega \bar{u} - z, \\
\bar{u} \in \partial I_{\{\|q\|_{C_\Gamma(\overline{\omega}_c)} \leqslant \alpha\}}(S_\omega^* \bar{q}),
\end{cases}
$$

where we have applied the equivalence (1.2.11) to the second relation only. Setting $\bar{p} = -S_\omega^* \bar{q} = S_\omega^*(S_\omega \bar{u} - z) \in C_\Gamma(\overline{\omega}_c)$ (i.e., introducing the adjoint state), we obtain the primal-dual optimality system for $(\bar{u}, \bar{p}) \in \mathcal{M}_\Gamma(\overline{\omega}_c) \times C_\Gamma(\overline{\omega}_c)$

(2.1.7)
$$
\begin{cases}
S_\omega^*(S_\omega \bar{u} - z) = \bar{p}, \\
\langle \bar{u}, \bar{p} - p \rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \leqslant 0,
\end{cases}
$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ with $\|p\|_{C_\Gamma(\overline{\omega}_c)} \leqslant \alpha$; see Theorem 8.2.3. Note that since S_ω is no longer bijective, we cannot solve the first equation for $\bar{u}$ as in (2.1.2).

Again, due to the low regularity of $\bar{u}$, we introduce a Moreau–Yosida regularization of (2.1.7):

(2.1.8)
$$
\begin{cases}
p_\gamma = S_\omega^*(S_\omega u_\gamma - z), \\
-u_\gamma = \gamma \max(0, p_\gamma - \alpha) + \gamma \min(0, p_\gamma + \alpha),
\end{cases}
$$

where S_ω is considered as an operator from $L^2(\omega_c) \to L^2(\omega_o)$. As in section 2.1.1, we deduce the existence of a unique solution $(u_\gamma, p_\gamma) \in L^2(\omega_c) \times W^{1,q}(\omega_c)$; see Theorem 8.3.1. For $\gamma \to \infty$, the family $\{u_\gamma\}_{\gamma>0}$ has a subsequence weakly-$\star$ converging to $\bar{u}$ in $\mathcal{M}_\Gamma(\overline{\omega}_c)$, and $\{p_\gamma\}_{\gamma>0}$ has a subsequence strongly converging to $\bar{p}$ in $W^{1,q}(\omega_c)$ and hence in $C_\Gamma(\overline{\omega}_c)$; see Theorem 8.3.2.

The regularized optimality system (2.1.8) can be written as an operator equation $F(u_\gamma) = 0$ for $F : L^2(\omega_c) \to L^2(\omega_c)$,

$$
F(u) = u + \gamma \max(0, S_\omega^*(S_\omega u - z) - \alpha) + \gamma \min(0, S_\omega^*(S_\omega u - z) + \alpha).
$$

Due to the smoothing properties of the adjoint solution operator S_ω^*, this equation is semismooth, with Newton derivative given by

$$
D_N F(u) h = h + \gamma \chi_{\{x : |S_\omega^*(S_\omega u - z)(x)| > \alpha\}}(S_\omega^* S_\omega h).
$$

Due to the presence of the first term and the continuity of S_ω and S_ω^*, the Newton derivatives have uniformly bounded inverses, and the semismooth Newton method converges locally superlinearly; see Theorem 8.4.1. The solution of the Newton step $D_F(u^k)\delta u = -F(u^k)$ can be computed using a matrix-free Krylov method such as GMRES, where the action of the Newton derivative on a given δu is computed by first solving the state equation $A\delta y = \chi_{\omega_c}\delta u$ followed by the adjoint equation $A^*\delta p = \chi_{\omega_o} y - z$ and setting $S_\omega^* S_\omega \delta u = \chi_{\omega_c}\delta p$. In practice, the Newton method is combined with the continuation strategy described above.

Figure 2.2 shows an example target and the corresponding optimal control u_γ for $A = -\nu\Delta - b \cdot \nabla$ with $\nu = 0.1$ and $b = (1,0)^\top$, $\alpha = 10^{-3}$, and $\gamma = 10^{12}$. It can be observed that

(a) z (b) u_γ
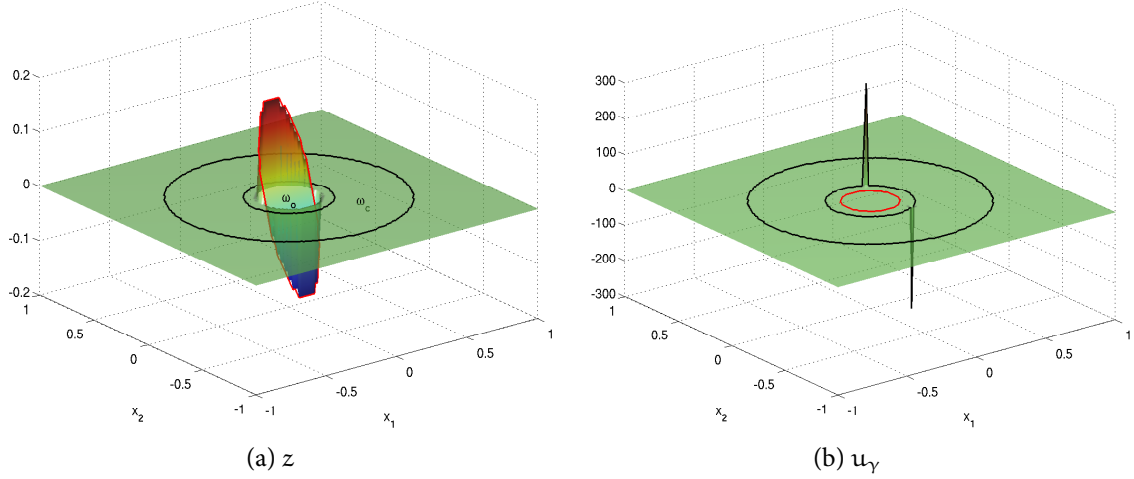
Figure 2.2: Target z and optimal control u_γ for $\gamma = 10^{12}$ and $\alpha = 10^{-3}$ (control domain ω_c and observation domain ω_o are shown in black and red, respectively)

the controls are concentrated on the boundary of the control domain ω_c (outlined in black) closest to the observation domain ω_o (in red). More examples can be found in section 8.5.

For some applications, it is important to ensure non-negativity of the controls; this is the case, e.g., if the controls represent light sources. This restriction can be incorporated by replacing $\mathcal{F}$ in the above framework with

$$\mathcal{F}_+ : \mathcal{M}_\Gamma(\overline{\omega}_c) \to \bar{\mathbb{R}}, \qquad \mathcal{F}_+(\nu) = \alpha \,\|\nu\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} + \delta_{\{\mu \in \mathcal{M}_\Gamma(\overline{\omega}_c) : \mu \geqslant 0\}}(\nu).$$

It follows from its definition that the Fenchel conjugate $\mathcal{F}_+^*$ is finite in $q \in C_\Gamma(\overline{\omega}_c)$ if and only if $q \leqslant \alpha$ everywhere, i.e.,

$$\mathcal{F}_+^* : C_\Gamma(\overline{\omega}_c) \to \bar{\mathbb{R}}, \qquad \mathcal{F}_+^*(q) = \delta_{\{\nu \in C_\Gamma(\overline{\omega}_c) : \nu \leqslant \alpha\}}(q).$$

This leads to the optimality system (recalling that $\bar{p} = -S_\omega^* \bar{q}$)

$$\begin{cases} S_\omega^*(S_\omega \bar{u} - z) = \bar{p}, \\ \langle \bar{u}, \bar{p} - p \rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \leqslant 0, \end{cases}$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ with $p \geqslant -\alpha$, whose Moreau–Yosida regularization is

$$\begin{cases} p_\gamma = S_\omega^*(S_\omega u_\gamma - z), \\ -u_\gamma = \gamma \min(0, p_\gamma + \alpha). \end{cases}$$

The semismooth Newton method discussed above can be applied after straightforward modifications; see Remark 8.2.5 ff.

2.1.3 CONFORMING APPROXIMATION FRAMEWORK

In the previous sections, we have introduced a regularization in order to apply semismooth Newton methods in function spaces. Since for every $\gamma > 0$ the regularized controls u_γ are in $L^2(\Omega)$, the Newton steps can be discretized in this case using a standard finite difference or finite element method (*optimize-then-discretize*). On the other hand, if we apply a conforming discretization to problem (2.1.1), the resulting finite-dimensional optimality system will be semismooth without additional regularization. This will allow the numerical solution of the (semi-discretized) problem in measure space.

The crucial idea here is to construct a finite-dimensional subspace of $\mathcal{M}(\Omega)$ by considering a conforming discretization of $C_0(\Omega)$ and then mirroring the duality of $C_0(\Omega)$ and $\mathcal{M}(\Omega)$ on a discrete level. We start from the standard finite element approximation of continuous functions. Let $\{\mathcal{T}_h\}_{h>0}$ be a family of shape regular triangulations of $\overline{\omega}$ and let $\{x_j\}_{j=1}^{N_h}$ denote the interior nodes of the triangulation $\mathcal{T}_h$; see section 9.3 for the precise definitions. Associated to these nodes we consider the nodal basis formed by the continuous piecewise linear functions $\{e_j\}_{j=1}^{N_h}$ such that $e_j(x_i) = \delta_{ij}$ for every $1 \leqslant i, j \leqslant N_h$. We now define

$$Y_h = \left\{ y_h \in C_0(\Omega) : y_h = \sum_{j=1}^{N_h} y_j e_j, \text{ where } \{y_j\}_{j=1}^{N_h} \subset \mathbb{R} \right\}$$

endowed with the supremum norm. Since any function $y_h \in Y_h$ attains its maximum and minimum at one of the nodes, we have

$$\|y_h\|_{C_0} = \max_{1 \leqslant j \leqslant N_h} |y_j| = |\vec{y}_h|_\infty,$$

where we have identified y_h with the vector $\vec{y}_h = (y_1, \ldots, y_{N_h})^T \in \mathbb{R}^{N_h}$ of its expansion coefficients, and $|\cdot|_p$ denotes the usual p-norm in $\mathbb{R}^{N_h}$. Similarly, we define

$$U_h = \left\{ u_h \in \mathcal{M}(\Omega) : u_h = \sum_{j=1}^{N_h} u_j \delta_{x_j}, \text{ where } \{u_j\}_{j=1}^{N_h} \subset \mathbb{R} \right\},$$

where δ_{x_j} is the Dirac measure corresponding to the node x_j, i.e., $\langle \delta_{x_j}, v \rangle_{\mathcal{M},C_0} = v(x_j)$ for all $v \in C_0(\Omega)$. For $u_h \in U_h$, we have

$$\|u_h\|_{\mathcal{M}} = \sup_{\|v\|_C = 1} \sum_{j=1}^{N_h} u_j \langle \delta_{x_j}, v \rangle = \sum_{j=1}^{N_h} |u_j| = |\vec{u}_h|_1.$$

Hence endowed with these norms, U_h is the topological dual of Y_h with respect to the duality pairing

$$(2.1.9) \qquad \langle u_h, y_h \rangle_{\mathcal{M},C_0} = \sum_{j=1}^{N_h} u_j y_j = \vec{u}_h^T \vec{y}_h.$$

The natural conforming discretization of $\mathcal{M}(\Omega)$ is thus by a linear combination of Dirac measures.

To analyze the discretization of the optimal control problem, it will be useful to define the linear operators $\Pi_h : C_0(\Omega) \to Y_h$ and $\Lambda_h : \mathcal{M}(\Omega) \to U_h$ by

$$\Pi_h y = \sum_{j=1}^{N_h} y(x_j) e_j \quad \text{and} \quad \Lambda_h u = \sum_{j=1}^{N_h} \langle u, e_j \rangle \delta_{x_j}.$$

It is straightforward to verify using (2.1.9) that Λ_h is the weak-$\star$ adjoint of Π_h and that

$$(2.1.10) \qquad \langle u, y_h \rangle_{\mathcal{M}, C_0} = \langle \Lambda_h u, y_h \rangle_{\mathcal{M}, C_0}$$

for all $u \in \mathcal{M}(\Omega)$ and $y_h \in Y_h$. Furthermore, $\Lambda_h u$ converges weakly-$\star$ in $\mathcal{M}(\Omega)$ to u as $h \to 0$ and $\|\Lambda_h\|_{\mathcal{L}(\mathcal{M}(\Omega), U_h)} \leqslant 1$; see Theorem 9.3.1.

We now consider the semi-discrete optimal control problem

$$(2.1.11) \qquad \begin{cases} \displaystyle\min_{u \in \mathcal{M}(\Omega)} \frac{1}{2}\|y_h - z\|_{L^2(\Omega_h)}^2 + \alpha\|u\|_{\mathcal{M}(\Omega)}, \\[2mm] \text{s.t.} \quad a(y_h, v_h) = \langle u, v_h \rangle_{\mathcal{M}, C_0} \quad \text{for all } v_h \in Y_h, \end{cases}$$

where $a : H^1(\Omega) \times H^1(\Omega) \to \mathbb{R}$ is the bilinear form associated with the operator A. Note that we have only discretized the state, but not the control; in this sense, this approach is related to the variational discretization method introduced in [Hinze 2005]. As before, we obtain the existence of an optimal control $\bar{u} \in \mathcal{M}(\Omega)$; however, since the mapping $u \mapsto y_h$ is not injective due to (2.1.10), the control is not unique. Nevertheless, by the same argument, there exists a unique $\bar{u}_h \in U_h$ such that every solution $\bar{u} \in \mathcal{M}(\Omega)$ satisfies $\Lambda_h \bar{u} = \bar{u}_h$; see Theorem 9.3.2. This means that we even if we restrict the control space to U_h, the computed control will be optimal for (2.1.11) as well.

Using the properties of Λ_h, one can show weak-$\star$ convergence of $\bar{u}_h$ to solutions of (2.1.1) in $\mathcal{M}(\Omega)$ and strong convergence of the corresponding states $\bar{y}_h$ to $\bar{y}$ in $L^2(\Omega)$ as $h \to 0$; see Theorem 9.3.5. If z is sufficiently smooth, we also obtain a rate for the latter:

$$\|\bar{y} - \bar{y}_h\|_{L^2(\Omega)} \leqslant Ch^{\frac{\kappa}{2}},$$

where $\kappa = 1$ if $n = 2$ and $\kappa = 1/2$ if $n = 3$; see Theorem 9.4.2.

To compute the optimal control $\bar{u}_h$, we formulate problem (2.1.11) in terms of the coefficient vectors $\vec{u}_h$ and $\vec{y}_h$. Introducing the stiffness matrix A_h corresponding to A, we have

$$\begin{cases} \displaystyle\min_{\vec{u}_h \in \mathbb{R}^{N_h}} \frac{1}{2}|\vec{y}_h - \vec{z}_h|_2^2 + \alpha|\vec{u}_h|_1, \\[2mm] \text{s.t.} \quad A_h \vec{y}_h = \vec{u}_h. \end{cases}$$

(Note that the "mass matrix" corresponding to $\langle u_h, v_h \rangle_{\mathcal{M}, C_0}$ is the identity.) Applying Fenchel duality as above and introducing the optimal state vector $\bar{y}_h \in \mathbb{R}^{N_h}$, we obtain for the vectors $\bar{u}_h, \bar{p}_h \in \mathbb{R}^{N_h}$ the optimality conditions

$$\begin{cases} A_h \bar{y}_h = \bar{u}_h, \\ A_h^\top \bar{p}_h = M_h(\bar{y}_h - y_{d,h}), \\ -\bar{u}_h = \max(0, -\bar{u}_h + \gamma(\bar{p}_h - \alpha)) + \min(0, -\bar{u}_h + \gamma(\bar{p}_h + \alpha)) \end{cases}$$

for any $\gamma > 0$, where M_h is the mass matrix corresponding to Y_h, and max and min should be understood componentwise in $\mathbb{R}^{N_h}$. Since we are in finite dimensions, this system can be solved using a semismooth Newton method. In practice, a continuation strategy based on a Moreau–Yosida regularization (obtained by dropping the terms $-\bar{u}_h$ on the right hand side of the last equation) is useful to compute a good starting point for the Newton iteration.

This framework can also be applied to the case of Neumann boundary controls in the space $\mathcal{M}(\Gamma)$; see section 9.5.

2.2   PARABOLIC PROBLEMS WITH RADON MEASURES

When applying the above framework to control problems involving parabolic partial differential equations, the situation is more difficult due to the low regularity of the states. For right hand sides in the space $\mathcal{M}(\Omega_T)$, where $\Omega_T := (0, T) \times \Omega$, the solution to the heat equation is only in $L^r(0, T; L^2(\Omega))$ for $r < 2$. (Using the duality technique, $r = 2$ would require $C(\Omega_T)$ regularity for solutions to the adjoint equation with right hand sides in $L^2(\Omega_T)$, which does not hold.) If we want to consider distributed L^2 tracking, we need to use controls that are more regular in time. This leads to the space $L^2(0, T; \mathcal{M}(\Omega))$ defined in section 1.1.2. The resulting controls are smooth in time, but exhibit sparsity in space; such controls can be used to model moving point sources. The spatio-temporal coupling of the corresponding control cost, however, presents a challenge for deriving numerically useful optimality conditions.

