# Aspects of parameter identification in semilinear reaction-diffusion systems

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Die aktuell veröffentlichte Version unterscheidet sich von der zur Bewertung eingereichten Version. Sie enthält Änderungen basierend auf den Gutachten. Insbesondere Kapitel 5 wurde grundlegend überarbeitet und ergänzt. Daraus resultierten entsprechende Anpassungen in Kapitel 6.

# Zusammenfassung

Die vorliegende Arbeit liefert einen Ansatz für die Parameteridentifikation in allgemeinen seminlinearen parabolischen partiellen Differentialgleichungen. Dabei wird auf zwei Dinge eingegangen. Zum einen wird ein Lösungsansatz via Tikhonov-Regularisierung vorgeschlagen um eventuelle unstetige Abhängigkeiten der Parameter von den Daten in den Griff zu bekommen und zum anderen wird die Eindeutigkeit einer Lösung des Problems diskutiert.

Dazu wird zunächst eine allgemeine Differentialgleichung formuliert, die tatsächlich als Grundlage von vielen Realweltmodellen dient. Anschließend wird das allgemeine Konzept der Parameteridentifikaton eingegangen. Bevor dieses auf die allgemeine Differentialgleichung angewendet wird, werden aktuelle Resultate aus der Lösungstheorie für ebensolche Gleichungen vorgestellt, welche vonnöten ist um Stetigkeits- und Differentierbarkeitseigenschaften des Operators zu zeigen, der Parameter auf eine Lösung der Differentialgleichung abbildet. Diese Eigenschaften, werden, soweit möglich, nachgewiesen und diskutiert. Außerdem wird sich der Interpretation von Quellbedingungen für diesen Operator gewidmet. Ein besonderes Augenmerk wird auch darauf gelegt, verschiedene Arten von Messoperatoren zu untersuchen. Dabei wird gezeigt, dass man ausgehend von limitierten Messungen unter gewissen Voraussetzungen tatsächlich eine eindeutige Lösung des Parameteridentifikationsproblems erhält. Im letzten Teil der Arbeit werden schließlich numerische Experimente anhand eines konkreten Beispiels vorgestellt, die die vorherigen theoretischen Ergebnisse bekräftigen.

# Abstract

This thesis provides an approach for parameter identification in general semilinear parabolic partial differential equations. We investigate the problem of parameter identification from two different angles. On one hand, Tikhonov regularization is proposed to deal with possible non continuous dependence of the parameters onto the data and on the other hand the uniqueness of a solution of the parameter identification problem is discussed.

For this, a general differential equation is formulated that serves as the basic model for many real world applications. Then the concept of parameter identification is addressed. Before we apply this concept to our general equation, recent results for the solution of such equations are introduced, because they are needed to show continuity and differentiability properties of the operator that maps a parameter to a solution. These properties then are, as far as possible, proved and discussed. Furthermore, source conditions for our kind of problems are investigated. Special attention is paid to different kinds of measurement operators. It is shown that the parameter identification can be uniquely solved under certain restrictions, if a concrete, applicationally relevant measurement operator is given. The last part of the work shows numerical results for a concrete example that support our theoretical findings.

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# Contents

# CHAPTER 1

## Introduction

If one wants to study the evolution of a certain process over time, the change of the object over time and space can be modeled mathematically by the help of physical laws. This usually leads to a partial differential equation or in the case of several interacting processes to a system of partial differential equations. For every process modeled in this way, there are certain quantities that determine the outcome of the process, which are the *parameters* in the partial differential equation. If one knows all of these parameters one can solve the equation and thus determine the function that describes the evolution of the quantity of interest. This problem is usually called the forward problem and can easily described by the operator equation

$$F(p) = u,$$

where $F$ is the operator that maps a parameter $p$ to the solution $u$. This operator is given implicitly through the differential equation and is usually a nonlinear map. The operator $F$ will be referred as *parameter-to-state* or *control-to-state map* throughout this work. However, in many real life problems, the situation is exactly the opposite. Here, one can observe (and also measure) the evolution of the quantity of interest $u$, at least partially. What remains unknown is the exact shape of the parameters. So one wants to find $p$ with $u$ given, or in other words, one wants to perform a *parameter identification.*

A first idea to deal with such a problem is the well known *data fitting* or *least squares approach*

$$\operatorname*{argmin}_p \|F(p) - u\|^2. \tag{1.1}$$

In the context of parameter identification this process is not ideal, because the fact that a parameter is unknown is not the only difficulty one has to deal with.

Parameter identification problems coming from partial differential equations tend to be *ill-posed*, which in common understandings can mean three things

1. Different parameters yield the same solution, i.e. $F$ is not injective.

2. For given (noisy) data $u$, there are no parameters that could have caused them, i.e. $F$ is not surjective.

3. The parameters do not depend continuously on the data.

For the moment, we will take a look at the third point. No matter, how good a measurement process is, there will always be noise, so instead of $u$, one measures a noisy version of $u$, which, for given noise level $\delta$ will be denoted as $u^\delta$. On top of this, in most applications it can not be expected that a measurement of $u$ is possible over the whole domain for every time point, so one faces limited and noisy data. If one includes this information, the fitting problem (1.1), becomes

$$\operatorname*{argmin}_p \|OF(p) - u^\delta\|^2, \tag{1.2}$$

where $O$ is an operator that describes the limitation in the measurements. Now, if the parameters do not depend continuously on the data, one adds an additional constraint to the functional (1.2) and gets

$$J_\alpha(p) := \operatorname*{argmin}_p \|OF(p) - u^\delta\|^2 + \alpha R(p)$$

$J_\alpha$ is called a *Tikhonov type functional.* The functional $R$ is called *penalty term* or *prior* and stabilizes the data fitting process. The name prior comes from the second feature of $R$. It forces the minimizer of $J_\alpha$ to have certain properties, which can be used to improve the quality of the solution based on a priori information. The parameter $\alpha$ fulfills two functions, it regulates the degree of stabilization as well as the degree of special features of $R$ that the function $p$ adapts. Originally, the Tikhonov functional was introduced for $R(p) = \|p\|^2$ in [67]. The classical Tikhonov functional, i.e. $R(p) = \|p\|^2$, is very well understood and comprehensive results can be found in the textbooks [23, 59]. In the past decade, one began to study more general convex penalty terms [11, 17, 36, 40, 56], especially *sparsity enforcing* priors have become very popular and were studied extensively [17, 31, 46]. The reason for this is that many natural problems inhibit a sparse structure in some suitable basis, where action and interaction only takes place locally.

It can be shown that the minimization of Tikhonov-type functionals is a *regularization* (in other words a stabilization of the inversion of $F$), i.e. it has certain properties that are wanted in practice, such as stability and a good approximation of the real solution for a small noise level if $F$ and $R$ fulfill the right continuity properties. There are other regularization techniques that perform equally well or even better in certain situations, but they are less general and often have special requirements, see for example the standard references [23, 59].

Among the large variety of partial differential equations, usually the ones that involve two space derivatives are the most interesting ones, because many real world applications lead to models involving this type of equations. These equations are classified in different types, elliptic, hyperbolic and parabolic equations [25] and each have their rich theory for solving them as well as for solving inverse problems arising from them. In this work we will focus on a very important subclass of parabolic equations, so called reaction-diffusion equations, motivated from chemical reactions happening in a medium or biochemical evolution in real world organisms and there is a broad range of applications modeled by these type of equations, see [12, 29, 45, 49, 51, 55] for a few examples. Throughout the work we consider a general open, bounded and connected subset $\Omega$ of $\mathbb{R}^d$ with sufficiently smooth boundary, where $d = 1, 2, 3$ and a real interval $I = [0, T]$. For the rest of the work, we will also use the notation $\Omega_T = \Omega \times (0, T)$. Then a general system of semilinear parabolic reaction-diffusion equations can be described in the following way:

$$
\begin{aligned}
\frac{\partial}{\partial t}u_i(x,t) - \nabla \cdot D_i(x,t)\nabla u_i(x,t) & \\
+g_i(p(x,t), u(x,t)) = f_i(x,t) & \qquad \text{in } \Omega_T, \\
z_1 u_i(x,t) + z_2 \frac{\partial}{\partial \nu} u_i(x,t) = 0 & \qquad \text{on } \partial\Omega \times [0,T], \\
u_i(x,0) = u_{0i}(x) & \qquad \text{on } \Omega \times \{0\},
\end{aligned}
\tag{1.3}
$$

where $i = 1, ..., N$, $u = (u_1, ..., u_N)$, $p = (p_1, ..., p_M)$, $z_1 \in \{0, 1\}$, $z_2 = 1 - z_1$ and $g : \mathbb{R}^M \times \mathbb{R}^N \to \mathbb{R}^N$. The parameters $D_i$ are diffusion coefficients for which we assume that $0 < D_i < C$, while the parameter $p$ can describe multiple things, like interaction of the solutions or just synthesis and decay of one solution. More concrete, the exact function of the parameter vector $p$ is determined by the application that is modeled. For the sake of readability we only consider homogeneous Dirichlet or Neumann boundary conditions. The extension of the theory we propose to more general (but linear) boundary conditions is mostly straightforward, in particular when it comes to analyzing the inverse problem. At places, where this comes into effect, we will make appropriate remarks.