We thus consider the optimal control problem

(2.2.1)
$$\begin{cases} \min_{u \in L^2(I, \mathcal{M}(\Omega))} \frac{1}{2}\|y - z\|_{L^2(\Omega_T)}^2 + \alpha\|u\|_{L^2(\mathcal{M})}, \\ \text{s.t.} \quad \partial_t y + Ay = u \quad \text{in } \Omega_T, \\ \qquad\qquad y(x, 0) = y_0 \quad \text{in } \Omega \end{cases}$$

for given $y_0 \in L^2(\Omega)$. If A (and A^*) enjoys maximal parabolic regularity, the state equation is well-posed in $L^2(0, T; W_0^{1, q'}(\Omega))$ for all $q' \in [1, \frac{n}{n-1})$; see Theorem 10.2.2 for the case $A = -\Delta$. The control problem (2.2.1) then has a unique solution $\bar{u} \in L^2(0, T; \mathcal{M}(\Omega))$; see Theorem 10.3.2. Although the derivation of optimality conditions is deferred to later, let us

note that we can again deduce sparsity properties of the optimal control from them: For almost every $t \in [0, T]$,

$$\text{supp}(\bar{u}^+(t)) \subset \{x \in \Omega : \bar{p}(x, t) = -\|\bar{p}(t)\|_{C_0}\},$$
$$\text{supp}(\bar{u}^-(t)) \subset \{x \in \Omega : \bar{p}(x, t) = +\|\bar{p}(t)\|_{C_0}\},$$

where $\bar{p}$ denotes the adjoint state; see Theorem 10.3.3. This implies that the control is active where the adjoint state attains its maximum or minimum over Ω independently at each time t, and hence a purely spatial sparsity structure for the controls.

The approximation framework for $L^2(0, T; \mathcal{M}(\Omega))$ is again based on applying discrete duality to a conforming discretization of $L^2(0, T; C_0(\Omega))$. For the spatial discretization, we take the framework introduced in section 2.1.3; the temporal discretization uses piecewise constant functions. This leads to a dG(0)cG(1) discontinuous Galerkin approximation of the state equation; see, e.g., [Thomée 2006]. Specifically, we introduce a temporal grid $0 = t_0 < t_1 < \ldots < t_{N_\tau} = T$ with $\tau_k = t_k - t_{k-1}$ and set $\tau = \max_{1 \leqslant k \leqslant N_\tau} \tau_k$. For every $\sigma = (\tau, h)$ we now define the discrete spaces

$$\mathcal{Y}_\sigma = \{y_\sigma \in L^2(0, T; C_0(\Omega)) : y_\sigma|_{(t_{k-1}, t_k]} \in Y_h, \ 1 \leqslant k \leqslant N_\tau\},$$

$$\mathcal{U}_\sigma = \{u_\sigma \in L^2(0, T; \mathcal{M}(\Omega)) : u_\sigma|_{(t_{k-1}, t_k]} \in U_h, \ 1 \leqslant k \leqslant N_\tau\}.$$

The elements $u_\sigma \in \mathcal{U}_\sigma$ and $y_\sigma \in \mathcal{Y}_\sigma$ can be represented in the form

$$u_\sigma = \sum_{k=1}^{N_\tau} u_{k,h}\chi_k \quad \text{and} \quad y_\sigma = \sum_{k=1}^{N_\tau} y_{k,h}\chi_k,$$

where χ_k is the characteristic function of the interval $(t_{k-1}, t_k]$, $u_{k,h} \in U_h$, and $y_{k,h} \in Y_h$. Identifying again u_σ with the vector $\vec{u}_\sigma$ of expansion coefficients u_{kj}, we have for all $u_\sigma \in \mathcal{U}_\sigma$ that

$$\|u_\sigma\|_{L^2(\mathcal{M})}^2 = \int_0^T \left\| \sum_{k=1}^{N_\tau} \sum_{j=1}^{N_h} u_{kj}\chi_k\delta_{x_j} \right\|_{\mathcal{M}}^2 dt = \sum_{k=1}^{N_\tau} \tau_k \left(\sum_{j=1}^{N_h} |u_{kj}| \right)^2 = \sum_{k=1}^{N_\tau} \tau_k |\vec{u}_k|_1^2$$

for $\vec{u}_k = (u_{k1}, \ldots, u_{kN_h})^T$, and similarly for all $y_\sigma \in \mathcal{Y}_\sigma$ that

$$\|y_\sigma\|_{L^2(C_0)}^2 = \sum_{k=1}^{N_\tau} \tau_k \left(\max_{1 \leqslant j \leqslant N_h} |y_{kj}| \right)^2 = \sum_{k=1}^{N_\tau} \tau_k |\vec{y}_k|_\infty^2.$$

It is thus straightforward to verify that endowed with these norms, $\mathcal{U}_\sigma$ is the topological dual of $\mathcal{Y}_\sigma$ with respect to the duality pairing

(2.2.2) $$\langle u_\sigma, y_\sigma \rangle_{L^2(\mathcal{M}), L^2(C_0)} = \sum_{k=1}^{N_\tau} \tau_k \sum_{j=1}^{N_h} u_{kj}y_{kj} = \sum_{k=1}^{N_\tau} \tau_k (\vec{u}_k^T \vec{y}_k).$$

As in the elliptic case, we now introduce the linear operators

$$\Phi_\sigma : L^2(0,T;\mathcal{M}(\Omega)) \to \mathcal{U}_\sigma, \qquad \Psi_\sigma : L^2(0,T;C_0(\Omega)) \to \mathcal{Y}_\sigma$$

by

$$\Phi_\sigma u = \sum_{k=1}^{N_\tau} \frac{1}{\tau_k} \int_{I_k} \Lambda_h u(t)\, dt\, \chi_k, \qquad \Psi_\sigma y = \sum_{k=1}^{N_\tau} \frac{1}{\tau_k} \int_{I_k} \Pi_h y(t)\, dt\, \chi_k,$$

which satisfy

$$\langle u, y_\sigma \rangle_{L^2(\mathcal{M}),L^2(C_0)} = \langle \Phi_\sigma u, y_\sigma \rangle_{L^2(\mathcal{M}),L^2(C_0)}$$

for all $u \in L^2(0,T;\mathcal{M}(\Omega))$ and $y_\sigma \in \mathcal{Y}_\sigma$. Furthermore, $\Phi_\sigma u$ converges weakly-$\star$ to u in $L^2(0,T;\mathcal{M}(\Omega))$ as $\sigma \to 0$ and $\|\Phi_\sigma\|_{\mathcal{L}(L^2(\mathcal{M}),\mathcal{U}_\sigma)} \leqslant 1$; see Theorem 10.4.2.

Since the dG(0)cg(1) discontinuous Galerkin approximation can be formulated as a variant of the implicit Euler method, the semi-discrete optimal control problem can be written as
(2.2.3)

$$\begin{cases} \displaystyle\min_{u \in L^2(0,T;\mathcal{M}(\Omega))} \frac{1}{2}\|y_\sigma - z\|^2_{L^2(\Omega_T)} + \alpha\|u\|_{L^2(\mathcal{M})}, \\[2ex] \quad \text{s.t.} \quad \left(\frac{y_{k,h} - y_{k-1,h}}{\tau_k}, v_h\right) + a(y_{k,h}, v_h) = \frac{1}{\tau_k}\int_{\tau_{k-1}}^{\tau_k} \langle u(t), v_h\rangle_{\mathcal{M},C_0}\, dt, \\[2ex] \qquad\qquad\qquad\qquad y_{0,h} = y_0, \end{cases}$$

Again, since only the state is discretized, the solution $\bar{u}$ is not unique in $L^2(0,T;\mathcal{M}(\Omega))$, but there exists a unique $\bar{u}_\sigma \in \mathcal{U}_\sigma$ such that every solution $\bar{u} \in L^2(0,T;\mathcal{M}(\Omega))$ satisfies $\Phi_\sigma \bar{u} = \bar{u}_\sigma$. Convergence as $\sigma \to 0$, including rates, can be obtained in a similar fashion as in the elliptic case; see sections 10.4 and 10.5.

For the computation of the optimal control $\bar{u}_\sigma$, we formulate (2.2.3) in terms of the expansion coefficients $u_{k,h}$ and $y_{k,h}$. Let $N_\sigma = N_\tau \times N_h$ and identify as above $u_\sigma \in \mathcal{U}_\sigma$ with the vector $\vec{u}_\sigma = (u_{11}, \ldots, u_{1N_h}, \ldots, u_{N_\tau N_h})^\mathsf{T} \in \mathbb{R}^{N_\sigma}$ of coefficients, and similarly $y_\sigma \in \mathcal{Y}_\sigma$ with $\bar{y}_\sigma$; see section 10.4.1. To keep the notation simple, we will omit the vector arrows from here on and fix $y_0 = 0$. Then the discrete state equation can be expressed as $L_\sigma y_\sigma = u_\sigma$ with

$$L_\sigma = \begin{pmatrix} \tau_1^{-1}M_h + A_h & 0 & 0 \\ -\tau_1^{-1}M_h & \tau_2^{-1}M_h + A_h & 0 \\ 0 & \ddots & \ddots \end{pmatrix} \in \mathbb{R}^{N_\sigma \times N_\sigma}.$$

Introducing for $v_\sigma \in \mathbb{R}^{N_\sigma}$ the vectors $v_k = (v_{k1}, \ldots, v_{kN_h})^\mathsf{T} \in \mathbb{R}^{N_h}$, $1 \leqslant k \leqslant N_\tau$, the discrete optimal control problem (2.2.3) can be stated in reduced form as

$$\min_{u_\sigma \in \mathbb{R}^{N_\sigma}} \frac{1}{2}\sum_{k=1}^{N_\tau} \tau_k [L_\sigma^{-1}u_\sigma - z_\sigma]_k^\mathsf{T} M_h [L_\sigma^{-1}u_\sigma - z_\sigma]_k + \alpha \left(\sum_{k=1}^{N_\tau} \tau_k |u_k|_1^2\right)^{1/2}.$$

We now set

$$\mathcal{F}: \mathbb{R}^{N_\sigma} \to \mathbb{R}, \qquad \mathcal{F}(v) = \alpha \left(\sum_{k=1}^{N_\tau} \tau_k |v_k|_1^2 \right)^{1/2},$$

$$\mathcal{G}: \mathbb{R}^{N_\sigma} \to \mathbb{R}, \qquad \mathcal{G}(v) = \frac{1}{2} \sum_{k=1}^{N_\tau} \tau_k (v_k - z_k)^\mathsf{T} M_h (v_k - z_k),$$

$$\Lambda: \mathbb{R}^{N_\sigma} \to \mathbb{R}^{N_\sigma}, \qquad \Lambda v = L_\sigma^{-1} v,$$

and calculate the Fenchel conjugates with respect to the topology induced by the duality pairing (2.2.2). For $\mathcal{G}$, direct calculation yields that

$$\mathcal{G}^*(q) = \frac{1}{2} \sum_{k=1}^{N_\tau} \tau_k \left((q_k + M_h z_k)^\mathsf{T} M_h^{-1} (q_k + M_h z_k) - z_k^\mathsf{T} M_h z_k \right)$$

For $\mathcal{F}$, we have by example (iii) in section 1.2.1 that

$$\mathcal{F}^*(q) = \delta_{B_\alpha}(q) = \begin{cases} 0 & \text{if } \left(\sum_{k=1}^{N_\tau} \tau_k |q_k|_\infty^2 \right)^{1/2} \leqslant \alpha, \\ \infty & \text{otherwise.} \end{cases}$$

This leads to the dual problem

$$\min_{p_\sigma \in \mathbb{R}^{N_\sigma}} \frac{1}{2} \sum_{k=1}^{N_\tau} \tau_k ([L_\sigma^\mathsf{T} p_\sigma]_k - M_h z_k)^\mathsf{T} M_h^{-1} ([L_\sigma^\mathsf{T} p_\sigma]_k - M_h z_k) + \delta_{B_\alpha}(p_\sigma).$$

Here, we cannot make direct use of the extremality relations since we have no pointwise characterization of the subdifferential of $\mathcal{F}^*$. We thus consider the following equivalent reformulation

$$\begin{cases} \displaystyle \min_{p_\sigma \in \mathbb{R}^{N_\sigma}, c_\sigma \in \mathbb{R}^{N_\tau}} \frac{1}{2} \sum_{k=1}^{N_\tau} \tau_k ([L_\sigma^\mathsf{T} p_\sigma]_k - M_h z_k)^\mathsf{T} M_h^{-1} ([L_\sigma^\mathsf{T} p_\sigma]_k - M_h z_k) \\ \\ \qquad \text{s.t.} \quad |p_k|_\infty \leqslant c_k \text{ for all } 1 \leqslant k \leqslant N_\tau \quad \text{and} \quad \sum_{k=1}^{N_\tau} \tau_k c_k^2 = \alpha^2, \end{cases}$$

where $c_\sigma = (c_1, \dots, c_{N_\tau})^\mathsf{T} \in \mathbb{R}^{N_\tau}$. Since the constraints satisfy a Maurer–Zowe regular point condition (that the feasible set contains an interior point), we obtain first order optimality conditions which can be reformulated as

$$\begin{cases} L_\sigma \bar{y}_\sigma - \bar{u}_\sigma = 0, \\ L_\sigma^\mathsf{T} \bar{p}_\sigma - M_\sigma(\bar{y}_\sigma - z_\sigma) = 0, \\ \bar{u}_k + \max(0, -\bar{u}_k + \gamma(\bar{p}_k - \bar{c}_k)) + \min(0, -\bar{u}_k + \gamma(\bar{p}_k + \bar{c}_k)) = 0, \\ \displaystyle \sum_{j=1}^{N_h} [-\max(0, -\bar{u}_k + \gamma(\bar{p}_k - \bar{c}_k)) + \min(0, -\bar{u}_k + \gamma(\bar{p}_k + \bar{c}_k))]_j + 2\lambda \bar{c}_k = 0, \\ \displaystyle \sum_{k=1}^{N_\tau} \tau_k \bar{c}_k^2 - \alpha^2 = 0, \end{cases}$$

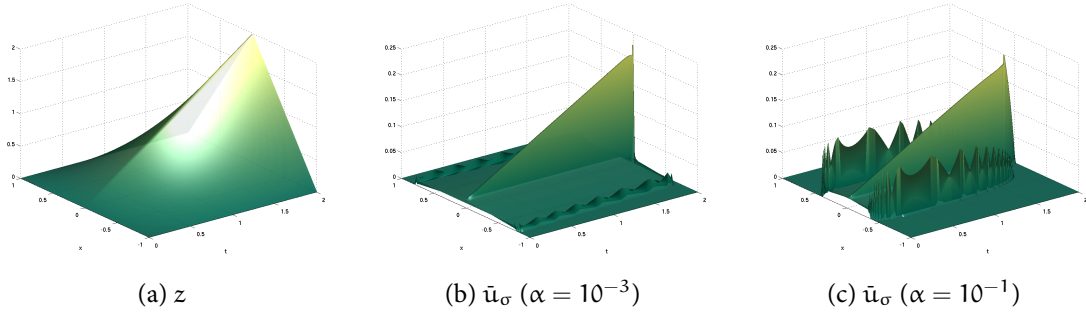(a) z (b) $\bar{u}_\sigma$ ($\alpha = 10^{-3}$)   (c) $\bar{u}_\sigma$ ($\alpha = 10^{-1}$)

Figure 2.3: Target z and corresponding measure space optimal controls $\bar{u}_\sigma$ for $\alpha = 10^{-3}$ and $\alpha = 10^{-1}$

where the third and fourth equations hold for all $1 \leqslant k \leqslant N_\tau$. This system can be solved by a semismooth Newton method; a good starting point again can be computed using a continuation strategy based on a Moreau–Yosida regularization of the complementarity conditions; see section 10.6.

Figure 2.3 shows an example target and the corresponding measure space optimal control $\bar{u}_\sigma$ for two different values of α. The results demonstrate the expected sparsity structure: For larger α, the controls are sparser in space, but smoother in time. More examples can be found in section 10.7.

2.3 ELLIPTIC PROBLEMS WITH FUNCTIONS OF BOUNDED VARIATION

To treat controls in the space $BV(\Omega)$, we follow the approach of section 2.1.1. We consider the problem

$$\begin{cases} \min_{u \in BV(\Omega)} \dfrac{1}{2} \|y - z\|_{L^2}^2 + \alpha \|u\|_{BV} \\ \text{s.t.} \quad Ay = u \end{cases}$$

under the same assumptions as in section 2.1.1. Due to the embedding $BV(\Omega) \hookrightarrow \mathcal{M}(\Omega)$, the state equation is well-posed and existence of a unique minimizer follows again from standard arguments.

Here, we make use of the dense embedding $(C_0^\infty(\Omega))^n \hookrightarrow H_{\text{div}}^2(\Omega)$ to apply Fenchel duality in a Hilbert space setting. In the following, Lebesgue spaces of vector valued functions are denoted by a blackboard bold letter corresponding to their scalar equivalent, e.g., $\mathbb{L}^2(\Omega) := (L^2(\Omega))^n$. Now let

$$H_{\text{div}}^2(\Omega) := \left\{ v \in \mathbb{L}^2(\Omega) : \text{div}\, v \in \mathcal{W}, \, v \cdot v = 0 \text{ on } \partial\Omega \right\},$$

31

endowed with the norm $\|v\|_{H^2_{\mathrm{div}}}^2 := \|v\|_{\mathbb{L}^2}^2 + \|\operatorname{div} v\|_{\mathcal{W}}^2$. We set

$$
\begin{aligned}
&\mathcal{F} : H^2_{\mathrm{div}}(\Omega)^* \to \mathbb{R}, &\quad& \mathcal{F}(u) = \frac{1}{2} \left\| A^{-1} u - z \right\|_{\mathbb{L}^2}^2, \\
&\mathcal{G} : H^2_{\mathrm{div}}(\Omega)^* \to \mathbb{R}, &\quad& \mathcal{G}(v) = \alpha \|v\|_{\mathcal{M}^n}, \\
&\Lambda : \mathcal{W}^* \to H^2_{\mathrm{div}}(\Omega)^*, &\quad& \Lambda v = Dv,
\end{aligned}
$$

where D is the distributional gradient, and deduce from the Fenchel duality theorem that the dual problem

$$
\begin{cases}
\displaystyle \min_{p \in H^2_{\mathrm{div}}(\Omega)} \frac{1}{2} \left\| A^* \operatorname{div} p + z \right\|_{\mathbb{L}^2}^2 - \frac{1}{2} \|z\|_{\mathbb{L}^2}^2 \\[2mm]
\text{s.\,t.} \quad \|p\|_{(C_0)^n} \leqslant \alpha
\end{cases}
$$

has a solution (which however may not be unique); see Theorem 7.2.11. From the extremality relations, we obtain first order optimality conditions: There exists $\bar{\lambda} := D\bar{u} \in H^2_{\mathrm{div}}(\Omega)^*$ such that

$$
\begin{cases}
\langle A^* \operatorname{div} \bar{p} + z, A^* \operatorname{div} v \rangle_{\mathbb{L}^2} + \langle \lambda^*, v \rangle_{H^2_{\mathrm{div}}{}^*, H^2_{\mathrm{div}}} = 0, \\[2mm]
\langle \lambda^*, p - \bar{p} \rangle_{H^2_{\mathrm{div}}{}^*, H^2_{\mathrm{div}}} \leqslant 0,
\end{cases}
$$

for all $v, p \in H^2_{\mathrm{div}}(\Omega)$ with $\|p\|_{(C_0)^n} \leqslant \alpha$; see Corollary 7.2.12. These conditions also imply that for any $p \in H^2_{\mathrm{div}}(\Omega)$, $p \geqslant 0$,

$$
\langle D\bar{u}, p \rangle_{H^2_{\mathrm{div}}{}^*, H^2_{\mathrm{div}}} = 0 \quad \text{if} \quad \operatorname{supp}(p) \subset \{x : |\bar{p}(x)|_\infty < \alpha\}.
$$

This can be interpreted as a sparsity condition on the gradient of the control: The optimal control $\bar{u}$ will be constant on sets where the constraints on the dual variable $\bar{p}$ are inactive.

Since $\|A^* \operatorname{div} p\|_{\mathbb{L}^2}$ is only a seminorm on $H^2_{\mathrm{div}}(\Omega)$, we need to add additional regularization to ensure a unique solution. Since furthermore $H^2_{\mathrm{div}}(\Omega)$ does not embed into $\mathbb{L}^q$ for $q > 2$ – which is necessary to apply a semismooth Newton method, – we set $\mathcal{H} := H^2_{\mathrm{div}}(\Omega) \cap \mathcal{W}^n$ and consider the regularization

$$
\begin{aligned}
\min_{p \in \mathcal{H}} \frac{1}{2} \left\| A^* \operatorname{div} p + z \right\|_{\mathbb{L}^2}^2 &+ \frac{\beta}{2} \|\Delta p\|_{\mathbb{L}^2}^2 - \frac{1}{2} \|z\|_{\mathbb{L}^2}^2 \\
&+ \frac{\gamma}{2} \|\max(0, p - \alpha)\|_{\mathbb{L}^2}^2 + \frac{\gamma}{2} \|\min(0, p + \alpha)\|_{\mathbb{L}^2}^2
\end{aligned}
$$

with the corresponding optimality system

$$
\begin{cases}
\langle A^* \operatorname{div} p_\gamma + z, A^* \operatorname{div} v \rangle_{\mathbb{L}^2} + \beta \langle \Delta p_\gamma, \Delta v \rangle_{\mathbb{L}^2} + \langle \lambda_\gamma, v \rangle_{H^2_{\mathrm{div}}{}^*, H^2_{\mathrm{div}}} = 0, \\[2mm]
\lambda_\gamma = \gamma \max(0, p_\gamma - \alpha) + \min(0, p_\gamma + \alpha),
\end{cases}
$$

for all $v \in H^2_{\mathrm{div}}(\Omega)$, where Δ denotes the componentwise Laplacian with homogeneous Dirichlet boundary conditions, and the max, min are understood to act componentwise.
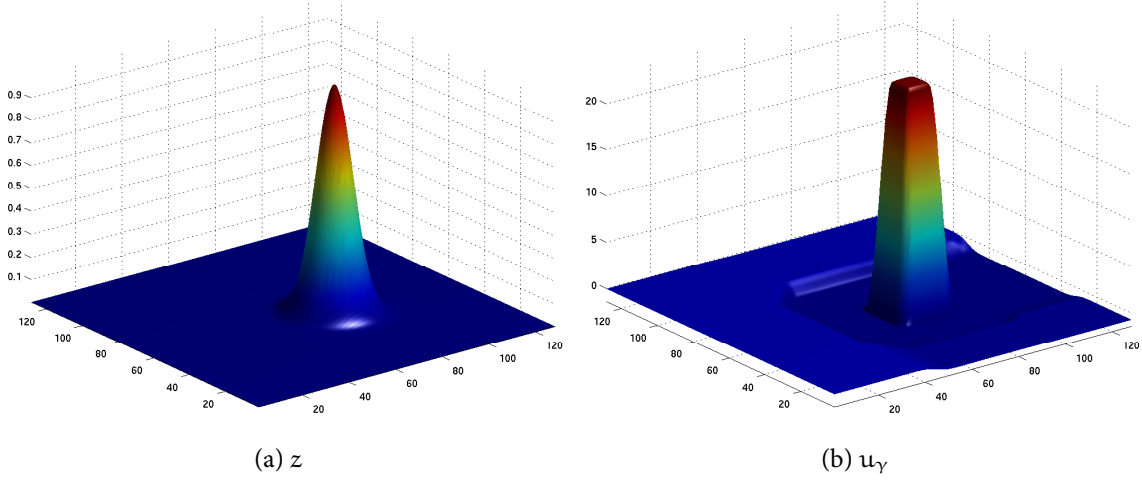
(a) z (b) u_γ

Figure 2.4: Target z and corresponding optimal control u_γ for $\alpha = 10^{-4}$, $\beta = 10^{-1}$, $\gamma = 10^7$

(Here and below, α stands for the vector $(\alpha, \ldots, \alpha) \in \mathbb{R}^n$.) This system can be written as a semismooth operator equation $F(p) = 0$ for $F : \mathcal{H} \to \mathcal{H}^*$,

$$\langle F(p), v \rangle_{\mathcal{H}^*, \mathcal{H}} := \langle A^* \operatorname{div} p + z, A^* \operatorname{div} v \rangle_{L^2} + \beta \langle \Delta p, \Delta v \rangle_{\mathbb{L}^2}$$
$$+ \gamma \langle \max(0, p - \alpha) + \min(0, p + \alpha), v \rangle_{L^2}$$

for all $v \in \mathcal{H}$. Its Newton derivative $D_N F$ is given by its action on h as

$$(2.3.1) \quad \langle D_N F(p)h, v \rangle_{\mathcal{H}^*, \mathcal{H}} = \langle A^* \operatorname{div} h, A^* \operatorname{div} v \rangle_{L^2} + \beta \langle \Delta h, \Delta v \rangle_{L^2}$$
$$+ \gamma \langle \chi_{\{x : |p(x)| > \alpha\}} h, v \rangle_{L^2},$$

where the last term is evaluated componentwise, i.e.,

$$(\chi_{\{x : |p(x)| > \alpha\}} h)_i(x) = \begin{cases} h_i(x) & \text{if } |p_i(x)| > \alpha, \\ 0, & \text{if } |p_i(x)| \leqslant \alpha, \end{cases}$$

for $i = 1, \ldots, n$. Since the weak form of the Newton derivative (2.3.1) by construction defines an inner product on $\mathcal{H}$, its inverse is uniformly bounded and the semismooth Newton method converges locally superlinearly; see Theorem 7.3.5.

Figure 2.4 shows an example target and the corresponding optimal control u_γ for $A = -\Delta$, $\alpha = 10^{-4}$, $\beta = 10^{-1}$ and $\gamma = 10^7$. It can be seen that the optimal controls tend to be piecewise constant. Note that although the target possesses rotational invariance, the optimal control does not; this is due to the anisotropy of the vector norm $|\cdot|_\infty$ used in the definition of the total variation. More examples can be found in section 7.4.

OPTIMAL CONTROL WITH L$^\infty$ FUNCTIONALS

3

This chapter treats optimal control problems where the functional to be minimized includes an L$^\infty$ norm. We can separate such problems into two classes, depending on the role of the norm:

- Problems with *tracking terms* in L$^\infty$ appear if the deviation from the target needs to be bounded uniformly everywhere in the domain; this amounts to a worst-case (in space) optimization problem.

- Problems with *control costs* in L$^\infty$ lead to optimal controls of bang-bang type (i.e., the control attains its upper or lower bound almost everywhere). This is relevant in cases where the control action is virtually cost-free, but the cost of constructing the control apparatus depends on the possible range of the control.

Note that such problems are related to but different from problems with pointwise constraints on the state or the control, since the constraints themselves are subject to optimization. Compared to problems with pointwise constraints, both types of L$^\infty$ optimal control problems have been studied relatively little in the context of partial differential equations.

The difficulty in their numerical solution arises from the fact that the subdifferential of the L$^\infty$ norm is difficult to characterize. This can be circumvented by a reformulation: The problem

$$\min_u \|f(u)\|_{L^\infty}^2$$

can equivalently be expressed as

$$\min_{c,v,u} c^2 \quad \text{s.t.} \quad \|v\|_{L^\infty} \leqslant c, \; f(u) = v,$$

see, e.g., [Ruszczyński 2006, Example 3.39], [Grund and Rösch 2001], and [Prüfert and Schiela 2009]. In this way, optimality conditions can be obtained under standard regular point conditions. The corresponding Lagrange multipliers are only in $(L^\infty(\Omega))^*$, but semismooth Newton methods can be applied after introducing a Moreau–Yosida regularization. The squared L$^\infty$ norm is considered in order to obtain positive definiteness of the Newton steps; note that this does not change the structural features of the problem, only the trade-off between minimizing the tracking term and the control cost for a fixed penalty parameter.

3.1 L^∞ TRACKING

We treat a slightly generalized problem

(3.1.1)
$$
\begin{cases}
\min_{c \in \mathbb{R}, u \in \mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2} |u|_2^2 \\[2mm]
\quad \text{s.t.} \quad Ay = f + \sum_{i=1}^{m} u_i \chi_{\omega_i}, \\[2mm]
\quad\quad -\beta_2 c + \psi_2 \leqslant y|_{\omega_0} \leqslant \beta_1 c + \psi_1,
\end{cases}
$$

where $\omega_i \subset \Omega, i = 0, \ldots, m$ are open and connected sets in Ω and $f \in L^q(\Omega)$ for some $q < \max(2, n)$. Further

$$
\beta_1, \beta_2 \in \mathbb{R} \text{ with } \beta_1, \beta_2 \geqslant 0 \quad \text{and} \quad \psi_1 \in L^\infty(\omega_0), \ \psi_2 \in L^\infty(\omega_0),
$$

and we assume that $\beta_1 + \beta_2 > 0$ as well as $\max \psi_2 \leqslant \min \psi_1$. To simplify notation, we introduce the control operator $B : \mathbb{R}^m \to L^\infty(\Omega)$, $Bu = \sum_{i=1}^{m} u_i \chi_{\omega_i}$.

This problem can be given the following interpretation: A pollutant f enters the groundwater and is (diffusively and/or convectively) transported throughout the domain Ω. To minimize the concentration y of a pollutant in a town ω_0, wells $\omega_1, \ldots, \omega_m$ are placed in Ω, through which a counter-agent u_i can be introduced. The problem is therefore to minimize the upper bound c in the formulation $y|_{\omega_0} \leqslant c$.

The case $\beta_1 = \beta_2 = 1$ and $\psi_1 = \psi_2 = 0$ corresponds to a problem with L^∞ tracking:

(3.1.2)
$$
\begin{cases}
\min_{u \in \mathbb{R}^m} \dfrac{1}{2} \|y\|_{L^\infty(\omega_0)}^2 + \dfrac{\alpha}{2} |u|_2^2 \\[2mm]
\text{s.t.} \quad Ay = f + Bu.
\end{cases}
$$

Since the functional in (3.1.1) is continuous and radially unbounded, the problem admits a unique solution $(\bar{u}, \bar{c})$; see Proposition 11.2.3. Optimality conditions follow from a Maurer–Zowe regular point condition; see Theorem 11.3.1. However, this leads to Lagrange multipliers that are only in $(L^\infty(\Omega))^*$, which is not amenable to numerical realization.

We thus consider the Moreau–Yosida regularization of (3.1.1),

$$
\begin{cases}
\min_{c \in \mathbb{R}, u \in \mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2} |u|_2^2 + \dfrac{\gamma}{2} \|\max(0, y|_{\omega_0} - \beta_1 c - \psi_1)\|_{L^2}^2 \\[3mm]
\quad\quad\quad\quad\quad\quad\quad + \dfrac{\gamma}{2} \|\min(0, y|_{\omega_0} + \beta_2 c - \psi_2)\|_{L^2}^2, \\[3mm]
\quad \text{s.t.} \quad Ay = f + Bu.
\end{cases}
$$

This is a smooth, strictly convex optimization problem with equality constraints satisfying a Slater condition (that the linearized constraint $(y, u) \mapsto Ay - Bu$ is surjective), and hence the necessary and sufficient optimality conditions are

$$
\begin{cases}
\alpha u_{\gamma,i} - \langle p_\gamma, \chi_{\omega_i} \rangle = 0, \quad i = 1, \ldots, m \\
c_\gamma - \langle \lambda_{\gamma,1}, \beta_1 \rangle + \langle \lambda_{\gamma,2}, \beta_2 \rangle = 0, \\
A^* p_\gamma + \tilde{\lambda}_\gamma = 0, \\
Ay_\gamma - f - Bu_\gamma = 0
\end{cases}
$$

where

$$
\begin{aligned}
\lambda_{\gamma,1} &= \gamma \max(0, y_\gamma|_{\omega_0} - \beta_1 c - \psi_1), \\
\lambda_{\gamma,2} &= \gamma \min(0, y_\gamma|_{\omega_0} + \beta_2 c - \psi_2), \\
\lambda_\gamma &= \lambda_{\gamma,1} + \lambda_{\gamma,2},
\end{aligned}
$$

and $\tilde{\lambda}_\gamma$ denotes the extension by zero to $\Omega \setminus \omega_0$ of λ_γ. As $\gamma \to \infty$, we have convergence of $(c_\gamma, u_\gamma, y_\gamma)$ to (c^*, u^*, y^*) in $\mathbb{R} \times \mathbb{R}^m \times W^{1,q}(\Omega)$; see Proposition 11.2.3. Furthermore, we have the rate

$$
\frac{1}{2}|c_\gamma - c^*|^2 + \frac{\alpha}{2}|u_\gamma - u^*|_2^2 = \mathcal{O}\left(\gamma^{-\frac{1-\theta}{1+\theta}}\right),
$$

where $\theta = \frac{nq}{nq + 2(q-n)}$; see Proposition 11.3.3.