## 1.1 Organization

In Chapter 2 we get more deeply into possible applications and give a more detailed motivation for what we are doing. Some general cases for the nonlinear function $g$ are discussed. After that we also give some real world applications that fit in our setting. One is coming from predator prey models, whilst the other one models the evolution of genes in simple organisms as the drosophila fly. Later on, we will use this last example for illustrations and numerical simulations.

Chapter 3 gathers all the necessary functional analytic tools that will help us with the analysis of the forward and the inverse problem.

Chapter 4 explains the difficulties in parameter identification. This section is split in two parts, the first one introduces the concept of identifiability and an example is given where identifiability fails. The second part then gives an overview over regularization of ill posed problems (ill posed in the sense of continuity) via Tikhonov-regularization, introduces source conditions and the application of sparsity constraints and discusses the minimization of Tikhonov-type functionals.

After that, in Chapter 5, we motivate the weak solution theory for (1.3) with the help of a simple example. Then we give a general concept for the solution theory of systems of parabolic partial differential equations with a special focus on solution spaces and their embeddings.

Chapter 6 then deals with the inverse problem. With the solution spaces from the previous section at hand, we will show necessary properties like differentiability and weak sequential closedness for our testproblem, that are needed for the application of Tikhonov-regularization, following the approach of [57, 58]. Also source conditions are discussed. We close this section with some remarks how the results can be generalized further.

The next big block, Chapter 7 then returns back to the identifiability of coefficients. For this, an adjoint approach derived in [21] is generalized for our needs and for a simple case identifiability is shown. Also the case if identifiability does not hold is discussed.

The last part of the work, Chapter 8, concentrates on concrete numerical tests with simulated data. Here, we explain, how numerical schemes for parabolic equations usually work and use this combined with existing theory to design a solver for the inverse problem. Then we will use a very special approach applying sparsity regularization, introduced in [30]. This approach uses the finite element basis for reconstructions. Finally, some numerical results are shown and commented.

## 1.2 Contribution of this work

The first main contribution of this work is the comprehensive discussion of the parameter identification problem itself, highlighting difficulties and certain properties of the problem. It is especially discussed how to deal with it when using Tikhonov-type regularization under various circumstances. Our work regarding this continues the approach of *Ressel* [57], where a similar analysis was performed for a concrete semilinear system. Staying close to the work [57], we consider a broad range of different nonlinear functions as well as the somewhat straightforward linear case which should give the reader a good understanding of what is going on. Also, we extend the theory proposed in [57] to space or time independent parameters and discuss *source conditions*, i.e. conditions that ensure a convergence rate for noisy data for this parameter identification problem. The second contribution is the identifiability, i.e. the injectivity of the forward operator in certain situations for space time dependent parameters. For this, recent results concerning an adjoint approach proposed in [21] are generalized and discussed for our type of equations. Also the case, if uniqueness does not hold is discussed. The last major contribution concerns the application of sparsity regularization to semilinear parameter identification problems and especially the numerical part where the finite element basis functions are used for reconstructions. It turns out, that this approach indeed is very potent for identifying space and time dependent parameters in a reaction term in the presence of noisy data.

# CHAPTER 2

## Examples for semilinear reaction diffusion equations of second order

Before we start addressing the parameter identification problem, we want to go into detail concerning equation (1.3). This especially concerns the possibly nonlinear function $g$. At first we examine some typical cases in an academic sense. Then we look into more specific examples that will help the reader to understand the abstract concepts in more concrete situations. The first example of this series is of simple nature, while the second and third examples are coming from real world applications.

## 2.1 Examples for typical nonlinearities $g$

Whilst one can imagine almost any nonlinearities, in applications only a few of them are really relevant. Here we will highlight some typical classes of nonlinear functions $g$ that often appear in applications. The reason we are doing this is because they have to be treated differently when it comes to the inverse problem context, especially when one has to choose a parameter space. For the rest of this section, let $\lambda_{ik} \in \{0,1\}, \phi_{ik} : \mathbb{R}^N \to \mathbb{R}$, $i = 1,\dots,N$, $k = 1,\dots,\tilde{M}$, with $\sum_{i=1}^N \sum_{k=1}^{\tilde{M}} \lambda_{ik} = M$. We give the following examples:

1. Linear combinations, where $N = \tilde{M}$, i.e.

$$g_i(p,u) = \sum_{k=1}^{N} \lambda_{ik} p_{ik} u_k.$$

   A special case of this is a matrix vector multiplication, where all $\lambda_{ik} = 1$, i.e. $g_i(p,u) = (Wu)_i$.

2. Functions that are a linear in $p$ and possibly nonlinear in $u$:

$$g_i(p,u) = \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N).$$

   A special case of this are functions that are polynomial in $u$:

$$g_i(p,u) = \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} u_1^{i1} u_2^{i2} ... u_N^{iN}.$$

3. General nonlinear functions $\psi_i : \mathbb{R} \to \mathbb{R}$ componentwise applied to the previous case, i.e.

$$g_i(p,u) = \psi_i \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right).$$

   .

4. Combinations of the above, where multiplications of different parameters are allowed, i.e.

$$g_i(p,u) = \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i \left( \sum_{k=L+1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right).$$

Each of these cases can and has to be treated differently when it comes to the inverse problem, since certain continuity and differentiability properties of the function $g$ do not carry over to the operator case, see Chapters 3.7 and 6.4 for details. So we will make different assumptions for the different examples discussed in this section and the involved function spaces.

## 2.2 Reaction diffusion networks with matrix interaction

A prototypical example for equations of type (1.3) that are linear are equations, where the interaction between the involved functions is singularly determined by a matrix vector multiplication:

$$\frac{\partial u_i(x,t)}{\partial t} - \nabla \cdot D_i(x,t) \nabla u_i(x,t) = (W(x,t)u(x,t))_i \qquad \text{in } \Omega_T, \tag{2.1}$$

$$\frac{\partial}{\partial \nu} u_i(x,t) = 0 \qquad \text{on } \partial\Omega \times [0,T], \tag{2.2}$$

$$u_i(0,x) = u_{0i}(x) \qquad \text{on } \Omega \times \{0\}, \tag{2.3}$$

The Neumann boundary condition ensures that diffusion over the boundary is not possible and therefore the system is not influenced by external factors. As one can see, the equation is of the form of (1.3), where $g(W, u) = Wu$. One can see that the values of $u_i$ are either decaying if $Wu$ is negative, or growing if $Wu$ is positive. Assuming $u_i \geq 0$, the entries of $W$ play the decisive role in this process. Negative entries describe a damaging influence, while positive entries a promoting influence.

In the later chapters we will use (2.1) as an introductory example to highlight the ideas of certain theories before we apply these to more complex and general partial differential equations. Now that we are familiar with the basic concept of neural network equations, we fill these equations with life.

## 2.3 Lotka-Volterra-like equations

A biological application, where semilinear parabolic evolution equations come into play are competetive models between species. These describe the development of a set of different species in an environment. A special case are for example so called predator prey models, where, the predator cannot survive, when the prey is not present. Also species radiate to new habitats, which can be modeled by a diffusion term. Here again, the growth and decay of a species is influenced by the presence or absence of other species (often in a certain manner that is known a priori). A typical two species model as proposed in [60] reads as

$$\begin{aligned} \frac{\partial u}{\partial t} - D_1 \Delta u + r_1 u &= a_{11} u^2 + a_{12} uv, \\ \frac{\partial v}{\partial t} - D_2 \Delta v + r_2 v &= a_{22} v^2 + a_{21} uv, \end{aligned}$$

with some additional boundary conditions, that have to be adapted to the respective habitat. Additional a priori information can be used to determine the structure coefficients $a_{ij}$. For example if species $u$ is a predator of species $v$, then $a_{ij}$ has a positive sign, while $a_{ji}$ has a negative sign. If both species compete for the same food sources, both signs are negative. Compared with the example from the last section, we have a similar structure but a nonlinearity of polynomial type. While general Lotka-Volterra models often assume constant competition rates, the situation in the real world is more complicated. For example if there are hideout places for the prey which predators can not reach. Time dependencies in a predator prey model are also a factor to be considered, since for example certain seasons may change the general behaviour and biological fitness drastically. A lot more examples of this type can be found in the textbook [12].