Due to the regularity of the state equation and the embedding $\mathbb{R} \hookrightarrow L^\infty(\Omega)$, the optimality system, seen as an operator equation from $\mathbb{R}^m \times \mathbb{R} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega)$ to $\mathbb{R}^m \times \mathbb{R} \times W^{-1,q'}(\Omega) \times W^{-1,q}(\Omega)$, is semismooth with respect to y and c. The Newton derivative can be calculated in the usual fashion; see section 11.4 (due to the necessary additional notation, it is not given here). It can be shown that the Newton derivative has a uniformly bounded inverse, implying local superlinear convergence of the semismooth Newton method; see Proposition 11.4.1. Again, the problem of local convergence can be remedied with a continuation strategy in γ.

Figure 3.1 shows a model example for problem (3.1.2): The circular observation domain ω_0 (the "town") is situated in the center of the unit square $[-1, 1]^2$. On one side, a contaminant given by the function $f = 100(1 + y)\chi_{\{x:x>.75\}}$ enters the computational domain. Around the town, $m = 4$ control domains ("wells") are spaced equally. We consider convective-diffusive transport, which is described by the operator $Ay = -\nu\Delta y + b \cdot \nabla y$ with $\nu = 0.1$ and $b = (-1, 0)^\top$. Compared to the uncontrolled state y^0, the optimal state $\bar{y}$ is uniformly reduced within the observation domain ω_0. Since the state is bilaterally bounded, the controls opposite the support of the source are positive to avoid decreasing the lower bound. More examples are given in section 11.5.

(a) Geometric setup

(b) Uncontrolled state y^0

(c) Optimal control $\bar{u}$

(d) Optimal state $\bar{y}$
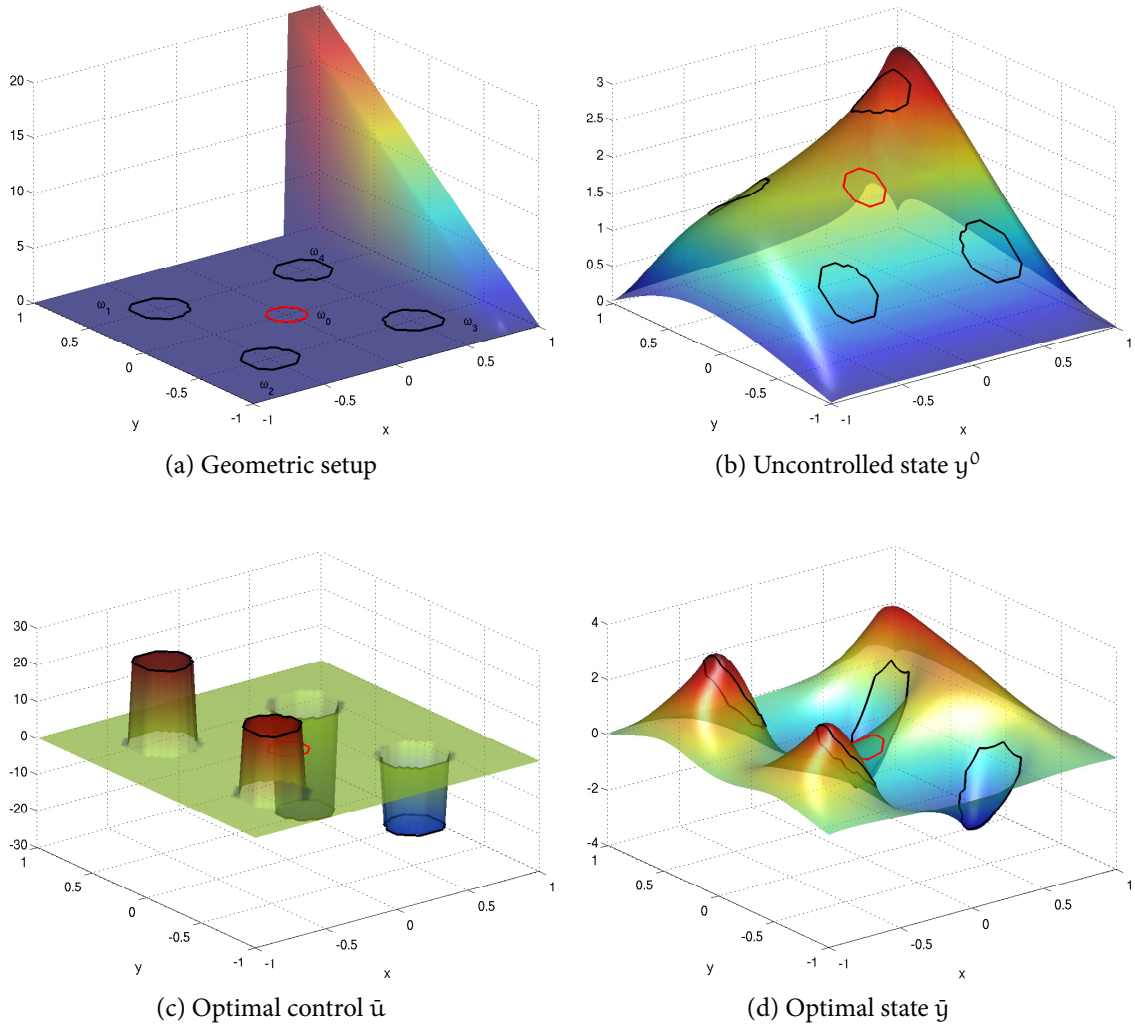
Figure 3.1: L$^\infty$ tracking problem. The upper left plot shows the pollutant f, while the circles give the observation domain ω_0 (red) and the control domains $\omega_1, \ldots, \omega_4$ (black). The upper right plot shows the uncontrolled state $y^0 = A^{-1}f$. The lower plots show the optimal control and state, respectively, for $\alpha = 10^{-6}$.

3.2 L^∞ CONTROL COST

We consider the optimal control problem

$$\begin{cases} \min_{u \in L^\infty(\Omega)} \frac{1}{2}\|y - z\|^2_{L^2} + \frac{\alpha}{2}\|u\|^2_{L^\infty} \\ \qquad \text{s.t.} \quad Ay = u. \end{cases}$$

Such problems are called *minimum effort problems* and have been studied in the context of ordinary partial differential equations; see, e.g., [Neustadt 1962]. They have received little attention for partial differential equations; see, e.g., [Zuazua 2007] and [Gugat and Leugering 2008] in the context of approximate and exact controllability of heat and wave equations. This may be related to the obvious difficulty arising from the non-differentiability appearing in the problem formulation.

Our approach rests on the equivalent formulation

(3.2.1)
$$\begin{cases} \min_{c \in \mathbb{R}, u \in L^\infty(\Omega)} \frac{1}{2}\|y - z\|^2_{L^2} + \frac{\alpha}{2}c^2 + \delta_{B_{L^\infty}}(u) \\ \qquad \text{s.t.} \quad Ay = cu, \end{cases}$$

which is strictly convex due to the square of the optimal L^∞ bound c. Here and in the following, we exclude the trivial case $\bar{c} = 0$. This problem admits a unique solution $(\bar{u}, \bar{c}) \in L^\infty(\Omega) \times \mathbb{R}$, which satisfies the first order optimality conditions

$$\begin{cases} \langle -\bar{p}, u - \bar{u}\rangle_{L^2} \geqslant 0 \quad \text{for all } u \text{ with } \|u\|_{L^\infty} \leqslant 1, \\ \alpha\bar{c} - \langle\bar{u}, \bar{p}\rangle_{L^2} = 0, \\ \bar{y} - z + A^*\bar{p} = 0, \\ A\bar{y} - \bar{c}\bar{u} = 0, \end{cases}$$

with the optimal state $\bar{y} \in H^1_0(\Omega)$ and the Lagrange multiplier $\bar{p} \in H^1_0(\Omega)$. Identifying $L^1(\Omega)$ with the weak-$\star$ dual of $L^\infty(\Omega)$ and applying the equivalence (1.2.11) to the first relation (which is the explicit form of $\bar{p} \in \partial\delta_{B_{L^\infty}}(\bar{u})$), we obtain

$$\bar{u} \in \partial(\|\cdot\|_{L^1})(\bar{p}) = \operatorname{sign}(\bar{p}).$$

Note that this relation directly implies the bang-bang nature of the optimal controls. Inserting this into the remaining equations and eliminating $\bar{y}$ yields the reduced optimality system

$$\begin{cases} AA^*\bar{p} + \bar{c}\operatorname{sign}(\bar{p}) = Az, \\ \alpha\bar{c} - \|\bar{p}\|_{L^1} = 0. \end{cases}$$

Since the multi-valued sign is not differentiable even in a generalized sense, we introduce for $\beta > 0$ a Huber-type smoothing of the L^1 norm and its derivative:

(3.2.2)
$$\begin{cases} AA^*p_\beta + c_\beta\operatorname{sign}_\beta(p_\beta) = Az, \\ \alpha c_\beta - \|p_\beta\|_{L^1_\beta} = 0, \end{cases}$$

where we have defined

$$(3.2.3) \qquad \|p\|_{L^1_\beta} := \int_\Omega |p(x)|_\beta \ dx, \qquad |p(x)|_\beta := \begin{cases} p(x) - \frac{\beta}{2} & \text{if } p(x) > \beta, \\ -p(x) - \frac{\beta}{2} & \text{if } p(x) < -\beta, \\ \frac{1}{2\beta} p(x)^2 & \text{if } |p(x)| \leqslant \beta, \end{cases}$$

and

$$\mathrm{sign}_\beta(p)(x) := \begin{cases} 1 & \text{if } p(x) > \beta, \\ -1 & \text{if } p(x) < -\beta, \\ \frac{1}{\beta} p(x) & \text{if } |p(x)| \leqslant \beta. \end{cases}$$

The optimality system (3.2.2) can also be obtained by adding the penalty $\frac{c}{2} \|u\|_{L^2}^2$ to (3.2.1) which allows deducing existence and uniqueness of solutions (c_β, p_β) to (3.2.2); see Proposition 12.3.1. The optimality condition $u_\beta = \mathrm{sign}_\beta(p_\beta)$ – corresponding to the first relation of (3.2.2) – implies that the regularized controls are of bang-zero-bang type: either $u_\beta(x) = \pm 1$ or $|u_\beta(x)| \ll 1$. As $\beta \to 0$, the family of regularized solutions (u_β, c_β) contains a subsequence that converges strongly in $L^q(\Omega) \times \mathbb{R}_+$ for any $q \in [1, \infty)$ to $(\bar{u}, \bar{c})$; see Proposition 12.3.5. It also holds that $\beta \mapsto c_\beta \|u_\beta\|_{L^2}^2$ is monotonically decreasing; see Lemma 12.3.4.

Due to the local quadratic smoothing, $\|\cdot\|_{L^1_\beta}$ is Fréchet differentiable with derivative sign_β. Furthermore, the mapping $\psi : \mathbb{R} \to \mathbb{R}, t \mapsto \mathrm{sign}_\beta(t)$ is continuous and piecewise differentiable and hence defines a semismooth Nemytskii operator from $L^q(\Omega)$ to $L^p(\Omega)$ for every $q > p$ with Newton derivative

$$D_N \mathrm{sign}_\beta(v)h = \frac{1}{\beta} \chi_{\{x : |v(x)| \leqslant \beta\}} h.$$

for every $h \in L^q(\Omega)$. The regularity of $\bar{p}$ thus implies that (3.2.2) defines a semismooth operator equation $T(p, c) = 0$ for $T : \mathcal{W} \times \mathbb{R}_+ \to \mathcal{W}^* \times \mathbb{R}$. Uniform boundedness of the Newton step

$$\begin{cases} AA^* \delta p + c^k \frac{1}{\beta} \chi_{\{x : |v(x)| \leqslant \beta\}} \delta p + \mathrm{sign}_\beta(p^k)\delta c = -(AA^* p^k + c\, \mathrm{sign}_\beta(p^k) - Az), \\ \alpha \delta c - \langle \mathrm{sign}_\beta(p^k), \delta p \rangle = -(\alpha c^k - \|p^k\|_{L^1_\beta}) \end{cases}$$

once more follows from the fact that by assumption AA^* is an isometry from $\mathcal{W}$ to $\mathcal{W}^*$; see Proposition 12.4.1. This implies local superlinear convergence of the semismooth Newton method.

To combine this with a practical continuation in β requires adapting the stepsizes: If the Newton iteration did not converge for $\beta_n = \sigma \beta_{n-1}$ with $\sigma < 1$ after a given number of iterations (as monitored by the change in active sets), the result is discarded and the Newton iteration is restarted for a new $\beta_n = \sigma' \beta_{n-1}$ for $\sigma' > \sigma$. This requires an appropriate stopping rule to prevent stagnation. Here, a model function approach based on the function

(a) target z (b) control u_β ($\alpha = 5 \cdot 10^{-3}$)   (c) control u_β ($\alpha = 5 \cdot 10^{-5}$)
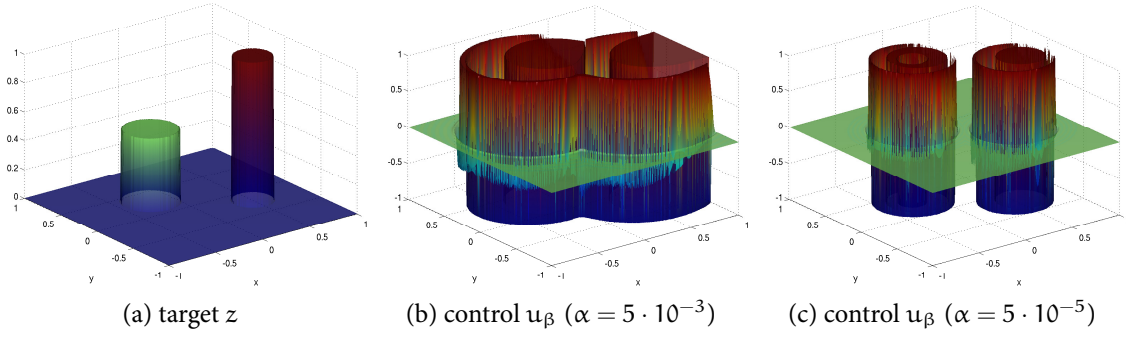
Figure 3.2: Minimum effort problem; shown are the target z and the corresponding optimal controls u_β for $\alpha = 5 \cdot 10^{-3}$ and $\alpha = 5 \cdot 10^{-5}$

$\beta \mapsto c_\beta \|u_\beta\|_{L^2}^2$ is followed: Using the current and the previous iterates, one constructs a two-parameter interpolant $m(\beta)$ and takes $m(0)$ as an estimate of $\bar{c} \|\bar{u}\|_{L^2}^2$. If $c_{\beta_n} \|u_{\beta_n}\|_{L^2}^2 > \mu m(0)$ for a given efficiency index $\mu < 1$, the continuation is terminated; see section 12.4.2 for details.

Figure 3.2 shows results for the convection-diffusion problem from Figure 3.1 for two different values of α. The continuation strategy terminated in both cases at $\beta \approx 2 \cdot 10^{-7}$. The bang-zero-bang nature of the regularized controls can be observed clearly. Comparing the optimal L^∞ bounds $c_\beta = 0.8788$ and $c_\beta = 6.8161$, respectively, with the unscaled controls u_β demonstrates the tradeoff between magnitude and support inherent in minimum effort problems. More examples are given in section 12.5.

INVERSE PROBLEMS WITH NON-GAUSSIAN NOISE

4

In this chapter, we consider the inverse problem

$$S(u) = y^\delta$$

for a compact (possibly nonlinear) operator S, where we are interested in recovering an unknown true solution $u^\dagger$ from measurements $y^\delta = S(u^\dagger) + \xi^\delta$, where ξ^δ is some (random or deterministic) observation error of magnitude δ (often called *noise level*). Since S is compact, this problem is ill-posed even if y^δ is in the range of S and S is invertible, in the sense that the solution u^δ does not depend continuously on the data. For this reason, one usually computes an approximation u_α of u^δ by minimizing the *Tikhonov functional*

$$(4.0.1) \qquad \mathcal{F}(S(u), y^\delta) + \alpha \mathcal{R}(u)$$

for an appropriate *discrepancy term* $\mathcal{F}$ and *regularization term* $\mathcal{R}$. If this problem has a unique solution u_α which converges to $u^\dagger$ as δ and α go to zero, this approach is called a *(Tikhonov) regularization* of the original inverse problem; the classical reference is [Engl, Hanke, and Neubauer 1996]. The choice of discrepancy and regularization term is crucial to achieve this, and the correct choice is intimately tied to a priori information about the problem. Specifically, the regularization term is often the (semi-)norm of an appropriate function space containing the true solution, and serves to enforce the desired structure of the solution. For example, higher order Sobolev or Lebesgue space norms yield smoother solutions, L^1-type norms promote sparsity, and total variation terms lead to piecewise constant solutions. This aspect, especially the last two examples, has attracted great interest in the last years. The discrepancy term has a similar connection with the observation error ξ^δ, and for random noise can often be deduced from statistical considerations. If ξ^δ is normally distributed, the appropriate discrepancy term is $\mathcal{F}(S(u), y^\delta) = \frac{1}{2} \left\| S(u) - y^\delta \right\|_{L^2}^2$, and this L^2 *data fitting term* is used in the vast majority of applications even if the Gaussian assumption is not justified. This is possibly due to the fact that the discrepancy terms for non-Gaussian noise may be nonsmooth, making the numerical solution challenging.

Here we will consider two such examples:

- *Impulsive noise* is characterized by significant outliers, i.e., large deviations which occur with much greater frequency than in Gaussian noise. On the other hand, not all data points are corrupted, i.e., there exist $x \in \Omega$ where $\xi^\delta(x) = 0$. Such noise frequently occurs in digital image acquisition and processing due to, e.g., malfunctioning pixels in camera sensors, faulty memory locations in hardware, or transmission in noisy channels. The assumption that there exist uncorrupted data points amounts to *sparsity* of the noise; this suggests choosing the discrepancy term

$$\mathcal{F}(S(u), y^\delta) = \left\| S(u) - y^\delta \right\|_{L^1}.$$

- *Uniform noise* can take any value between, say, $-\delta$ and δ with equal probability. Noise distributions of this type appear as statistical models of quantization errors and are therefore of relevance in any inverse problem where digital acquisition and processing of measured data plays a significant role, e.g., in the context of wireless sensor networks. Statistical considerations suggest that the choice

$$\mathcal{F}(S(u), y^\delta) = \left\| S(u) - y^\delta \right\|_{L^\infty}$$

is appropriate in this case.

Although the choice of discrepancy terms has received less attention than the choice of regularization terms, there has been considerable recent progress in the general theory of inverse problems in Banach spaces which covers the above cases; see, e.g., [Burger and Osher 2004; Resmerita 2005; Pöschl 2009; Scherzer et al. 2009]. Efficient methods for their numerical solution, however, are less well studied.

One issue that distinguishes minimizing the Tikhonov functional (4.0.1) from optimal control problems with a similar structure is the role played by the parameter α, which governs the trade-off between attaining the data (or target) and enforcing the desired structural properties of the minimizer. In optimal control, this trade-off is usually part of the model and thus fixed in advance. For inverse problems, on the other hand, there exists an optimal choice for α, namely the one that yields a minimizer u_α that is as close as possible to $u^\dagger$. The parameter choice thus depends on y^δ and is part of the problem.

Of course, without knowing the true solution $u^\dagger$, this optimal choice is not possible. There are two classes of practical choice rules: The rules in the first class are based on the noise level δ and allow proving error estimates for u_α in terms of the noise level. One popular rule is the *Morozov discrepancy principle*, where α is chosen such that the discrepancy term is on the order of the noise level δ. On the other hand, *heuristic rules* such as the quasi-optimality principle do not require knowledge of the noise level. Although one can construct for any such rule a worst-case example for which convergence does not hold (known as the "Bakushinskii veto"; see [Bakushinskii 1984]), they are desirable in practice since the noise level may not be available. This is especially the case for non-Gaussian noise.

Here, a heuristic choice rule is proposed that involves auto-calibration of the noise level for non-Gaussian noise. Specifically, α is chosen such that the *balancing principle*

$$(4.0.2) \qquad \sigma\mathcal{F}(S(u_\alpha), y^\delta) = \alpha\mathcal{R}(u_\alpha)$$

is satisfied. The parameter σ is a proportionality constant which depends on S and $\mathcal{R}$, but not on δ. The motivation is that if S is compact, $S(u)$ is smooth for any "reasonable" u, while non-Gaussian noise in general is not. If the discrepancy term is chosen appropriately, $\mathcal{F}(S(u), y^\delta)$ will therefore be a good estimate of the noise level δ for u reasonably close to $u^\dagger$. A similar assumption on the structural difference of noise and data allows proving (average-case) convergence rates for minimization-based heuristic choice rules; see [Kindermann 2011]. Of course, this is not a rigorous justification; but the rule performs quite well in practice and can be implemented using a simple fixed point iteration: For α_0 chosen sufficiently large, the iterates

$$(4.0.3) \qquad \alpha_{k+1} := \sigma\frac{\mathcal{F}(S(u_{\alpha_k}), y^\delta)}{\mathcal{R}(u_{\alpha_k})}$$

define a monotonically decreasing sequence that converges to a solution of (4.0.2). This follows from the fact that by the minimizing property of u_α, the mappings $\alpha \mapsto \mathcal{F}(S(u_\alpha), y^\delta)$ and $\alpha \mapsto \mathcal{R}(u_\alpha)$ are monotonically decreasing and monotonically increasing, respectively, as $\alpha \to 0$; see [Clason, Jin, and Kunisch 2010] and section 15.3. In practice, convergence is achieved within a few iterations.

4.1 L^1 DATA FITTING

We first consider inverse problems with data corrupted by impulsive noise. Specifically, we assume that y^δ is defined pointwise as

$$y^\delta(x) = \begin{cases} S(u^\dagger)(x) & \text{with probability } 1-d, \\ S(u^\dagger)(x) + \xi(x) & \text{with probability } d, \end{cases}$$

where $\xi(x)$ is a random variable, e.g., normally distributed with mean zero and typically large variance. The parameter $d \in (0, 1)$ represents the percentage of corrupted data points. As discussed above, this implies that $y^\delta - S(u^\dagger)$ is sparse, suggesting use of the L^1 norm as discrepancy term. To avoid additional complications, we further assume in the following that $u^\dagger$ is an element of a Hilbert space $\mathcal{X}$ and correspondingly fix $\mathcal{R}(u) = \frac{1}{2}\|u\|_{\mathcal{X}}^2$.

4.1.1 LINEAR INVERSE PROBLEMS

We begin with linear inverse problems, i.e., $S(u) = Ku$ for a bounded linear operator $K : L^2(\Omega) \to L^2(\Omega)$, and consider

$$\min_{u \in L^2(\Omega)} \|Ku - y^\delta\|_{L^1(\Omega)} + \frac{\alpha}{2}\|u\|_{L^2}^2 .$$

Since $u \in L^2(\Omega)$, standard results ensure the well-posedness of this problem: There exists a unique solution u_α which depends continuously on the data y^δ, and if $\alpha \to 0$ and $\delta/\alpha \to 0$, the minimizers u_α converge to $u^\dagger$. Furthermore, under a so-called source condition (that $u^\dagger$ lies in the range of K^*, which implies additional regularity of the true solution) one obtains rates for this convergence; see section 13.2.1.

We now apply Fenchel duality. Setting

$$\mathcal{F} : L^2(\Omega) \to \mathbb{R}, \qquad \mathcal{F}(v) = \frac{\alpha}{2} \|v\|_{L^2}^2,$$
$$\mathcal{G} : L^2(\Omega) \to \mathbb{R}, \qquad \mathcal{G}(v) = \|v - y^\delta\|_{L^1},$$
$$\Lambda : L^2(\Omega) \to L^2(\Omega), \qquad \Lambda v = K v,$$

and computing the Fenchel conjugates (with respect to the weak duality between $L^1(\Omega)$ and $L^\infty(\Omega)$ in case of $\mathcal{G}$), we obtain the dual problem

$$(4.1.1) \qquad \min_{p \in L^2(\Omega)} \frac{1}{2\alpha} \|K^* p\|_{L^2}^2 - \langle p, y^\delta \rangle_{L^2} + \delta_{B_{L^\infty}}(p),$$

where we have used (1.2.4) together with the transformation rules (1.2.2) (for $\mathcal{F}$) and (1.2.3) (for $\mathcal{G}$). The Fenchel duality theorem then yields existence of at least one minimizer $p_\alpha \in L^2(\Omega)$, which satisfies the extremality relations

$$(4.1.2) \qquad \begin{cases} K^* p_\alpha = \alpha u_\alpha, \\ \langle K u_\alpha - y^\delta, p_\alpha - p \rangle_{L^2} \leqslant 0, \end{cases}$$

for all $p \in L^2(\Omega)$ with $\|p\|_{L^\infty} \leqslant 1$, where we have again used the equivalence (1.2.11) to obtain the second relation; see Theorem 13.2.5. From the latter, we immediately deduce the following structural information:

$$\operatorname{supp}((K u_\alpha - y^\delta)^+) \subset \{x : p_\alpha(x) = 1\},$$
$$\operatorname{supp}((K u_\alpha - y^\delta)^-) \subset \{x : p_\alpha(x) = -1\}.$$

This can be interpreted as follows: the data is attained exactly at points where the bound constraint on p_α is inactive, and the sign of p_α is determined by the sign of the noise. The dual variable thus serves as a noise indicator.

If the inversion of K is ill-posed, solving the optimality system (4.1.2) is ill-posed as well. In addition, the low regularity $p_\alpha \in L^2(\Omega)$ prohibits application of semismooth Newton methods. We thus add a H^1 regularization term for p_α: For $\beta > 0$, we consider

$$(4.1.3) \qquad \min_{p \in H^1(\Omega)} \frac{1}{2\alpha} \|K^* p\|_{L^2}^2 + \frac{\beta}{2} \|\nabla p\|_{L^2}^2 - \langle p, y^\delta \rangle_{L^2} + \delta_{B_{L^\infty}}(p).$$

Under the assumption that $\ker K^* \cap \ker \nabla = \{0\}$, i.e., constant functions do not belong to the kernel of K^*, probem (4.1.3) is strictly convex and hence admits a unique solution. The family

of minimizers $\{p_\beta\}_{\beta>0}$ contains a subsequence converging weakly in $L^2(\Omega)$ to a minimizer p_α of (4.1.1); see Theorem 13.3.2. Since a regular point condition is satisfied for the box constraint, we obtain the optimality system

$$\begin{cases} \dfrac{1}{\alpha}KK^*p_\beta - \beta\Delta p_\beta - y^\delta + \lambda_\beta = 0, \\[2mm] \langle\lambda_\beta, p - p_\beta\rangle_{L^2} \leqslant 0, \end{cases}$$

for all $p \in H^1(\Omega)$ with $\|p\|_{L^\infty} \leqslant 1$ and a $\lambda_\beta \in (H^1(\Omega))^*$. Again, the low regularity of the Lagrange multiplier λ_β prevents a semismooth complementarity formulation, and we introduce for $\gamma > 0$ the Moreau–Yosida regularization

$$(4.1.4) \qquad \begin{cases} \dfrac{1}{\alpha}KK^*p_\gamma - \beta\Delta p_\gamma - y^\delta + \lambda_\gamma = 0, \\[2mm] \lambda_\gamma = \gamma\max(0, p_\gamma - 1)) + \gamma\min(0, p_\gamma + 1). \end{cases}$$

One can show convergence for $(p_\gamma, \lambda_\gamma)$ as $\gamma \to \infty$ for fixed $\beta \geqslant 0$; see Theorem 13.3.1 and Theorem 13.A.1.

Due to the regularity of $p_\beta \in H^1(\Omega)$, the optimality system (4.1.4) defines a semismooth nonlinear equation $F(p) = 0$ with $F : H^1(\Omega) \to (H^1(\Omega))^*$,

$$F(p) = \frac{1}{\alpha}KK^*p - \beta\Delta p + \gamma(\max(0, p - 1) + \min(0, p + 1)) - y^\delta,$$

which has the Newton derivative

$$D_N F(p)h = \frac{1}{\alpha}KK^*h - \beta\Delta h + \gamma\chi_{\{x:|p(x)|>1\}}h.$$

Since by assumption the inner product $\beta\langle\nabla\cdot, \nabla\cdot\rangle_{L^2} + \frac{1}{\alpha}\langle K^*\cdot, K^*\cdot\rangle_{L^2}$ induces an equivalent norm on $H^1(\Omega)$ for any $\beta > 0$, the Lax–Milgram theorem implies uniform invertibility of $D_N F(p)$ for fixed $\beta, \gamma > 0$ and hence local superlinear convergence of the semismooth Newton method. Since β should be chosen as small as possible without making $D_N F(p)$ numerically singular, one can apply a continuation strategy which is terminated as soon as the computed p_β becomes infeasible, i.e., $\|p_\beta\|_{L^\infty} \gg 1$. In practice, the continuation strategy for β is sufficient to deal with the local convergence of the Newton method, and the parameter γ can be fixed at a large value, e.g., $\gamma = 10^9$.

Figure 4.1 shows a typical realization of noisy data for an inverse heat conduction problem with $d = 0.3$ and compares the performance of L^1 fitting with L^2 fitting, demonstrating the increased robustness of the former. For comparison, in both cases the parameter was chosen from a range of 100 logarithmically spaced values to give the lowest L^2 reconstruction error. The reconstruction with the parameter $\alpha_b = 2.239 \times 10^{-2}$ chosen according to the balancing principle (4.0.2) is very close to the optimal reconstruction with $\alpha_{opt} = 2.009 \times 10^{-2}$. Details and further one- and two-dimensional examples can be found in section 13.5.

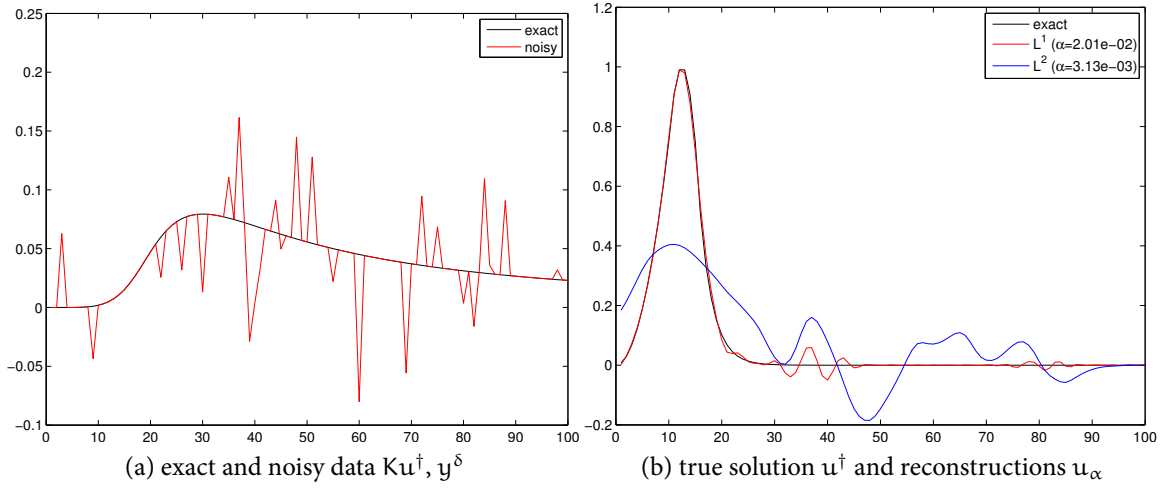(a) exact and noisy data $Ku^\dagger$, y^δ (b) true solution $u^\dagger$ and reconstructions u_α

Figure 4.1: Comparison of linear $L^1(\Omega)$ and $L^2(\Omega)$ fitting for inverse heat conduction problem ($d = 0.3$)

4.1.2 NONLINEAR INVERSE PROBLEMS

We now consider L^1 fitting for nonlinear inverse problems, in particular, for parameter identification for partial differential equations. Let $S : \mathcal{X} \to \mathcal{Y}$ denote the parameter-to-observation mapping, where $\mathcal{X}$ is a Hilbert space and the space $\mathcal{Y}$ compactly embeds into L^q for some $q > 2$. We also assume that y^δ is bounded almost everywhere, which is the case for data subject to impulsive noise. The spaces $\mathcal{X}$ and $\mathcal{Y}$ are defined on the bounded domains $\omega \subset \mathbb{R}^n$ and $D \subset \mathbb{R}^m$, respectively. To apply our approach, we assume that S is uniformly bounded in $U \subset \mathcal{X}$, completely continuous, and twice Fréchet differentiable with bounded first and second derivatives. These are generic assumptions in the context of parameter identification problems for partial differential equations, and are satisfied, for example, in the following situations.

- *Inverse potential problems* consist in recovering the potential u defined on $\omega = \Omega$ from noisy observational data y^δ in the domain $D = \Omega$, i.e., S maps $u \in U \subset \mathcal{X} = L^2(\Omega)$ to the solution $y \in \mathcal{Y} = H^1(\Omega)$ to

$$\begin{cases} -\Delta y + uy = f & \text{in } \Omega, \\ \dfrac{\partial y}{\partial n} = 0 & \text{on } \Gamma. \end{cases}$$

  Such problems arise in heat transfer, e.g., damping design and identifying heat radiative coefficients.