## 2.4 Biochemical evolution in embryogenesis

Another practical example is given by a nonlinear system that is directly derived from a biochemical application. In biochemical evolution, processes are often following equations like (1.3). A very special example is the early embryotic development of small organisms, where gene networks control the development of some very specific expressions or properties of the embryo. Most times, a specific genetic network consists of a few genes and is often controlled by a maternal gene. A very special example is the drosophila fly, where the first few stages of embryogenesis take place in only on multinuclear cell [51, 55]. If one tries to keep the model as simple as possible only very few natural processes have to be considered in the network. These are diffusion, decay and synthesis. Further we want to keep the interaction as direct as possible, meaning, that the synthesis rate is only controlled by the presence or absence of other genes. This ignores the interaction between mRNA and proteins, but for simple organisms like drosophila, it is believed that a model like this is sufficient for describing the evolutionary process [51]. The model is then given as a semilinear PDE. Here we only state the equation in its simplest form, where we ignore the presence of maternal genes, transport terms for moving cells or mRNA/gene interaction:

$$\begin{aligned} \frac{\partial u_i(x,t)}{\partial t} - \nabla \cdot D_i(x,t)\nabla u_i(x,t) + \lambda_i(x,t)u_i(x,t) \\ -R_i(x,t)\phi((W(x,t)u(x,t))_i) &= 0 && \text{in } \Omega_T, \\ \frac{\partial}{\partial \nu} u_i(x,t) &= 0 && \text{on } \partial\Omega \times (0,T], \\ u_i(x,0) &= u_{0i}(x) && \text{on } \Omega \times \{0\}. \end{aligned} \tag{2.4}$$

The function $\phi : \mathbb{R} \to \mathbb{R}$ is a smooth sigmoidal signal response function. In our example we utilize the function

$$\phi(z) = \frac{1}{2}\left(\frac{z}{\sqrt{z^2+1}} + 1\right).$$

Note that its derivative is given as

$$\phi'(z) = \frac{1}{2(\sqrt{z^2+1})^3},$$

which we will need later on.

More complex models would lead to similar equations, but would probably include transport terms due to moving cells as well as the interaction of mRNA concentrations with the respective gene concentrations. This would lead to another set of PDEs following its own laws [13]. Also the resulting systems would be way more complex, but we believe that the techniques that are discussed in this thesis can be used to treat these equations in a similar fashion.

Analytic properties for this example have been studied extensively in [57]. Also, this example will accompany us throughout the thesis and will help us to understand certain key features of semilinear equations. Further, we will develop our numerical framework mainly for this example, i.e. (2.4), which will be highlighting some properties of sparsity regularization for these types of equations.

# CHAPTER 3

# Preliminaries

In this chapter, we introduce the functional analysis necessary for the regularization of parameter identification problems. Although we try to keep our work as self contained as possible, we expect that the reader is familar with basic functional analysis. This especially includes the concepts of dual spaces, weak and weak* convergence and $L_p$ spaces. Also knowledge of classical theorems like the Banach-Steinhaus Theorem, the Banach-Alaoglu Theorem or the Dominated Convergence Theorem for $L_p$ spaces are assumed to be known. If this is not the case, we refer to the textbooks [1, 70]. Also basic knowledge about the weak solution theory for elliptic PDEs will be helpful for understanding the concepts presented in the later sections, but is not necessary to follow this work.

## 3.1 Bochner integration

For the right treatment of equation (1.3), namely the definition of weak solutions, we need a more general concept of integration. It turns out that a right concept to handle this is the Bochner integral which allows the integration of Banach space valued functions. For the sake of simplicity, we restrict ourselves to real intervals, which is all we need in this work. The generalization to arbitrary Lebesgue spaces with finite measure is mostly straight forward. For more information about Bochner integration, we refer to the standard references [18, 70], where most of the statements made can be found in general fashion. For the rest of this section let $I := [0, T] \subset \mathbb{R}$ and $Y$ a Banach space.

**Definition 3.1.1.** *A function $u : [0, T] \to Y$ is called* simple*, if there is a finite* *number of subsets $I_k$ of $[0,T], k = 1,..,N$ with*

$$\bigcup_{k=1}^{N} I_k = I$$

*and it holds $u(t) := y_k$ on $I_k$ for $k = 1,\dots,N$. Further, the integral of a simple function is defined as*

$$\int_0^T u(t)\ dt := \sum_{i=1}^{N} \mu(I_k) y_k,$$

*where $\mu$ is the Lebesgue measure on $\mathbb{R}$.*

Now, as in the case of Lebesgue integration, one can define measurable and integrable functions as the limit of simple functions.

**Definition 3.1.2.** *A function $u : [0,T] \to Y$ is called* Bochner measurable *if there exists a sequence of simple functions $\{u_k\}_{k\in\mathbb{N}}$, such that*

$$\lim_{k\to\infty} u_k(t) \to u(t)$$

*for almost every $t \in [0,T]$. Further, if*

$$\lim_{k\to\infty} \int_0^T \|u_k(t) - u(t)\|_Y\ dt = 0$$

*the function $f$ is called* Bochner integrable *and*

$$\int_0^T u(t)\ dt := \int_0^T u_n(t)\ dt$$

*is called the* Bochner integral *of $u$.*

An important characterization of Bochner integrable functions is the following one:

**Theorem 3.1.3** ([70, Theorem 5.1])**.** *A function $u : [0,T] \to Y$ is Bochner integrable, if and only if $\|u\|_Y : [0,T] \to \mathbb{R}$ is integrable.*

Similar to Lebesgue integrable functions, one can define the seminorm

$$\|u\|_{L_p([0,T],Y)} := \left( \int_0^T \|u(t)\|_Y^p\ dt \right)^{1/p} \tag{3.1}$$

for $1 \leq p < \infty$ and

$$\|u\|_{L_\infty([0,T],Y)} := \operatorname*{esssup}_{t \in I} \|u(t)\|_Y$$

for $p = \infty$. Then one can define the spaces

$$\tilde{L}_p([0,T],Y) := \{u \text{ Bochner measurable} \mid \|u\|_{L_p([0,T],Y)} < \infty\}$$

and the set

$$\mathcal{N} := \{f \text{ Bochner measurable} \mid f = 0 \text{ almost everywhere}\}.$$

If one now builds the quotient space, the following holds true:

**Proposition 3.1.4** ([63, Ch. III.1])**.** *The space*

$$L_p([0,T],Y) := \tilde{L}_p([0,T],Y)/\mathcal{N}$$

*equipped with* (3.1) *is a Banach space for* $1 \leq p \leq \infty$.

We can also get a generalization of the well known Hölder inequality:

**Proposition 3.1.5** ([57, Remark 2.25])**.** *Let* $p, q \in \mathbb{R}$ *with* $1/p + 1/q = 1$. *For* $u \in L_p([0,T],Y)$ *and* $v \in L_q([0,T],Y^*)$, *the function* $\langle v(t), u(t) \rangle_{(Y^*,Y)}$ *is Lebesgue measurable and it holds*

$$\int_0^T \langle v(t), u(t) \rangle_{(Y^*,Y)} \, dt \leq \|v\|_{L_p([0,T],Y^*)} \|u\|_{L_q([0,T],Y)}.$$

An important property of Bochner integrable functions is the following, also known as Phillip's theorem, which characterizes the dual space of a Bochner space:

**Theorem 3.1.6** ([63, Theorem 1.5])**.** *Let* $1 < p < \infty$ *with* $1/p + 1/q = 1$. *Let* $Y$ *be reflexive. Then it holds*

$$(L_p([0,T],Y))^* \cong L_q([0,T],Y^*).$$

It is also good to know that testing a Bochner integral with a function out of the dual space of $Y$ and integration over the dual product yield the same results

**Proposition 3.1.7** ([25, Theorem E.5.8])**.** *Suppose* $u \in L_p([0,T],Y)$ *and* $v \in Y^*$, *then it holds*

$$\left\langle v, \int_0^T u(t) \, dt \right\rangle_{(Y^*,Y)} = \int_0^T \langle v, u(t) \rangle_{(Y^*,Y)} \, dt$$

Next, we cite a few results concerning embeddings and the Bochner integral:

**Proposition 3.1.8** ([70, Corollary 5.1]). *Let $J : X \hookrightarrow Y$ be a continuous embedding and $u : [0,T] \to X$, then it holds*

$$J\left(\int_0^T u \, dt\right) = \int_0^T Ju \, dt.$$

**Proposition 3.1.9.** *Let the embedding $J : X \hookrightarrow Y$ be continuous, then the embedding*

$$L_p([0,T],X) \hookrightarrow L_p([0,T],Y)$$

*are also continuous.*

*Proof.* Let $u$ in $X$. Then the assertion follows directly from $\|Ju\|_Y \leq \|J\|\|u\|_X$. □

The last statement we will need is the following useful isometry

**Proposition 3.1.10** ([57, Remark 2.8]). *For $1 \leq p < \infty$ it holds*

$$L_p([0,T],L_p(\Omega))^N \cong L_p([0,T] \times \Omega)^N.$$

We will use this isometry very frequently throughout the work, without explicitly mentioning it.