- *Inverse Robin coefficient problems* consist in recovering the Robin coefficient u defined on the boundary part $\omega = \Gamma_i$ from noisy observational data y^δ on the boundary part

$D = \Gamma_c$, i.e., S maps $u \in U \subset \mathcal{X} = L^2(\Gamma_i)$ to $y|_{\Gamma_c} \in \mathcal{Y} = H^{\frac{1}{2}}(\Gamma_c)$, where $v \mapsto v|_{\Gamma_c}$ denotes the Dirichlet trace operator and y is the solution to

$$\begin{cases} -\Delta y = 0 & \text{in } \Omega, \\ \dfrac{\partial y}{\partial n} = f & \text{on } \Gamma_c, \\ \dfrac{\partial y}{\partial n} + uy = 0 & \text{on } \Gamma_i. \end{cases}$$

This class of problems arises in corrosion detection and thermal analysis of quenching processes.

- *Inverse diffusion coefficient problems* consist in recovering the diffusion coefficient u defined on $\omega = \Omega$ from the noisy observational data y^δ in the domain $D = \Omega$, i.e., S maps $u \in U \subset \mathcal{X} = H^1(\Omega)$ to the solution $y \in \mathcal{Y} = W_0^{1,q}(\Omega)$, $q > 2$, to

$$\begin{cases} -\nabla \cdot (u\nabla y) = f & \text{in } \Omega, \\ y = 0 & \text{on } \Gamma. \end{cases}$$

Such problems arise in estimating the permeability of underground flow and the conductivity of heat transfer.

Under the above assumptions, the Tikhonov functional

(4.1.5) $$\min_{u \in U} \|S(u) - y^\delta\|_{L^1} + \frac{\alpha}{2}\|u\|_{\mathcal{X}}^2$$

is well-posed by standard arguments, and convergence rates can be obtained under the usual source conditions on $u^\dagger$; see section 14.2.1.

Since S is nonlinear, we cannot apply the Fenchel duality theorem. We therefore proceed as in section 2.1.2. Due to the differentiability assumptions, S is strictly differentiable, and hence the Tikhonov functional is Lipschitz continuous. We can therefore use Clarke's calculus for generalized gradients to obtain for any local minimizer u_α of (4.1.5) the optimality system

$$\begin{cases} S'(u_\alpha)^* p_\alpha + \alpha j(u_\alpha - u_0) = 0, \\ \langle S(u_\alpha) - y^\delta, p - p_\alpha \rangle_{L^1, L^\infty} \leqslant 0 & \text{for all } \|p\|_{L^\infty} \leqslant 1, \end{cases}$$

with a $p_\alpha \in L^\infty(D)$ with $\|p_\alpha\|_{L^\infty} \leqslant 1$. Here $S'(u)^*$ denotes the adjoint of $S'(u)$ with respect to $L^2(D)$, and $j : \mathcal{X} \to \mathcal{X}^*$ is the (linear) duality mapping, i.e., $j(u) = \partial(\frac{1}{2}\|\cdot\|_{\mathcal{X}}^2)(u)$; see Theorem 14.2.7.

As in section 3.2, we now apply the equivalence (1.2.11) to the second relation (which is the explicit form of $S(u_\alpha) - y^\delta \in \partial \delta_{B_{L^\infty}}(p_\alpha)$) to obtain

$$p_\alpha \in \partial(\|\cdot\|_{L^1})(S(u_\alpha) - y^\delta) = \text{sign}(S(u_\alpha) - y^\delta).$$

Inserting this into the first relation yields the necessary optimality condition

$$0 \in \alpha j(u_\alpha) + S'(u_\alpha)^*(\operatorname{sign}(S(u_\alpha) - y^\delta)).$$

Again, the non-differentiability of the multi-valued sign prevents application of Newton-type methods. We therefore consider for $\beta > 0$ the smoothed problem

$$\min_{u \in U} \|S(u) - y^\delta\|_{L^1_\beta} + \frac{\alpha}{2}\|u\|_\mathcal{X}^2,$$

with $\|\cdot\|_{L^1_\beta}$ defined as in (3.2.3). As $\beta \to 0$, the family of minimizers $\{u_\beta\}_{\beta > 0}$ contains a subsequence converging strongly in $\mathcal{X}$ to u_α; see Theorem 14.3.2.

Differentiability of $\|\cdot\|_{L^1_\beta}$ yields the necessary optimality condition

$$\alpha j(u_\beta) + S'(u_\beta)^*(\operatorname{sign}_\beta(S(u_\beta) - y^\delta)) = 0,$$

which defines a semismooth equation $F(u) = 0$ from $\mathcal{X}$ to $\mathcal{X}^*$ due to the linearity of the duality mapping in Hilbert spaces and the smoothing properties of S. By the chain rule for Newton derivatives we find the action of the Newton derivative on $\delta u \in \mathcal{X}$ as

$$D_N F(u)\delta u = \alpha j'(u^k)\delta u + (S''(u^k)\delta u)^* \operatorname{sign}_\beta(S(u^k) - y^\delta)) + \beta^{-1}S'(u^k)^*(\chi_{\mathcal{J}^k} S'(u^k)\delta u).$$

Given a way to compute the action of the derivatives $S'(u)h$, $S'(u)^*h$ and $[S''(u)h]^*p$ for given u, p and h, the Newton system can be solved using a matrix-free Krylov method. In the context of parameter identification for partial differential equations, this involves solving linearized forward and adjoint equations; see section 14.A for the explicit form of these derivatives for the model problems listed above.

To deduce superlinear convergence of the semismooth Newton method, it remains to show uniform invertibility of $D_N F(u)$. Since the operator S is nonlinear and the functional is thus in general non-convex, we need to assume a local quadratic growth condition at a minimizer u_β: There exists a constant $\gamma > 0$ such that

$$\langle S''(u_\beta)(h, h), \operatorname{sign}_\beta(S(u_\beta) - y^\delta)\rangle_{L^2} + \alpha\|h\|_\mathcal{X}^2 \geqslant \gamma\|h\|_\mathcal{X}^2$$

holds for all $h \in \mathcal{X}$. This is related to standard second-order sufficient optimality conditions in PDE-constrained optimization; see , e.g., [Tröltzsch 2010, Chapter 4.10]. The condition is satisfied for either large α or small noise (in the sense that $S(u_\beta) - y^\delta$ is sparse), which is a reasonable assumption for parameter fitting problems with impulsive noise. Under this condition, the inverse of $D_N F$ is uniformly bounded and thus local superlinear convergence holds; see Proposition 14.3.3. The Newton method is again combined with a continuation strategy in β, which is terminated if the semismooth Newton method failed to converge (as indicated by the change in active sets and the norm of the residual) after a given number of iterations.
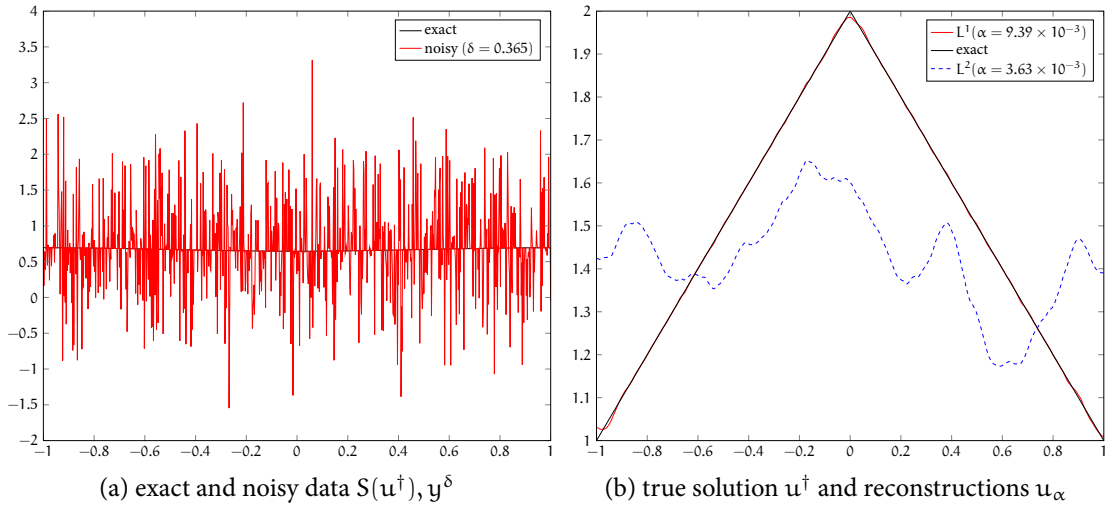
(a) exact and noisy data $S(u^\dagger), y^\delta$

(b) true solution $u^\dagger$ and reconstructions u_α

Figure 4.2: Comparison of nonlinear L^1 and L^2 fitting for inverse potential problem ($d = 0.6$)

Figure 4.2 shows a typical realization of noisy data for the inverse potential problem with $d = 0.6$, and compares the performance of L^1 fitting with L^2 fitting. For L^1 fitting, the regularization parameter α was chosen according to the balancing principle; the fixed point iteration (4.0.3) converged after 4 iterations. For L^2 fitting, the parameter is chosen from a range to give the smallest reconstruction error. Again, L^1 fitting is much more robust than L^2 fitting. More results for the model problems in one and two dimensions are given in section 14.4.

4.2 L^∞ DATA FITTING

We now consider linear inverse problems with data corrupted by uniformly distributed noise. Specifically, we assume that $S(u) = Ku$ for a bounded linear operator $K : \mathcal{X} \to L^\infty(\Omega)$, and $y^\delta \in L^\infty(\Omega)$ is defined pointwise as

$$y^\delta(x) = Ku^\dagger(x) + \xi(x),$$

where $\xi(x)$ is a uniformly distributed random value in the range $[-d\, y_{max}, d\, y_{max}]$ for a noise parameter $d > 0$ and $y_{max} = \|Ku^\dagger\|_\infty$. The main assumption on K is that

$$u_n \rightharpoonup u^\dagger \text{ in } \mathcal{X} \quad \text{implies} \quad Ku_n \to Ku^\dagger \text{ in } L^\infty(\Omega).$$

This holds if K is a compact operator or maps into a space compactly embedded into $L^\infty(\Omega)$ (as is commonly the case if K is the solution operator for a partial differential equation). We then consider for $p \in [1, \infty)$ the Tikhonov regularization

$$(4.2.1) \qquad \min_{u \in \mathcal{X}} \frac{1}{p} \left\| Ku - y^\delta \right\|_{L^\infty(\Omega)}^p + \frac{\alpha}{2} \|u\|_{\mathcal{X}}^2 .$$

Similar to the L^1 fitting case, well-posedness and convergence rates follow from standard results; see section 15.2. The reason for allowing $p > 1$ is to obtain positive definiteness of the Newton matrix; the value of p only influences the trade-off between minimizing the L^∞ norm of the residual and minimizing the norm of x, but not the relevant structural properties of the functional (in particular the geometry of the unit ball with respect to $\|\cdot\|_{L^\infty}^p$).

For the numerical solution of (4.2.1), we follow the approach presented in section 3.1. Fixing $p = 2$, we introduce the equivalent reformulation

$$\begin{cases} \min_{(u,c)\in X\times\mathbb{R}} & \dfrac{c^2}{2} + \dfrac{\alpha}{2}\|u\|_X^2 \\ \text{s.t.} & \left\|Ku - y^\delta\right\|_{L^\infty(\Omega)} \leqslant c. \end{cases}$$

Since a regular point condition is satisfied for the bound constraint, there exist Lagrange multipliers $\lambda_1, \lambda_2 \in L^\infty(\Omega)^*$ with

$$\langle \lambda_1, \varphi \rangle_{L^\infty(\Omega)^*, L^\infty(\Omega)} \leqslant 0, \qquad \langle \lambda_2, \varphi \rangle_{L^\infty(\Omega)^*, L^\infty(\Omega)} \geqslant 0$$

for all $\varphi \in L^\infty(\Omega)$ with $\varphi \geqslant 0$ such that the minimizer (u_α, c_α) satisfies the optimality conditions

$$\begin{cases} \alpha j(u_\alpha) = K^*(\lambda_1 + \lambda_2), \\ \quad c_\alpha = \langle \lambda_1 - \lambda_2, -1 \rangle_{L^\infty(\Omega)^*, L^\infty(\Omega)}, \\ \quad 0 = \left\langle \lambda_1, Ku_\alpha - y^\delta - c_\alpha \right\rangle_{L^\infty(\Omega)^*, L^\infty(\Omega)}, \\ \quad 0 = \left\langle \lambda_2, Ku_\alpha - y^\delta + c_\alpha \right\rangle_{L^\infty(\Omega)^*, L^\infty(\Omega)}, \end{cases}$$

see Theorem 15.4.1. Low regularity of the Lagrange multipliers once more prevents a semismooth complementarity formulation, and we introduce the Moreau–Yosida regularization

$$\min_{(u,c)\in X\times\mathbb{R}} \frac{c^2}{2} + \frac{\alpha}{2}\|u\|_X^2 + \frac{\gamma}{2}\left\|\max(0, Ku - y^\delta - c)\right\|_{L^2}^2 + \frac{\gamma}{2}\left\|\min(0, Ku - y^\delta + c)\right\|_{L^2}^2$$

which admits a unique minimizer $(u_\gamma, c_\gamma) \in X \times \mathbb{R}$. For $\gamma \to \infty$, the sequence of minimizers converges strongly to (u_α, c_α); see Theorem 15.4.2. Straightforward computation yields the (necessary and sufficient) optimality conditions

$$\begin{cases} \alpha j(u_\gamma) + \gamma K^* \left(\max(0, Ku_\gamma - y^\delta - c_\gamma) + \min(0, Ku_\gamma - y^\delta + c_\gamma)\right) = 0, \\ c_\gamma + \gamma \left\langle -\max(0, Ku_\gamma - y^\delta - c_\gamma) + \min(0, Ku_\gamma - y^\delta + c_\gamma), 1 \right\rangle_{L^2(\Omega)} = 0. \end{cases}$$

This defines a semismooth equation $F(u, c) = 0$ from $X \times \mathbb{R}$ to $X^* \times \mathbb{R}$ due to the mapping properties of $K : X \to L^\infty(\Omega)$ and the embedding that maps $c \in \mathbb{R}$ to the constant function $x \mapsto c \in L^\infty(\Omega)$. The Newton derivative of F is defined by its action on $(\delta u, \delta c)$ as

$$D_N F(u,c)(\delta u, \delta c) = \begin{pmatrix} \alpha j'(u)\delta u + \gamma K^*((\chi_{A_1} + \chi_{A_2})K\delta u) + \gamma \delta c K^*(-\chi_{A_1} + \chi_{A_2}) \\ \gamma \left\langle -\chi_{A_1} + \chi_{A_2}, K\delta u \right\rangle_{L^2(\Omega)} + \left(1 + \gamma \left\langle \chi_{A_1} + \chi_{A_2}, 1 \right\rangle_{L^2(\Omega)}\right)\delta c \end{pmatrix},$$

(a) exact and noisy data $Ku^\dagger, y^\delta$ (b) true solution $u^\dagger$ and reconstructions u_α
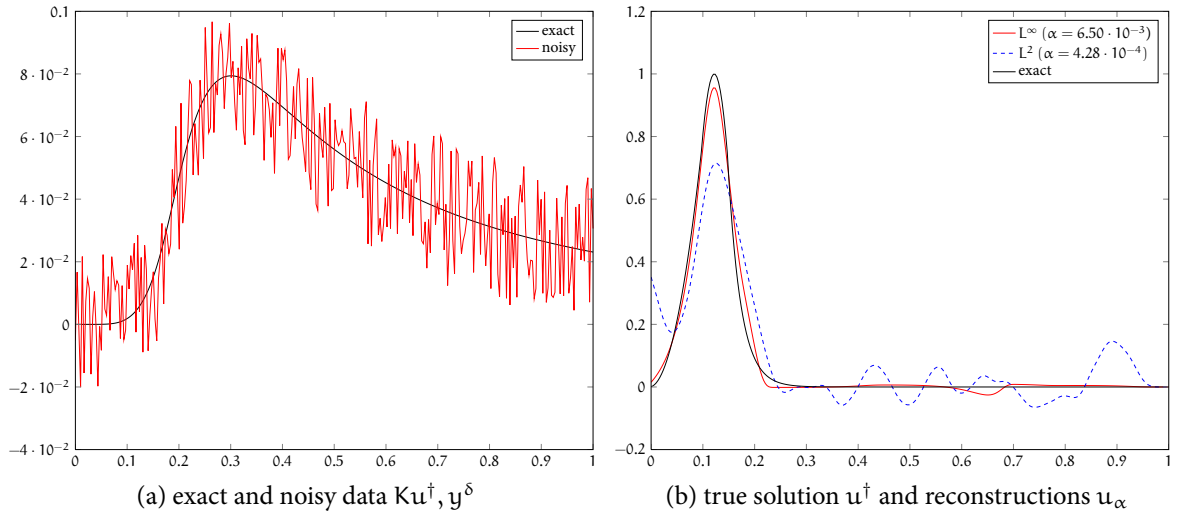
Figure 4.3: Comparison of linear L^∞ and L^2 fitting for inverse heat conduction problem ($d = 0.3$)

with

$$\mathcal{A}_1 = \left\{x : (Ku - y^\delta)(x) > c\right\}, \qquad \mathcal{A}_2 = \left\{x : (Ku - y^\delta)(x) < -c\right\}.$$

Since $\mathcal{A}_1$ and $\mathcal{A}_2$ are disjoint sets, straightforward calculation verifies that $D_N F$ is a positive definite operator independent of (u, c) and thus has a uniformly bounded inverse. This implies local superlinear convergence of the Newton method; see Theorem 15.4.4. Again, this is combined with a continuation strategy in γ.

Figure 4.3 shows a typical realization of noisy data for the inverse heat conduction problem with $d = 0.3$ and compares the performance of L^∞ fitting with L^2 fitting, demonstrating the increased robustness of the former. For L^∞ fitting, the regularization parameter α was chosen according to the balancing principle; the fixed point iteration (4.0.3) converged after 6 iterations. For L^2 fitting, the parameter is chosen from a range to give the smallest reconstruction error. More details and two-dimensional examples for deterministic quantization errors can be found in section 15.5.

APPLICATIONS IN BIOMEDICAL IMAGING

<div style="text-align: right">5</div>

The final chapter of this part illustrates the relevance of non-reflexive Banach spaces in real-world applications with two examples from biomedical imaging: Optimal light source placement in *diffuse optical imaging*, which can be formulated as an optimal control problem in the space of Radon measures, and image reconstruction in *parallel magnetic resonance imaging*, which amounts to a bilinear inverse problem where regularization terms of total variation type can lead to improved reconstruction quality. These works arose from cooperations with the Institute of Medical Engineering of the TU Graz in the framework of the SFB "Mathematical Optimization and Applications in Biomedical Sciences".

5.1 DIFFUSE OPTICAL IMAGING

Fluorescent diffuse optical tomography is an imaging methodology where a biological sample is illuminated by near-infrared light emitted from point-like light sources (so-called *optodes*) such as optical fibers or lasers after a fluorescent marker has been introduced which selectively binds to inclusions to be detected, e.g., cancer cells. The light then diffuses through the tissue while being scattered and absorbed by inhomogeneities including the markers. The photons absorbed by the latter are reemitted at a different wavelength and are then transported back to the surface, where they are captured and used to reconstruct a tomographic image of the marked tissue. However, the diffusive nature of the photon transport makes this task challenging. The reconstruction would be facilitated if the photon density of the illuminating light can be made homogeneous within a region of interest, so that any variation in contrast must be due to the marker distribution. A similar problem occurs in photodynamic cancer therapy, where instead of a fluorescent marker, a photo-activable cytotoxin is used to selectively destroy cancer cells, and homogeneous illumination is critical to avoid local under- an overdoses.

Due to the complex surface shape of biological samples, the configuration of optodes required to achieve this is far from obvious. Previously published methods were based on a discrete approach, where a (large) set of possible locations was specified beforehand, from which the best locations are chosen such that a certain performance criterion is minimized; this

amounts to a combinatorial problem with exponential complexity. The corresponding optimal source magnitudes would then be computed in a second step. In contrast, the measure space optimal control approach described in section 2.1 yields both location and magnitude of point sources in a single step, without requiring an initial feasible configuration or specification of the desired number of optodes.

The model of the steady state of light propagation in a scattering medium is based on the diffusion approximation of the radiative transfer equation. This leads to a stationary elliptic partial differential equation for the photon distribution $\varphi \in H^1(\Omega)$,

$$(5.1.1) \quad \begin{cases} -\nabla \cdot (\kappa(x)\nabla\varphi(x)) + \mu_a(x)\varphi(x) = q(x) & \text{in } \Omega, \\ \kappa(x)\,\nu(x) \cdot \nabla\varphi(x) + \rho\varphi(x) = 0 & \text{on } \Gamma. \end{cases}$$

The geometry of the sample is given by the domain $\Omega \subset \mathbb{R}^n$, $n \in \{2, 3\}$, with boundary Γ whose outward normal vector is denoted by ν. The medium is characterized by the absorption coefficient μ_a, the reduced scattering coefficient μ'_s, and the diffusion coefficient $\kappa = n\,[(\mu_a + \mu'_s)]^{-1}$. The coefficient ρ models the reflection of a part of the photons at the boundary due to a mismatch in the index of refraction. Finally, the source term q models the light emission from the optodes.

The objective is to minimize the deviation from a constant illumination z in an observation region $\omega_o \subset\subset \Omega$. Due to the linearity of the forward problem, we can take $z = 1$ without loss of generality. In addition, we restrict the possible light source locations to a control region $\omega_c \subset\subset \Omega$ and enforce non-negativity of the source term q (which represents the optodes). This leads to the optimization problem

$$\begin{cases} \displaystyle\min_{q \in \mathcal{M}(\overline{\omega}_c)} \frac{1}{2}\|\varphi|_{\omega_o} - z\|^2_{L^2(\omega_o)} + \alpha\|q\|_{\mathcal{M}(\overline{\omega}_c)} + \delta_{\{\mu:\,\mu \geqslant 0\}}(q) \\ \text{s.\,t.} \quad (5.1.1). \end{cases}$$

Applying the approach of section 2.1.2 yields for $\gamma > 0$ the family of optimality conditions

$$q_\gamma + \gamma \min(0, p_\gamma + \alpha) = 0,$$

where p_γ is again the adjoint state, i.e., the solution of the (selfadjoint) differential equation (5.1.1) with right hand side $\varphi_\gamma - z$. Instead of a matrix-free Krylov method, we first apply the discretization described in section 2.1.3 to obtain the discrete optimality system

$$\begin{cases} A_h\varphi_h - q_h = 0, \\ -M_o\varphi_h + A_h^\top p_h = -M_o z, \\ q_h + \gamma \min(0, p_h|_{\omega_c} + \alpha) = 0, \end{cases}$$

where A_h denotes the stiffness matrix corresponding to (5.1.1), M_o the restricted mass matrix with entries $\langle e_i, e_j\rangle_{L^2(\omega_o)}$, and the last equation is to be understood componentwise in $\mathbb{R}^{N_h}$. Due to the discretization chosen for q_γ, we can eliminate the control using the first
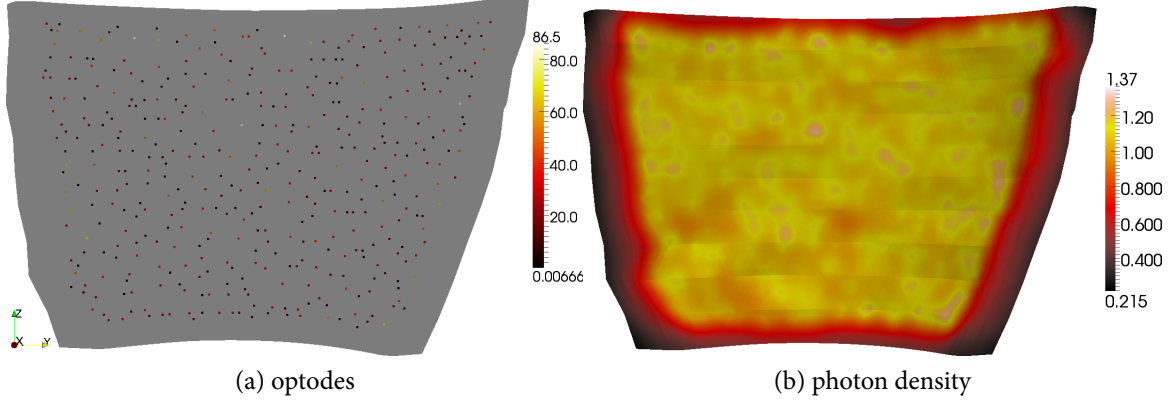
(a) optodes

(b) photon density

Figure 5.1: Optode positions and magnitudes (left) and photon densities (right, normalized to unit mean) for $\alpha = 0.8$

equation and apply a semismooth Newton method. In each Newton step, we have to solve for (φ^{k+1}, p^{k+1}) the block system

$$\begin{pmatrix} A_h & D_k \\ -M_o & A_h^T \end{pmatrix} \begin{pmatrix} \varphi^{k+1} \\ p^{k+1} \end{pmatrix} = \begin{pmatrix} -\alpha d^k \\ -M_o z \end{pmatrix},$$

where D_k is a diagonal matrix with the entries of the vector d^k,

$$d_j^k = \begin{cases} \gamma & \text{if } (p^k|_{\omega_c})_j < -\alpha, \\ 0 & \text{else,} \end{cases}$$

on the diagonal. This is once more combined with a continuation strategy in γ.

The feasibility of this approach is demonstrated for the practically relevant problem of designing light applicators in photodynamic therapy for mesotheliomas in the intrathoracic cavity, i.e., light-activated destruction of cancer cells on the surface of the lung. The goal is to achieve homogeneous illumination of the target region using a flexible diffuser with embedded light sources, taking into account the curvature of the surface. This is illustrated using a realistic three-dimensional diffuser model constructed from a CT scan of a human thorax, where the observation region ω_o is defined as the outer and inner surface of the model and ω_c is an interior manifold equidistant from both. Figure 5.1 shows the computed optimal light sources q_γ and resulting photon density φ_γ for $\alpha = 0.8$. The resulting deviation from a homogeneous illumination (with a coefficient of variation of 0.204) would be acceptable in practice. More results and quantitative evaluations are given in section 16.4.

5.2 PARALLEL MAGNETIC RESONANCE IMAGING

Magnetic resonance imaging (MRI) is a medical imaging method that employs radio pulse echoes to measure the density of hydrogen atoms in a sample, which allows the discrimination

of different types of tissue. The spatial information is encoded, using a combination of spatially varying magnetic fields, in the phase and frequency of the time-dependent echo, which is then measured by coils surrounding the patient. A Fourier transform of the recorded signal will therefore yield an image of the sample. Mathematically, MRI can thus be thought of as direct measurement of the Fourier coefficients of the image. One of the major drawbacks of MRI in current practice is the speed of the image acquisition, since in principle each (discrete) Fourier coefficient $k(i, j)$ has to be acquired separately: Each coordinate pair (i, j) needs to be encoded by the gradient fields and measured by a separate radio pulse. By employing a phase encoding instead of a frequency encoding for one coordinate, a "line" of Fourier coefficients $k(i, \cdot)$ can be read out in parallel for every radio excitation. The standard approach for further speeding up the process acquires only a subset of these lines (e.g., every second, $k(2i, \cdot)$, or every fourth, $k(4i, \cdot)$); other strategies (so-called *trajectories*) such as sampling along radial and spiral "lines" are possible.

This, however, leads to aliasing, as the signal is now sampled below the Nyquist frequency, resulting in visible image corruption. As a remedy, parallel magnetic resonance imaging (PMRI) measures the radio echo using multiple independent coils, which are usually placed in a circle around the patient; in this way one hopes to compensate for the lost information. Since these coils have only limited aperture compared to a single coil, the resulting measurements are non-uniformly modulated. It is, therefore, necessary to recover both the missing Fourier coefficients and the unknown modulations (the so-called *sensitivities*) from a set of modulated and aliased coil images.

Mathematically, PMRI can be formulated as a nonlinear inverse problem where the sampling operator $\mathcal{F}_S$ (e.g., Fourier transform followed by multiplication with a binary mask) and the correspondingly acquired Fourier coefficients $g = (g_1, \ldots, g_N)^\mathsf{T}$ from N receiver coils are given, and the spin density u and the unknown (or not perfectly known) set of coil sensitivities $c = (c_1, \ldots, c_N)^\mathsf{T}$ have to be found such that

$$F(u, c) := (\mathcal{F}_S(u \cdot c_1), \ldots, \mathcal{F}_S(u \cdot c_N))^\mathsf{T} = g$$

holds. Since this problem is bilinear, Newton-type methods are not applicable. A standard approach for nonlinear inverse problems, the *iteratively regularized Gauß–Newton* (IRGN) method, consists in solving a sequence of quadratic problems obtained by linearization. Specifically, one computes in each step k for given $x^k := (u^k, c^k)$ the solution $\delta x := (\delta u, \delta c)$ to the minimization problem

$$\min_{\delta x} \frac{1}{2} \|F'(x^k)\delta x + F(x^k) - g\|^2 + \frac{\alpha_k}{2} \mathcal{W}(c^k + \delta c) + \beta_k \mathcal{R}(u^k + \delta u)$$

for given $\alpha_k, \beta_k > 0$, and then sets $x^{k+1} := x^k + \delta x$, $\alpha_{k+1} := q_\alpha \alpha_k$ and $\beta_{k+1} := q_\beta \beta_k$ with $0 < q_\alpha, q_\beta < 1$. Here, the term $\mathcal{W}(c) = \|w \cdot \mathcal{F}c\|^2$ is a penalty on the high-frequency Fourier coefficients of the sensitivities (enforcing smoothness of the modulations) and $\mathcal{R}$ is a regularization term for the image. In this work total variation-type penalties are used to prevent noise amplification as $\alpha_k, \beta_k \to 0$. For the solution of the quadratic subproblems, a

first order method is chosen which requires only application of Fourier transforms and point-wise operations and hence can be implemented efficiently on modern multi-core hardware such as graphics processing units. Inserting the characterization (1.1.2) of the total variation seminorm yields the nonsmooth convex-concave saddle-point problem

$$\min_{\delta x} \max_{p} \frac{1}{2} \|F'(x^k)\delta x + F(x^k) - g\|^2 + \frac{\alpha_k}{2} \mathcal{W}(c^k + \delta c) + \langle u^k + \delta u, -\operatorname{div} p \rangle + \delta_{C_{\beta_k}}(p)$$

with

$$C_\beta = \left\{ p \in L^2(\Omega; \mathbb{C}^2) : \operatorname{div} p \in L^2(\Omega; \mathbb{C}),\ |p(x)|_2 \leqslant \beta \text{ for almost all } x \in \Omega \right\},$$

which is solved using a projected primal-dual extra-gradient method adapted from [Chambolle and Pock 2010]; see Algorithm 17.1. A similar approach can be applied when $\mathcal{R}$ is the *total generalized variation*, a higher order total variation-type penalty that promotes piecewise affine solutions; see [Bredies, Kunisch, and Pock 2010] and Algorithm 17.2.

Figure 5.2 shows reconstructions of real-time images of a beating heart using radial sampling with 25, 12 and 19 acquired lines (corresponding to undersampling of approximately 8.0, 9.6 and 10.6 times below the Nyquist limit, respectively), comparing L^2 regularization (IRGN) with total variation regularization (IRGN TV). The ability of the latter to prevent the noise amplification occuring in the former is evident. Additional results for different sampling strategies and total generalized variation are given in section 17.4.
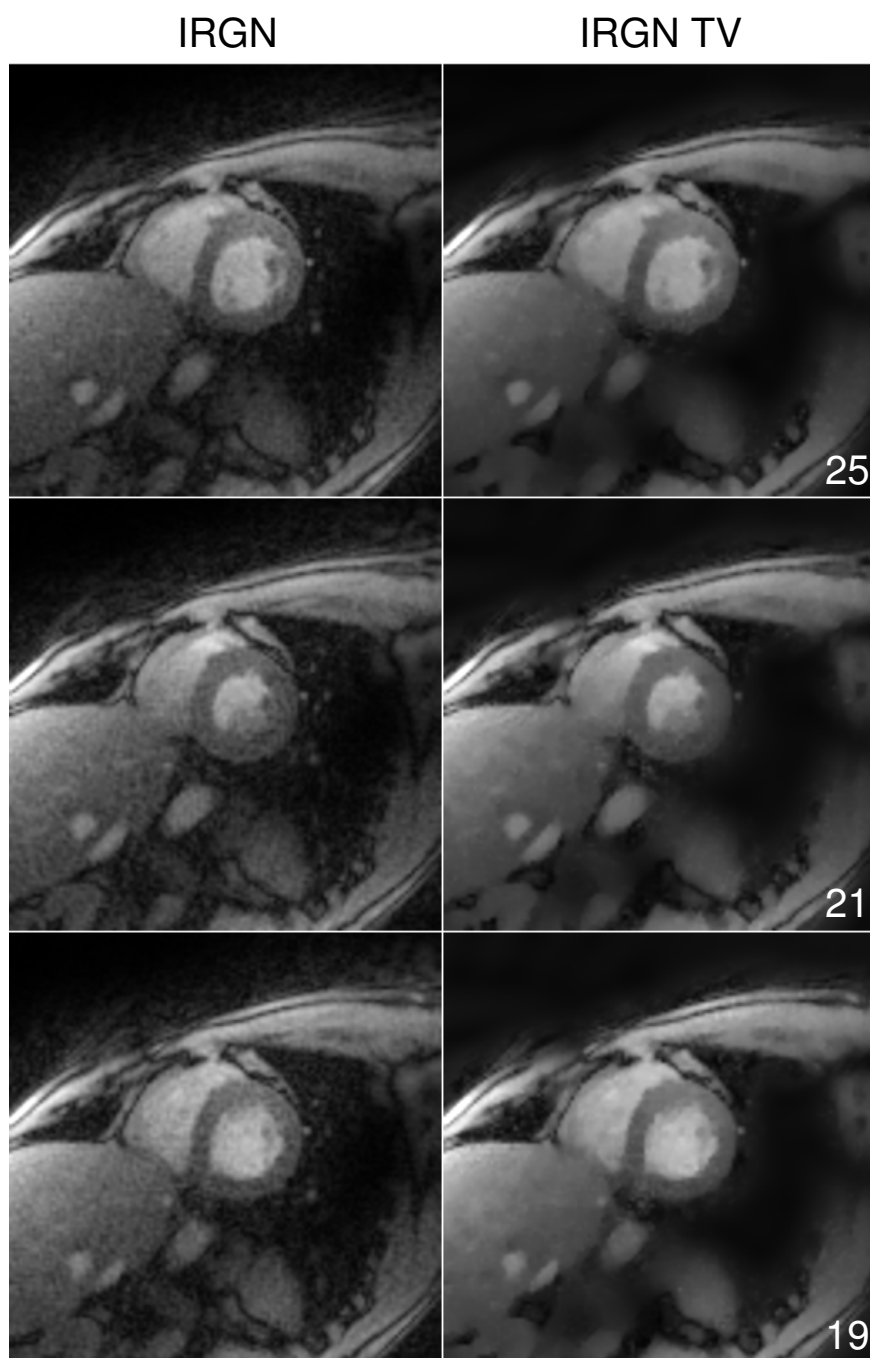
IRGN   IRGN TV

Figure 5.2: Reconstructions of real-time images of a beating heart from 25, 12 and 19 acquired radial lines with L^2 regularization (IRGN) and with total variation regularization (IRGN TV)

OUTLOOK

The results described in this thesis can be extended in many directions. Clearly, nonlinear optimal control problems, both in measure spaces and with L^∞ functionals, can be considered. Of interest would be nonlinear partial differential equations with controls on the right hand side as well as control of linear equations by lower order coefficients, e.g., potential terms. Also of practical relevance are controls with sparsity properties not in physical space but in a transform space, e.g., optimal control of the wave equation using controls that are a superposition of few frequencies. This problem can be treated using the approach proposed in section 2.3, with the Fourier transform in place of the distributional gradient. Tracking terms of L^1 and L^∞ type also appear as appropriate distance functionals in the context of optimal control of probability density functions (there known as *Kantorovich* and *Kolmogorov* distances, respectively).