## 3.2 Controllability of parabolic equations

In partial differential equations, one usually speaks of *control* and *state*. The state is the outcome of the equation, located at a solution space and the control is a parameter that allows us to control the outcome. Basically, every parameter in a differential equation can be used as control. If one speaks of a controllable problem, one usually means that every function at a certain time point in an appropriate function space can be reached by inserting the right control in the equation. As before, we restrict ourselves to equations that will matter for our analysis.

**Definition 3.2.1.** *A parabolic differential equation, where the solution $u$ is interpreted as a mapping $F$ from a control space $C$ to a solution space $W$ is said to be* controllable*, if for every initial data $u_0$, it holds $F(C) = W$.*

Exact controllability is a rather strong condition and thus is unlikely to hold for complex equations, thus one slightly weakens the above definition:

**Definition 3.2.2.** *A parabolic differential equation, where the solution $u$ is interpreted as a mapping $F$ from a control space $C$ to a solution space $W$ is said to be* approximately controllable*, if for every initial data $u_0$ it holds that $F(C) \subset W$ is dense.*

Note that both of these definitions are rather vague regarding the spaces $C$, $W$ and which parameter to use as control. Equations of type (1.3) are usually approximately controllable if $N = 1$, if one uses the right hand side $f$ as control or certain boundary data.

## 3.3 Weak derivatives

It turns out that the classical concept of differentiation from functions $u : \mathbb{R}^n \to \mathbb{R}$ is often too strict. Instead, one uses the formula for partial integration to generalize it and allow a much wider range of functions to be differentiable. So we introduce weak derivatives of functions.

**Definition 3.3.1.** *Let $\Omega \subset \mathbb{R}^n$, $u \in L_1(\Omega)$ and $\alpha = (\alpha_1, ..., \alpha_n)$ a multiindex. Then the function $u$ has a $\alpha$-th* weak derivative*, if there exists a function $u_\alpha \in L_1(\Omega)$ with*

$$\int\limits_\Omega D^\alpha u \varphi \; dx = (-1)^{|\alpha|} \int\limits_\Omega u_\alpha D^\alpha \varphi \; dx \qquad \forall \varphi \in C_0^\infty(\Omega).$$

**Remark 3.3.2.** The weak derivative of a function is unique, if it exists. Further, if a function is differentiable in a classical sense, it is also weakly differentiable.

A similar concept can also be applied in the case of Bochner integration and is a straight forward generalization of the definition of the weak derivative in the case of real valued functions.

**Definition 3.3.3.** *Let $X$ be a separable Banach space, $u \in L_1([0,T], X)$ and $\alpha = (\alpha_1, ..., \alpha_n)$ a multiindex. Then the function $u$ has a $\alpha$-th* weak derivative*, if there exists a function $u_\alpha \in L_1([0,T], X)$ with*

$$\int\limits_0^T u(t) D^\alpha \varphi(t) \; dt = (-1)^{|\alpha|} \int\limits_0^T u_\alpha(t) D^\alpha \varphi(t) \; dt \qquad \forall \varphi \in C_0^\infty([0,T]).$$

Using this concept of a weak derivative, one gets the following important embedding theorem.

**Theorem 3.3.4** (Lions-Aubin)**.** *Let $X, Y, Z$ be reflexive Banach spaces with embeddings $Y_1 \hookrightarrow Z \hookrightarrow Y_2$, where the first embedding is compact and the second embedding is continuous. Then for*

$$W := \{u \in L_p([0,T], Y_1) \mid u' \in L_p([0,T], Y_2)\}$$

*the embedding $W \hookrightarrow L_p([0,T], Z)$ is compact.*

## 3.4 Sobolev spaces

Similar to spaces of continuously differentiable functions, one can introduce the same concept of spaces for weakly differentiable functions.

**Definition 3.4.1.** *Let $m \in \mathbb{N}$, $1 \leq p \leq \infty$ and $\alpha = (\alpha_1, ..., \alpha_n)$ a multiindex, then*

$$H^{m,p}(\Omega) := \{u \in L_p(\Omega) \mid D^\alpha u \in L_p(\Omega)\ \forall \alpha : |\alpha| \leq m\}$$

*is called* Sobolev space of order *$m$.*

**Remark 3.4.2.** For $p = 2$, we use the notation $H^m(\Omega)$ instead of $H^{m,2}(\Omega)$.

**Proposition 3.4.3.** *The spaces $H^{m,p}(\Omega)$ equipped with the norm*

$$\|u\|_{H^{m,p}} := \left( \sum_{|\alpha| \leq m} \|D^\alpha u\|_{L_p}^p \right)^{\frac{1}{p}}$$

*for $1 \leq p < \infty$ and*

$$\|u\|_{H^m_\infty} := \max_{|\alpha| \leq m} \|D^\alpha u\|_{L_\infty}$$

*for $p = \infty$ are Banach spaces for all $m \in \mathbb{N}_0$. For $p = 2$, the spaces $H^m(\Omega)$ equipped with the inner product*

$$\langle u, v \rangle_{H^m} = \sum_{0 \leq |\alpha| \leq m} \int_\Omega D^\alpha u D^\alpha v \ dx.$$

*are Hilbert spaces*

Another interesting property of Sobolev spaces is the relation to their dual spaces. Let $1/q + 1/q' = 1$. It is not hard too see that one can identify any element of $(H^{m,q}(\Omega))^*$ by a sequence of $L_{q'}$ functions [19, Chapter 6.9]. Yet, this fact itself is not that useful for our work. More important for our analysis is the following. It is well known that $(L_q(\Omega))^* \cong L_{q'}(\Omega)$ for $1 < q < \infty$, i.e. for any element $L \in (L_q(\Omega))^*$, there exists a $v \in L_{q'}(\Omega)$, such that

$$L(u) = \int_\Omega vu \ dx. \tag{3.2}$$

Now suppose that $u$ is an element of $H^{m,q}(\Omega)$. The element $v \in L_{q'}(\Omega)$ also defines a linear functional on $H^{m,q}(\Omega)$ in the same way it does on $L_q(\Omega)$ and therefore $v$ can be viewed as an element of $(H^{m,q}(\Omega))^*$. This way one gets a natural embedding of dual spaces, i.e. $L_{q'}(\Omega) \cong (L_q(\Omega))^* \hookrightarrow (H^{m,q}(\Omega))^*$. Further, by the definition of the norm of a linear functional, one gets for $v \in L_q(\Omega)$:

$$(H^{m,q}(\Omega))^* = \sup_{u \in H^{m,q}(\Omega), \|u\|_{H^{m,q}} \leq 1} \int_\Omega vu \ dx$$

and therefore applying the Hölder inequality, combined with the continuity of the embedding $H^{m,q} \hookrightarrow L_q$ yields

$$\|v\|_{(H^{m,q}(\Omega))^*} \leq C\|v\|_{L_{q'}}.$$

So the embedding $L_{q'}(\Omega) \hookrightarrow (H^{m,q}(\Omega))^*$ is indeed continuous. By the canonical embedding $H^{m,q'}(\Omega) \hookrightarrow L_{q'}(\Omega)$ one gets the triple inclusion

$$H^{m,q'}(\Omega) \hookrightarrow L_{q'}(\Omega) \cong (L_q(\Omega))^* \hookrightarrow (H^{m,q}(\Omega))^*. \tag{3.3}$$

In fact, we can even get a little bit more than that:

**Proposition 3.4.4.** *Let $q, p \in (1, \infty)$, such that*

$$1 - \frac{d}{q} \geq -\frac{d}{p}, \tag{3.4}$$

*and $p'$, $q'$ the respective dual exponents. Then the following embeddings are continuous*

$$H^{1,q}(\Omega) \hookrightarrow L_p(\Omega)$$

*and*

$$L_{p'}(\Omega) \hookrightarrow (H^{1,q}(\Omega))^*.$$

*Proof.* The first embedding follows directly from the Sobolev embedding Theorem [1, Theorem 8.9]. Using this embedding, we find for $v \in L_{p'}(\Omega)$ that $\int vu\ dx$ is a linear functional on $H^{1,q}(\Omega)$. Thus we can define an embedding $L_{p'}(\Omega) \hookrightarrow (H^{1,q}(\Omega))^*$ via $v \mapsto \int vu\ dx$. Obviously this operator is linear and it is also continuous due to:

$$\begin{aligned}
\|v\|_{(H^{1,q}(\Omega))^*} &= \sup_{u \in H^{1,q}(\Omega), \|u\|_{H^{1,q}} \leq 1} \int_\Omega vu\ dx \\
&\leq \sup_{u \in H^{1,q}(\Omega), \|u\|_{H^{1,q}} \leq 1} \|v\|_{L_{p'}} \|u\|_{L_p} \\
&\leq \sup_{u \in H^{1,q}(\Omega), \|u\|_{H^{1,q}} \leq 1} C\|v\|_{L_{p'}} \|u\|_{H^{1,q}} \\
&\leq C\|v\|_{L_{p'}}.
\end{aligned}$$

□

**Corollary 3.4.5.** *For $q > \max\{1, 2d/(d+2)\}$, the embeddings*

$$H^{1,q}(\Omega) \hookrightarrow L_2(\Omega) \hookrightarrow (H^{1,q}(\Omega))^*$$

*are continuous.*

*Proof.* Follows directly from the previous proposition with $p = 2$. □

## 3.5 Differentiation of operators

Differentiation of functions plays a crucial role in their analysis, especially when it comes to an optimization task. Since in our case we are working with functions that are operating between Banach spaces, an appropriate concept of differentiation has to be introduced.

**Definition 3.5.1.** *Let $X, Y$ be Banach spaces and $U \subset X$ open. A function $F : U \subset X \to Y$ is called* Fréchet-differentiable *at $x \in U$ if there exists a linear and bounded function $A : X \to Y$ with*

$$F(x+h) = F(x) + Ah + r(h), \qquad \lim_{\|h\|_X \to 0} \frac{r(h)}{\|h\|_X} \to 0.$$

*The operator $A$ then is called the* (Fréchet-)derivative *of $F$ in $x$ and is denoted by $F'(x)$.*

Due to special domains that are needed in parameter identification problems (in our case almost everywhere bounded subsets of $L_p$ spaces), we are using a more adapted version of the derivative. The main reason behind this is the fact that a set of almost everywhere bounded functions has no open subsets regarding the $L_p$ topology. We state an explicit definition, which is taken from [57], for such an adapted derivative. Such a version of differentiability is commonly used for operators between function spaces with restricted domain of definition.

**Definition 3.5.2.** *Let $U \subset X$. A function $F : U \subset X \to Y$ is called* strongly differentiable *in $x \in U$ if there exists a linear and bounded function $A : X \to Y$ with*

$$F(x+h) = F(x) + Ah + r(h), \qquad \lim_{h \in DspV(x), \|h\|_X \to 0} \frac{r(h)}{\|h\|_X} \to 0,$$

*where $DspV(x) := \{h \in X \mid x + h \in U\}$ is the set of admissable displacement vectors. The operator $A$ then is called (strong) derivative of $F$ in $x$ and is denoted by $F'(x)$.*

By the above definitions it is clear that every Fréchet differentiable function is also strongly differentiable on any subset of the space, but the converse is obviously not true. However, any results that are holding for the Fréchet derivative mainly relying on norm estimates (which are all the statements we do need in our work) do also hold in the case of a strong derivative. In the rest of the work, we will often only speak of differentiable functions, especially when it is clear from the context if a strong or Fréchet-derivative is meant.

**Remark 3.5.3.** The strong derivative can be interpreted as the Fréchet derivative with respect to the subspace topology on $U$, i.e. in the subspace topology a set $S \subset U$ is open, if and only if the intersection of $S$ with $X$ is an open set.

A weaker version of the derivative can be given via the Gâteaux derivative:

**Definition 3.5.4.** *Let $X, Y$ be Banach spaces and $U \subset X$. A function $F : U \subset X \to Y$ is called* strongly Gâteaux-differentiable *at $x \in U$ if there exists a linear and bounded function $A : X \to Y$ with*

$$\lim_{t \to 0} \frac{F(x + th) - F(x)}{t} = Ah, \quad \forall h \in DspV(x).$$

*The function $A$ then is called* strong Gâteaux derivative *of $F$ in direction $h$ and is denoted by $F'_h(x)$. If further $U \subset X$ is open, then $F$ is called Gâteaux-differentiable and $F'_h(x)$ is called* Gâteaux derivative

If a function $F$ is Fréchet-differentiable at a point $x$, it is also Gâteaux differentiable. The same goes for the strong version. An important result related to differentiability is the Implicit Function Theorem.

**Theorem 3.5.5** (Implicit Function Theorem, [57, Theorem 8.7.8, Theorem 8.7.9])**.** *Let $W$ be a Banach space, $P$ a subset of a normed vector space and $Z$ be a normed vector space. For the map*

$$C : P \times W \to Z$$

*we assume*

1. *$C$ is continuous, $C(p_0, u_0) = 0$ for $(p_0, u_0) \in P \times W$.*
2. *The (partial) derivative $C_p$ exists and is continuous in a neighborhood $M \times N$ of $(p_0, u_0)$.*
3. *The (partial) derivative $C_u$ exists and is continuous in a neighborhood $M \times N$ of $(p_0, u_0)$, and at each point in $(p, u)$ of this neighborhood, $C_u$ is invertible.*
4. *The neighbourhood $N$ can be chosen convex.*

*Then we can find a constant $r > 0$ such that for all $p \in B_r(p_0)$ there exists exactly one $u(p)$, such that $C(p, u(p))) = 0$ and the resulting map*

$$\begin{aligned} u : B_r(p) \subset P &\to W \\ p &\mapsto u(p) \end{aligned}$$

*is continuously differentiable and the derivative is given as*

$$u_p(p) = (C_u(p, u(p)))^{-1} C_p(p, u(p)).$$

## 3.6 Convex analysis

Convex functions play an important role in the analysis of general Tikhonov functionals. Thus we give a short overview over their basis properties.

**Definition 3.6.1.** *Let $X$ be a normed space. A function $f : X \to \overline{\mathbb{R}}$ is called* convex, *if $\mathcal{D}(f) := \{x \in X \mid f(x) < \infty\}$ is convex and for all $x, y \in X$ it holds:*

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y).$$

*$f$ is called* proper *if $\mathcal{D}(f)$ is nonempty and $f(x) > -\infty$ for all $x \in X$.*

For a convex function one can generalize the notion of a derivative

**Definition 3.6.2.** *Let $X$ be a Banach space, let $f : X \to \overline{\mathbb{R}}$ be convex. $x^* \in X^*$ is called* subderivative *of $f$ at a point $x$, when*

$$f(y) \geq f(x) + \langle x^*, y - x \rangle_{(X^*,X)} \qquad \forall y \in X.$$

*The set of all subderivatives of $f$ at a point $x$ is called* subdifferential *of $f$.*

If $f$ is convex, lower semicontinuous and has a nonempty domain of definition, one can show that the subdifferential is nonempty for every $x \in \mathcal{D}(f)$. One now can show that the notion of a subdifferential is indeed a generalization of the derivative.

**Proposition 3.6.3** ([52, Proposition 2.3.10])**.** *If $f : X \to \overline{\mathbb{R}}$ is convex and Gâteaux differentiable at a point $x \in X$, then it holds*

$$\partial f(x) = \{f'(x)\}.$$

An important property when it comes to optimization of functionals is the following one:

**Proposition 3.6.4.** *If $f : X \to \overline{\mathbb{R}}$ is convex, $x \in X$ is a minimizer of $f$ if and only if $\mathcal{D}(f)$ is nonempty and $0 \in \partial f(x)$.*

*Proof.* This follows immediately from the definition of subdifferential. □

The sum of convex functions is indeed convex and we can compute the subdifferential in a very natural way:

**Proposition 3.6.5** ([52, Proposition 2.4.4])**.** *Let $f_1, f_2, ..., f_n : X \to \overline{\mathbb{R}}$ be convex and let all $f_i$ except one be continuous. Let $\mathcal{D} := \mathcal{D}(f_1) \cap \mathcal{D}(f_2) \cap ... \cap \mathcal{D}(f_n)$ nonempty. Then the sum $f_1 + f_2 + ... + f_n$ is a convex function and for each $x \in \mathcal{D}$ it holds*

$$\partial\left(\sum_{i=1}^{n} f(x)\right) = \sum_{i=1}^{n} \partial f(x).$$

An important concept in convex optimization is the following one:

**Proposition 3.6.6** ([15, Chapter 2])**.** *Let $X$ be a Hilbert space and $f : X \to \overline{\mathbb{R}}$ a proper, convex, lower semicontinuous function, then for $x \in \mathcal{D}(f)$, the operator $prox_f(x) : X \to X$ defined by*

$$\operatorname{prox}_f(x) = \operatorname*{argmin}_{y \in X} \frac{\|y - x\|^2}{2} + f(y)$$

*exists, is well defined and is called* proximal mapping *of $f$ at a point $x$.*

The following characterization for the proximal mapping can be given:

**Proposition 3.6.7.** *Let $X$ be a Hilbert space and $f : X \to \overline{\mathbb{R}}$ proper, convex and lower semicontinuous then the proximal mapping at a point $x$ is given by*

$$\operatorname{prox}_f(x) = (I + \partial f)^{-1}(x),$$

*where $I : X \to X$ is the identity mapping.*

*Proof.* From Proposition 3.6.4 it follows that

$$0 \in y - x + \partial f(y) \quad \Longleftrightarrow \quad x \in (I + \partial f)y,$$

which immediately proves the claim. □

The above assertion will play an important role when we analyze the minimization of Tikhonov type functional later on. Another

**Definition 3.6.8.** *Let $X$ be a Banach space and $f : X \to \overline{\mathbb{R}}$ convex. Further let $y \in \mathcal{D}(f)$ and $\xi \in \partial f(y)$, then $d_\xi : X \times X \to \mathbb{R}$ given by*

$$d_\xi(x, y) = f(x) - f(y) - \langle \xi, x - y \rangle_{(X^*, X)}$$

*is called* Bregman distance *with respect to $f$ and $\xi$.*

The Bregman distance is at least always greater or equal than zero, but it does not hold $d_\xi(x) \neq d_\xi(y)$, if $x \neq y$.