For inverse problems, it would be of interest to extend the L^1 data fitting to the case of mixed noise (e.g., combined Gaussian–impulsive or Cauchy-distributed noise). For such noise, the regularization of the L^1 norm introduced in section 4.1.2 turns out to be the statistically appropriate discrepancy term (known as the *Huber norm*); it remains to replace the continuation strategy in β with a suitable parameter choice method. Still missing is a rigorous stochastic framework for impulsive noise models in function spaces, which would lead to inverse problems with data fitting in measure spaces. Besides applying the L^∞ fitting approach to nonlinear parameter identification problems, it would be possible to combine it with the approach for L^1-type regularization terms to obtain a numerical method for the so-called *Dantzig selector*. Of course, any method for solving inverse problems has to be tested with real-world data; hence applying the developed methods to practical inverse problems is of great interest.

A long-term goal is to combine the measure space approach for source placement with sensitivity maximization techniques to solve optimal light source and sensor placement problems in optical tomography. In parallel magnetic resonance imaging, formulating the image reconstruction problem as an inverse problem allows the inclusion of physiological parameters, either as additional penalties or as unknown parameters to be reconstructed.

These extensions are the topic of future research.

Part II

OPTIMAL CONTROL WITH MEASURES

Part III

OPTIMAL CONTROL WITH L$^\infty$ FUNCTIONALS

Part IV

INVERSE PROBLEMS WITH NON-GAUSSIAN NOISE

Part V

APPLICATIONS IN BIOMEDICAL IMAGING

BIBLIOGRAPHY

Alibert, J.-J. and Raymond, J.-P. (1997). *Boundary control of semilinear elliptic equations with discontinuous leading coefficients and unbounded controls*. Numer. Funct. Anal. Optim. 18.3-4, pp. 235–250. DOI: 10.1080/01630569708816758 (cit. on pp. 5, 6).

Attouch, H., Buttazzo, G., and Michaille, G. (2006). *Variational Analysis in Sobolev and BV Spaces*. Vol. 6. MPS/SIAM Series on Optimization. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (cit. on pp. 5, 7).

Bakushinskii, A. B. (1984). *Remarks on choosing a regularization parameter using the quasi-optimality and ratio criterion*. USSR Computational Mathematics and Mathematical Physics 24.4, pp. 181–182. DOI: 10.1016/0041-5553(84)90253-2 (cit. on p. 42).

Boccardo, L. and Gallouët, T. (1989). *Nonlinear elliptic and parabolic equations involving measure data*. J. Funct. Anal. 87.1, pp. 149–169. DOI: 10.1016/0022-1236(89)90005-0 (cit. on p. 6).

Bredies, K., Kunisch, K., and Pock, T. (2010). *Total Generalized Variation*. SIAM J. Imaging Sci. 3.3, pp. 492–526. DOI: 10.1137/090769521 (cit. on p. 56).

Brezis, H. (2010). *Functional Analysis, Sobolev Spaces and Partial Differential Equations*. Springer, New York (cit. on pp. 3, 4).

Burger, M. and Osher, S. (2004). *Convergence rates of convex variational regularization*. Inverse Problems 20.5, pp. 1411–1421. DOI: 10.1088/0266-5611/20/5/005 (cit. on p. 42).

Casas, E., Herzog, R., and Wachsmuth, G. (2012). *Optimality conditions and error analysis of semilinear elliptic control problems with L^1 cost functional*. SIAM J. Control Optim. 22.3, pp. 795–820. DOI: 10.1137/110834366 (cit. on p. 18).

Casas, E. (1986). *Control of an elliptic problem with pointwise state constraints*. SIAM J. Control Optim. 24.6, pp. 1309–1318. DOI: 10.1137/0324078 (cit. on pp. 5, 6).

Casas, E. (1993). *Boundary control of semilinear elliptic equations with pointwise state constraints*. SIAM J. Control Optim. 31.4, pp. 993–1006. DOI: 10.1137/0331044 (cit. on p. 6).

Casas, E. (1997). *Pontryagin's principle for state-constrained boundary control problems of semilinear parabolic equations*. SIAM J. Control Optim. 35.4, pp. 1297–1327. DOI: 10.1137/S0363012995283637 (cit. on p. 6).

Chambolle, A. and Pock, T. (2010). *A first-order primal-dual algorithm for convex problems with applications to imaging*. J Math Imaging Vis online first. DOI: 10.1007/s10851-010-0251-1 (cit. on p. 56).

Chen, X., Nashed, Z., and Qi, L. (2000). *Smoothing methods and semismooth methods for nondifferentiable operator equations*. SIAM J. Numer. Anal. 38.4, pp. 1200–1216. DOI: 10.1137/S0036142999356719 (cit. on p. 15).

Clarke, F. H. (1990). *Optimization and Nonsmooth Analysis*. 2nd ed. Classics Appl. Math. 5. SIAM, Philadelphia (cit. on p. 9).

Clason, C., Jin, B., and Kunisch, K. (2010). *A duality-based splitting method for ℓ^1-TV image restoration with automatic regularization parameter choice*. SIAM J. Sci. Comput. 32.3, pp. 1484–1505. DOI: 10.1137/090768217 (cit. on p. 43).

Dunford, N. and Schwartz, J. T. (1988). *Linear operators. Part I*. Wiley Classics Library. John Wiley & Sons Inc., New York (cit. on p. 4).

Edwards, R. E. (1965). *Functional Analysis. Theory and Applications*. Holt, Rinehart and Winston, New York (cit. on pp. 5, 18).

Ekeland, I. and Témam, R. (1999). *Convex Analysis and Variational Problems*. Classics Appl. Math. 28. SIAM, Philadelphia (cit. on pp. 7, 9, 11, 12).

Elstrodt, J. (2005). *Maß- und Integrationstheorie*. 5th ed. Springer-Verlag, Berlin (cit. on p. 4).

Engl, H. W., Hanke, M., and Neubauer, A. (1996). *Regularization of Inverse Problems*. Kluwer, Dordrecht (cit. on p. 41).

Gilbarg, D. and Trudinger, N. S. (2001). *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics. Reprint of the 1998 edition. Springer-Verlag, Berlin (cit. on p. 6).

Grund, T. and Rösch, A. (2001). *Optimal control of a linear elliptic equation with a supremum norm functional*. Optimization Methods and Software 15.3-4, pp. 299–329. DOI: 10.1080/10556780108805823 (cit. on p. 34).

Gugat, M. and Leugering, G. (2008). *L^∞-norm minimal control of the wave equation: On the weakness of the bang-bang principle*. ESAIM Control Optim. Calc. Var. 14.2, pp. 254–283. DOI: 10.1051/cocv:2007044 (cit. on p. 38).

Hintermüller, M., Ito, K., and Kunisch, K. (2002). *The primal-dual active set strategy as a semismooth Newton method*. SIAM J. Optim. 13.3, 865–888 (2003). DOI: 10.1137/S1052623401383558 (cit. on pp. 15, 16).

Hintermüller, M. and Ulbrich, M. (2004). *A mesh-independence result for semismooth Newton methods*. Math. Program. 101.1, Ser. B, pp. 151–184. DOI: 10.1007/s10107-004-0540-9 (cit. on p. 17).

Hinze, M. (2005). *A variational discretization concept in control constrained optimization: The linear-quadratic case*. Comp. Optim. Appls. 30, pp. 45–61. DOI: 10.1007/s10589-005-4559-5 (cit. on p. 26).

Ito, K. and Kunisch, K. (2008). *Lagrange Multiplier Approach to Variational Problems and Applications*. Vol. 15. Advances in Design and Control. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (cit. on pp. 12, 15–17).

Kindermann, S. (2011). *Convergence analysis of minimization-based noise level-free parameter choice rules for linear ill-posed problems*. Electron. Trans. Numer. Anal. 38, pp. 233–257. URL: http://etna.math.kent.edu/vol.38.2011/pp233-257.dir/ (cit. on p. 43).

Kummer, B. (1988). *Newton's method for non-differentiable functions*. Mathematical Research 45, pp. 114–125 (cit. on p. 14).

Kummer, B. (2000). *Generalized Newton and NCP-methods: Convergence, regularity, actions*. Discuss. Math. Differ. Incl. Control Optim. 20.2, pp. 209–244. DOI: 10.7151/dmdico.1013 (cit. on p. 15).

Ladyzhenskaya, O. A. and Ural'tseva, N. N. (1968). *Linear and Quasilinear Elliptic Equations*. Translated from the Russian by Scripta Technica, Inc. Translation editor: Leon Ehrenpreis. Academic Press, New York (cit. on p. 6).

Maurer, H. and Zowe, J. (1979). *First and second order necessary and sufficient optimality conditions for infinite-dimensional programming problems*. Math. Programming 16.1, pp. 98–110. DOI: 10.1007/BF01582096 (cit. on p. 12).

Meyer, C., Panizzi, L., and Schiela, A. (2011). *Uniqueness criteria for solutions of the adjoint equation in state-constrained optimal control*. Numerical Functional Analysis and Optimization 32.9, pp. 983–1007. DOI: 10.1080/01630563.2011.587074 (cit. on p. 6).

Mifflin, R. (1977). *Semismooth and semiconvex functions in constrained optimization*. SIAM J. Control Optimization 15.6, pp. 959–972. DOI: 10.1137/0315061 (cit. on p. 14).

Neustadt, L. W. (1962). *Minimum effort control systems*. J. SIAM Control Ser. A 1, pp. 16–31. DOI: 10.1137/0301002 (cit. on p. 38).

Pöschl, C. (2009). *An overview on convergence rates for Tikhonov regularization methods for non-linear operators*. J. Inverse Ill-Posed Probl. 17.1, pp. 77–83. DOI: 10.1515/JIIP.2009.009 (cit. on p. 42).

Prüfert, U. and Schiela, A. (2009). *The minimization of a maximum-norm functional subject to an elliptic PDE and state constraints*. ZAMM 89.7, pp. 536–551. DOI: 10.1002/zamm.200800097 (cit. on p. 34).

Qi, L. Q. and Sun, J. (1993). *A nonsmooth version of Newton's method*. Math. Programming 58.3, Ser. A, pp. 353–367. DOI: 10.1007/BF01581275 (cit. on p. 14).

Resmerita, E. (2005). *Regularization of ill-posed problems in Banach spaces: Convergence rates*. Inverse Problems 21.4, pp. 1303–1314. DOI: 10.1088/0266-5611/21/4/007 (cit. on p. 42).

Ruszczyński, A. (2006). *Nonlinear Optimization*. Princeton University Press, Princeton, NJ (cit. on p. 34).

Scherzer, O., Grasmair, M., Grossauer, H., Haltmeier, M., and Lenzen, F. (2009). *Variational Methods in Imaging*. Vol. 167. Applied Mathematical Sciences. Springer, New York (cit. on p. 42).

Schiela, A. (2008). *A simplified approach to semismooth Newton methods in function space*. SIAM J. on Opt. 19.3, pp. 1417–1432. DOI: 10.1137/060674375 (cit. on pp. 12, 17).

Schirotzek, W. (2007). *Nonsmooth Analysis*. Universitext. Springer, Berlin (cit. on pp. 7, 9–11).

Stadler, G. (2009). *Elliptic optimal control problems with L^1-control cost and applications for the placement of control devices*. Computational Optimization and Applications 44.2, pp. 159–181. DOI: 10.1007/s10589-007-9150-9 (cit. on p. 18).

Stampacchia, G. (1965). *Le problème de Dirichlet pour les équations elliptiques du second ordre à coefficients discontinus*. Ann. Inst. Fourier (Grenoble) 15.fasc. 1, pp. 189–258. DOI: 10.5802/aif.204 (cit. on pp. 5, 6).

Thomée, V. (2006). *Galerkin Finite Element Methods for Parabolic Problems*. 2nd. Vol. 25. Springer Series in Computational Mathematics. Springer-Verlag, Berlin (cit. on p. 28).

Troianiello, G. M. (1987). *Elliptic Differential Equations and Obstacle Problems*. The University Series in Mathematics. Plenum Press, New York (cit. on p. 6).

Tröltzsch, F. (2010). *Optimal Control of Partial Differential Equations: Theory, Methods and Applications*. Translated from the German by Jürgen Sprekels. American Mathematical Society, Providence, RI (cit. on p. 48).

Ulbrich, M. (2002). *Semismooth Newton methods for operator equations in function spaces*. SIAM J. Optim. 13.3, 805–842 (2003). DOI: 10.1137/S1052623400371569 (cit. on pp. 15, 17).

Ulbrich, M. (2011). *Semismooth Newton methods for variational inequalities and constrained optimization problems in function spaces*. Vol. 11. MOS-SIAM Series on Optimization. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA. DOI: 10.1137/1.9781611970692 (cit. on pp. 12, 14).

Vossen, G. and Maurer, H. (2006). *On L^1-minimization in optimal control and applications to robotics*. Optimal Control Appl. Methods 27.6, pp. 301–321. DOI: 10.1002/oca.781 (cit. on p. 18).

Wachsmuth, D. and Wachsmuth, G. (2011a). *Convergence and regularization results for optimal control problems with sparsity functional*. ESAIM: Control Optim. Calc. Var. 17, pp. 858–886. DOI: 10.1051/cocv/2010027 (cit. on p. 18).

Wachsmuth, D. and Wachsmuth, G. (2011b). *Regularization error estimates and discrepancy principle for optimal control problems with inequality constraints*. Control and Cybernetics 40.4, pp. 1125–1154. URL: http://www.tu-chemnitz.de/mathematik/part_dgl/publications/Wachsmuth_Wachsmuth__On_the_regularization_of_optimization_problems_with_inequality_constraints.pdf (cit. on p. 18).

Warga, J. (1972). *Optimal Control of Differential and Functional Equations*. Academic Press, New York (cit. on p. 5).

Werner, D. (2011). *Funktionalanalysis*. 7th ed. Springer-Verlag, Berlin (cit. on p. 2).

Ziemer, W. P. (1989). *Weakly differentiable functions*. Vol. 120. Graduate Texts in Mathematics. Sobolev spaces and functions of bounded variation. Springer-Verlag, New York (cit. on p. 13).

Zuazua, E. (2007). *Controllability and observability of partial differential equations: Some results and open problems*. In: Handbook of differential equations: Evolutionary equations. Vol. III.

Elsevier/North-Holland, Amsterdam, pp. 527–621. DOI: 10.1016/S1874-5717(07)80010-7 (cit. on p. 38).