## 3.7 Superposition operators

Let us consider a general, possibly nonlinear function $f : \mathbb{R} \to \mathbb{R}$. If $f \circ u \in L_q(\Omega)$ for all $u \in L_p(\Omega)$, we surely can define an operator $F : L_p(\Omega) \to L_q(\Omega)$, $u \mapsto f(u)$. This operator is called a *superposition operator*. In many situations one wants to survey analytical properties of the function $F$ regarding continuity and Fréchet differentiability. One might even think that the continuity and differentiability properties of $f$ directly carry over to the function $F$. But this is not always the case. In fact, the function $f$ has to fulfill a certain growth estimate to guarantee the differentiability of the operator $F$, along with certain restrictions onto the exponents $p$ and $q$. In this section, we will give a short overview over these facts. The statements we cite in this section are quite technical and thus we will give a short explanation afterwards. Also we try to keep this section as short as possible and refer to the standard reference [5] for more information about superposition operators.

**Definition 3.7.1.** *Let $\Omega \subset \mathbb{R}^n$. A function $f : \Omega \times \mathbb{R} \to \mathbb{R}$ is called* Caratheodory function *if $f$ is measurable in the first argument and continuous in the second argument.*

First of all we address the existence question concerning superposition operators:

**Theorem 3.7.2** ([5, Theorem 3.1])**.** *Let $f : \Omega \times \mathbb{R} \to \mathbb{R}$ be a Caratheodory function and $1 < p < \infty$. The superposition operator $F$ generated by $f$ maps $L_p(\Omega)$ into $L_q(\Omega)$ if and only if there exists a function $a \in L_q(\Omega)$ and a constant $C \geq 0$ such that*

$$|f(x, u)| \leq a(x) + C|u|^{p/q}.$$

Usually, superposition operators generated by Caratheodory functions are continuous between $L_p(\Omega)$ and $L_q(\Omega)$ for appropriate $p$ and $q$ (cf. [5] for this statement). So the first result we cite is concerning the Lipschitz continuity of superposition operators

**Theorem 3.7.3** ([5, Theorem 3.10])**.** *Let $f$ be a Caratheodory function and suppose that the superposition operator $F$ generated by $f$ acts from $L_p(\Omega) \to L_q(\Omega)$ with $p \geq q$. Then the following conditions are equivalent*

1. *The operator $F$ satisfies a Lipschitz condition*

$$\|F(h_1) - F(h_2)\|_{L_q} \leq k(r)\|h_1 - h_2\|_{L_p}, \qquad h_1, h_2 \in B_r(L_p).$$

2. *The function $f$ satisfies a Lipschitz condition*

$$|f(x, u) - f(x, v)| \leq g(x, w)|u - v| \quad (|u|, |v| \leq w),$$

*where the function $g$ generates a superposition operator $G$, which maps the ball $B_r(L_p(\Omega))$ into the ball $B_{k(r)}(L_{\frac{pq}{p-q}}(\Omega))$ in the case $p > q$ and into the ball $B_{k(r)}(L_\infty(\Omega))$ in the case $p = q$.*

So, roughly speaking superposition operators generated by Lipschitz continuous functions are at least locally Lipschitz continuous. Global Lipschitz continuity holds for example if the operator $G$ generated by $g$ is a linear operator and then the global Lipschitz constant is given by $\|G\|$ [57, Theorem 3.2.8].

**Theorem 3.7.4** ([5, Theorem 3.12])**.** *Let $f$ be a Caratheodory function and suppose that the superposition operator $F$ generated by $f$ acts from $L_p(\Omega) \to L_q(\Omega)$. If $F$ is differentiable at $u \in L_p$, the derivative has the form*

$$F'(u(x))h(x) = a(x)h(x) \tag{3.5}$$

*with*

$$a(x) = \lim_{z\to 0} \frac{f(x, u(x) + z) - f(x, u(x))}{z}. \tag{3.6}$$

*In case $p > q$ the function $a$ belongs to $L_{\frac{pq}{p-q}}(\Omega)$. In the case $p = q$ the function $f$ has the form*

$$f(x, u(x)) = c(x) + a(x)u(x)$$

*with $u \in L_q(\Omega)$ and $a \in L_\infty(\Omega)$. In case $p < q$ the function $f$ is constant. Conversely, if $p > q$ and the superposition operator $G$ generated by the function*

$$g(x, z) = \begin{cases} \frac{1}{z}(f(x, u(x) + z) - f(x, u(x))) & z \neq 0 \\ a(x) & z = 0 \end{cases} \tag{3.7}$$

*is continuous from $L_p(\Omega) \to L_{\frac{pq}{p-q}}(\Omega)$, then $F$ is differentiable with derivative* (3.5)*.*

Theorem 3.7.4 essentially says, that if a function $f(x, u(x))$ is truly nonlinear in $u$, then its superposition operator can only be differentiable if $p > q$. Further, in condition (3.7) a sufficient condition for differentiability is given in the case $p > q$. Since this is the only interesting case, we are looking deeper into it in the following theorem.

**Theorem 3.7.5** ([5, Theorem 3.13])**.** *Let $p > q$ and suppose that the superposition operator $F$ generated by $f$ acts from $L_p(\Omega) \to L_q(\Omega)$. Then $F$ is differentiable if and only if the limit* (3.6) *exists, belongs to $L_{\frac{pq}{p-q}}(\Omega)$ and satisfies the following condition: for each $\lambda > 0$ there exists $a_\lambda \in L_1(\Omega)$, such that $\|a_\lambda\| \to 0$ as $\lambda \to \infty$ and*

$$|f(x, u(x) + h) - f(x, u(x)) - a(x)h|^q \leq \lambda^{-q} a_\lambda(x) + \lambda^{p-q}|h|^p. \tag{3.8}$$

**Remark 3.7.6.** The exponent $pq/(p - q)$ is exactly chosen in a way that the multiplication in (3.5) for $a \in L_{pq/(p-q)}$ with a function $h \in L_p$ is in $L_q$, as one can derive from the Hölder inequality.

**Remark 3.7.7.** By Theorem 3.7.4 the derivative of a superposition operator $F$ coming from a differentiable function $f$ is a multiplication operator. The reader is encouraged to remember that, since it will be very important later on. This multiplication operator consists of the two components $a = f'$ and the direction $h$. This also explains the restrictions that have to be made on the exponents. For example if we consider an operator $F : L_2 \to L_2$, it must hold $\|ah\|_{L_2} \leq C\|h\|_{L_2}$, which only holds if $a \in L_\infty$. Finally, the growth condition (3.8) from Theorem 3.7.5 basically ensures the convergence of the remainder $r(h)$ for $h \to 0$. So if one wants to check differentiability of superposition operators, one has basically to check if the condition (3.8) holds. Note that for well behaved functions $f$, one might assume growth conditions on the superposition operator that are easier to verify than (3.8) to achieve differentiability as it has been done in [57].

Since we will also be dealing with weak convergences between $L_p$ spaces the following result will be also of interest

**Theorem 3.7.8** ([5, Theorem 3.9]). *Let $f$ be a Caratheodory function, and suppose that the superposition operator $F$ generated by $f$ acts from $L_p(\Omega)$ into $L_q(\Omega)$. Then $F$ is weakly continuous if and only if $f$ satisfies*

$$f(x, u(x)) = c(x) + a(x)u(x).$$

So superposition operators that come from a truly nonlinear function $f$ can not be weakly continuous.

**Remark 3.7.9.** The theorems regarding differentiability and weak continuity will explain the extended analysis that we have to make for the parameter identification problem compared to the usual analysis of parameter identification problems in Hilbert spaces. We will come back to this when we analyze the parameter-to-state map of our parameter identification problem in Chapter 6.

## 3.8 Unbounded operators

Let us consider a linear operator $A : \mathcal{D}(A) \subset X \to Y$, where $X$ and $Y$ are Banach spaces. Further we do not assume that this operator is bounded. Typical examples for unbounded operators are differential operators mapping between $L_2$ spaces, i.e.

$$\begin{aligned} A : H^1(\Omega) \subset L_2(\Omega) &\to L_2(\Omega) \\ u &\mapsto \nabla u. \end{aligned}$$

The following concept will be helpful:

**Definition 3.8.1.** *Let $\{u_n\} \subset \mathcal{D}(A)$ with $u_n \to u \in X$ and $Au_n \to v \in Y$. Then $A$ is called* closed *if $u \in \mathcal{D}(A)$ and $Au = v$.*

For an unbounded operator with a dense domain of definition, i.e. $\overline{\mathcal{D}(A)} = X$, it is possible to define an adjoint operator.

**Theorem 3.8.2** ([42, Chapter 5]). *Let $A : \mathcal{D}(A) \subset X \to Y$ be densely defined. Then, there exist a unique linear operator $A^* : \mathcal{D}(A^*) \subset Y^* \to X^*$ such that*

$$\langle y^*, Ax\rangle_{(Y^*,Y)} = \langle A^*y^*, x\rangle_{(X^*,X)}, \qquad \forall x \in \mathcal{D}(A), y^* \in \mathcal{D}(A^*)$$

*and for any other linear operator $B$ satisfying*

$$\langle y^*, Ax\rangle_{(Y^*,Y)} = \langle By^*, x\rangle_{(X^*,X)}, \qquad \forall x \in \mathcal{D}(A), y^* \in \mathcal{D}(B),$$

*$B$ is a restriction of $A^*$. $A^*$ then is called the adjoint of $A$.*

In particular, we need the following

**Theorem 3.8.3** ([42, Theorem 5.30])**.** *Let* $A : \mathcal{D}(A) \subset X \to Y$ *be a linear, closed and densely defined operator. If* $A^{-1}$ *exists and is bounded, then* $(A^*)^{-1} : Y^* \to X^*$ *exists and is bounded and it holds*

$$(A^*)^{-1} = (A^{-1})^*.$$

# CHAPTER 4

# Parameter identification

In a parameter identification problem, the outcome of a system like in (1.3) is at least partially known, that means one can measure the solutions of the differential equation on a subset $\Omega_0 \subset \overline{\Omega}_T$, and one wants to extract certain parameters from these measurements. For example, in (2.4) we can measure the genetic concentrations at certain time instances and one wants to know the interaction of different genes. A problem that almost always comes with this task is the ill-posedness of this inverse problem. We distinguish two different kinds of ill-posedness. The first question one always has to ask if there is a unique dependence of the parameters onto the data or mathematically spoken, if the forward operator is injective. The second question then is, if the parameters depend continuously on the data. Especially in problems involving partial differential equations this is usually not the case and one has to deal with this.

## 4.1 Identifiability

The first question one may ask is, if for a given solution of a differential equation one can obtain an at least locally unique set of parameters. To examine this question further, we introduce the concept of identifiability, which we adapt from [7]:

**Definition 4.1.1.** *Let $P$ be the parameter space of a parameter identification problem $F : P \to Y$ and $d : P \times P \to \mathbb{R}$ be a distance function. In a parameter identification problem $F(p) = y$, $p$ is called globally identifiable if $F$ is injective. The parameter $p$ is called locally identifiable if there exists a $\varepsilon > 0$ such that for each $p^*$ with $d(p, p^*) < \varepsilon$ and $F(p) = F(p^*)$ it holds $p = p^*$. Otherwise, $p$ is called unidentifiable.*

Local non identifiability in fact is much worse than non continuous dependence of the parameters on the data, because even with perfect data, one can not expect to come close to the true solution in general. In this case, one can only hope to characterize the set of parameters $S := \{p \in P \mid F(p) = F(p^\dagger)\}$ and possibly use a priori information to pick the right parameter. However, depending on the structure of the problem, characterizing such a set might be impossible.

### 4.1.1 Identifiability in parabolic systems

In systems of differential equations, identifiability is always a problem and often only holds under strong restrictions on the parameters [60, 16]. In scalar equations, where only one parameter has to be identified, identifiability often can be shown, at least locally under mild assumptions on the measurements, see Chapter 7. The more variables are involved in a system and the bigger the system becomes, it seems more and more unlikely that identifiability holds and thus the conditions needed to show identifiability become more and more restrictive. Especially in parabolic equations or systems with more than one parameter involved, one cannot expect identifiability in general if all parameters are space and time dependent. To show this, we consider our example from Section 2.2.

**Theorem 4.1.2.** *Let $N \geq 2$. Let $P$ and $U$ be Banach spaces, with $\mathcal{P} = P \times ... \times P$ and $\mathcal{W} = U \times ... \times U$ and let both spaces be equipped with the product-one-norm. Assume that for every parameter $W \in \mathcal{P}$ the equation* (2.1) *has a unique solution in the space $\mathcal{W}$. Further assume $U \hookrightarrow P$. Then the interaction parameter $W \in \mathcal{P}$ in equation* (2.1) *is unidentifiable with respect to the $\mathcal{P}$-norm.*

*Proof.* Without loss of generality we assume $N = 2$. We show that in any $\varepsilon$-neighbourhood of a given parameter $W \in \mathcal{W}$ there is at least one $W^*$ with $\|W - W^*\| \leq \varepsilon$ but $F(W) = F(W^*)$. Let $\varepsilon > 0$, $W \in \mathcal{W}$ and let $u$ be the solution corresponding to $W$. Without loss of generality, we assume $u \neq 0$. Note that if $u_i(x,t) = 0$, then the parameter $W$ has no influence at the point $(x,t)$. Let $\|u\| = \|u_1\|_P + \|u_2\|_P$ and define

$$W_{11}^* := W_{11} - \frac{\varepsilon}{2}\frac{u_2}{\|u\|_{\mathcal{P}}} \quad \text{and} \quad W_{12}^* := W_{12} + \frac{\varepsilon}{2}\frac{u_1}{\|u\|_{\mathcal{P}}}$$

as well as

$$W_{21}^* := W_{21} \quad \text{and} \quad W_{22}^* := W_{22}.$$

The parameter $W^*$ is a well defined element from $\mathcal{P}$ because of the continuous embedding $U \hookrightarrow P$. Further, let $u^*$ be the solution to (2.1) with the parameter

$W^*$. For $t \in (0,T]$ we get

$$\begin{aligned} & -\frac{u_2}{\|u\|}u_1^* + \frac{u_1}{\|u\|}u_2^* \\ =& -\frac{u_2}{\|u\|}u_1^* + \frac{u_1}{\|u\|}u_2^* + \frac{u_2}{\|u\|}u_1 - \frac{u_1}{\|u\|}u_2 \\ =& -\frac{u_2}{\|u\|}(u_1^* - u_1) + \frac{u_1}{\|u\|}(u_2^* - u_2). \end{aligned}$$

Since both, $u$ and $u^*$ solve a differential equation, we get by subtracting the respective equations

$$\begin{aligned} & (u_1^* - u_1)_t - \nabla \cdot D\nabla(u_1^* - u_1) + W_{11}(u_1^* - u_1) + W_{12}(u_2^* - u_2) \\ & - \frac{\varepsilon}{2}\frac{u_2}{\|u\|}u_1^* + \frac{\varepsilon}{2}\frac{u_1}{\|u\|}u_2^* \\ =& (u_1^* - u_1)_t - \nabla \cdot D\nabla(u_1^* - u_1) + W_{11}(u_1^* - u_1) + W_{12}(u_2^* - u_2) \\ & - \frac{\varepsilon}{2}\frac{u_2}{\|u\|}(u_1^* - u_1) + \frac{\varepsilon}{2}\frac{u_1}{\|u\|}(u_2^* - u_2) \\ =& (u_1^* - u_1)_t - \nabla \cdot D\nabla(u_1^* - u_1) + W_{11}^*(u_1^* - u_1) + W_{12}^*(u_2^* - u_2) = 0 \end{aligned}$$

and

$$(u_2^* - u_2)_t - \nabla \cdot D\nabla(u_2^* - u_2) + W_{21}^*(u_1^* - u_1) + W_{22}^*(u_2^* - u_2) = 0.$$

Hence, $v = u^* - u$ solves the differential equation

$$\begin{aligned} v_t - \nabla \cdot D\nabla v + W^* v = 0 \qquad & \text{in} \qquad \Omega_T \\ \frac{\partial}{\partial \nu} v(0,t) = 0 \qquad & \text{on} \qquad \partial\Omega \times [0,T] \\ v(x,0) = 0 \qquad & \text{on} \qquad \Omega \times \{0\}. \end{aligned}$$

Clearly, $v = 0$ is a solution of this differential equation as well. Thus, by our assumption that the solution is unique, it must hold $u = u^*$. Hence, $F(W) = F(W^*)$. Further it holds

$$\begin{aligned} \|W - W^*\|_{\mathcal{P}} &= \sum_{i=1}^{2}\sum_{j=1}^{2} \|W_{ij} - W_{ij}^*\|_P \\ &\le \frac{\varepsilon}{2\|u\|}\|u_2\|_P + \frac{\varepsilon}{2\|u\|}\|u_1\|_P \\ &\le \varepsilon. \end{aligned}$$

This concludes the proof. □

**Remark 4.1.3.** The assumptions we made to show the non-uniqueness are not very strong. For example, if one chooses $P = L_2(\Omega)$ and $U = \mathbb{W}_1^2$ (and restricts the domain of $F$ in an appropriate way), existence and uniqueness follows by classical weak solution theory (see Chapter 5 or cf. [25]).

**Remark 4.1.4.**

i) In the case of Theorem 4.1.2, $N^2$ space and time dependent parameters have to be identified, but there is only data for two space and time dependent functions. So the data is highly underspecified.

ii) One can easily construct similar examples for non uniqueness in the case that multiple parameters that have to be identified in a scalar equation (or in a system).

iii) We have used the norm of the parameter space as distance function in Theorem 4.1.2. But even for more general distance functions that can be related to the spaces $\mathcal{P}$ and $\mathcal{W}$ the parameter stays unidentifiable. This is especially interesting for Tikhonov-regularization, because here, usually certain norms are used as a prior to highlight properties of the function.

For now on, we will leave the identifiability issue and will return to it in Section 7.

## 4.2 Tikhonov type regularization

Usually, when someone speaks of ill-posedness of a problem, he means that the parameters are not continuously dependent on the data. In this case, one needs to perform some kind of regularization (which means a stabilization of the inversion process). A very general regularization method is Tikhonov type regularization. For this section, let $X$ and $Y$ be arbitrary Hilbert spaces and $F : \mathcal{D}(F) \subset X \to Y$ an arbitrary operator. In the respective inverse problem, one wants to find $x \in X$, with $F(x) = y$, if only a noisy version $y^\delta$ of $y$ is known. As already stated in the introduction, Tikhonov type regularization is the minimization of the functional

$$J_\alpha(x) := \|F(x) - y^\delta\|_Y^2 + \alpha R(x), \tag{4.1}$$

where $R : X \to [0, \infty]$. In the following we will denote a minimizer of $J_\alpha$ by $x_\alpha^\delta$ and the true solution by $x^\dagger$. First of all one might ask questions about existence of a minimizer as well as the behaviour of the Tikhonov functional for $\alpha \to 0$. Remember that the penalty $R$ should be chosen in a way to include a priori information about the true solution in order to find a good approximation of $x^\dagger$, especially if the solution of $F(x) = y$ is not unique. If the parameter is at least locally identifiable, the right choice of $R$ can improve the quality of the solution drastically, depending on available a priori information of $x^\dagger$. To put this concept into mathematical language, we introduce the notation of an $R$ minimizing solution:

**Definition 4.2.1.** *A solution $x^\dagger$ to the problem $F(x) = y$ is called $R$ minimizing-solution, if $F(x^\dagger) = y$ and*

$$R(x^\dagger) \leq R(x) \qquad \forall x \in \{x \mid F(x) = y\}.$$

Note that an $R$ minimizing solution might not be unique either. To ensure regularizing properties, one usually has to make some assumptions on $F$ and $R$. Note that we are dealing with a somewhat special problem. Therefore we modify the standard assumptions from [36] to better fit our parameter identification problem. The reason for this is that the key ingredient for regularization to happen, the so called *weak sequential closedness* introduced in [24], can often not be shown with standard weak topologies for nonlinear PDEs. This is a direct consequence of Theorem 3.7.8, where it is stated that a truly nonlinear superposition operator between $L_p$ spaces (which are the preferred choice for our problem) cannot be weak to weak continuous. The approach we are using here was introduced in [57] and is further extended to fit our needs.

**Assumption 4.2.2.**

*(i)* $\tilde{X}$ *is a Banach space and* $\tilde{X} \hookrightarrow X$ *continuously.*

*(ii)* $\tilde{X}$ *can be equipped with a topology* $\tau$ *and* $x_n \overset{\tau}{\to} x$ *in* $\tilde{X}$ *implies* $x_n \rightharpoonup x$ *in* $X$.

*(iii)* $\mathcal{D}(F) \subset \tilde{X}$.

*(iv)* $F$ *is* $\tau$*-weakly sequentially closed, i.e.* $x_n \overset{\tau}{\to} x$ *and* $F(x_n) \rightharpoonup y$ *implies* $x \in \mathcal{D}(F)$ *and* $F(x) = y$.

*(v)* $R : X \to \mathbb{R}$ *is proper, convex and weakly lower semicontinuous.*

*(vi)* $\mathcal{D} := \mathcal{D}(R) \cap \mathcal{D}(F)$ *is nonempty and* $x^\dagger \in \mathcal{D}$.

*(vii)* *The level sets*

$$\mathcal{M} := \{x \in \mathcal{D} \mid R(x) \leq C,\ C \geq 0\}$$

*are* $\tau$ *sequentially precompact in the following sense: every sequence* $\{x_k\} \subset \mathcal{M}$ *has a subsequence, that is convergent in* $\mathcal{M}$ *with respect to the* $\tau$*-topology.*

*One might replace the assumption (vii) by the following one*

*(vii') The domain* $\mathcal{D}$ *is* $\tau$ *sequentially precompact.*

**Remark 4.2.3.** A typical example for a topology $\tau$ that fulfills Assumption 4.2.2 conditions (i) and (ii) is of course the weak topology on $X$. Another one is the strong topology. Another trivial example is the case, where $\Omega \subset \mathbb{R}^d$ is bounded, $X = L_2(\Omega)$, $\tilde{X} = L_\infty(\Omega)$ and $\tau$ is the weak$^*$ topology on $L_\infty(\Omega)$, since weak$^*$ convergence in $L_\infty$ implies weak convergence in $L_2$.

One can now show regularization properties for Tikhonov type regularization, which consists of three parts. The proofs of the following theorems can mostly be done along the lines of the equivalent ones in [36]. For the sake of completeness, we include them here. The first one is existence of solutions

**Theorem 4.2.4.** *Let Assumption 4.2.2 hold. Then for any $\alpha > 0$, there exists a minimizer of $J_\alpha$.*

*Proof.* Since $\mathcal{D}$ is nonempty, there exists an $\bar{x} \in X$ such that $J_\alpha(\bar{x}) := C < \infty$. Further it holds $J_\alpha \geq 0$ and hence there exists $M_J = \inf_{x\in\mathcal{D}} J_\alpha(x)$ and therefore a sequence $\{x_k\}$ with $J_\alpha(x_k) \to M_J$ and $J_\alpha(x_k) \leq C$. One can easily show that the sequences $\{F(x_k)\}$ and $\{R(x_k)\}$ are bounded. By Assumption 4.2.2 $(vii)$ the sequence $\{x_k\}$ has a $\tau$ convergent subsequence that we again denote by $\{x_k\}$. By $(ii)$ this sequence also converges weakly in $X$. Further, by the boundness of the sequence $F(x_k)$ there exists subsequence $\{x_n\}$ of $\{x_k\}$ with $x_n \rightharpoonup y$ in $Y$. By the $\tau$-weak sequential closedness of $F$ we therefore get $F(x) = y$. Now we use the weak lower semicontinuity of the norm and the penalty to arrive at

$$\|F(x) - y^\delta\|^2 + \alpha R(x) \leq \liminf \|F(x_n) - y^\delta\|^2 + \alpha R(x_n) = M_J.$$

Hence, $x$ is a minimum of the Tikhonov functional. □

The second part is the continuity in the data, if $y^\delta$ varies in a small portion, also the minimizer should only vary a small bit. Note that for general penalty terms we only obtain a weak continuity result:

**Theorem 4.2.5.** *Let Assumption 4.2.2 hold. Further, let $\{y_k\}_{k\in\mathbb{N}}$ converge to $y^\delta$ in $Y$ and let*

$$x_k \in \operatorname*{argmin}_{x\in\mathcal{D}(F)} \|F(x) - y_k\|^2 + \alpha R(x).$$

*Then there exists a $\tau$ convergent subsequence of $\{x_k\}_{k\in\mathbb{N}}$ converging to a minimizer $x_\alpha^\delta$ of $J_\alpha$ with $R(x_k) \to R(x_\alpha^\delta)$.*

*Proof.* The definition of $\{x_k\}$ implies that

$$\|F(x_k) - y_k\|^2 + \alpha R(x_k) \leq \|F(x) - y_k\|^2 + \alpha R(x) \qquad \forall x \in \mathcal{D}. \tag{4.2}$$

Using the norm convergence of $y_k \to y^\delta$ and (4.2) we get

$$\begin{aligned} \|F(x_k) - y^\delta\|^2 + \alpha R(x_k) &\leq (\|F(x_k) - y_k\|^2 + \|y_k - y^\delta\|^2) + \alpha R(x_k) \\ &\leq 2\|F(x) - y_k\|^2 + 2\|y_k - y^\delta\|^2 + 2\alpha R(x) \\ &\leq 2C_1 + 2C_2 + 2\alpha R(x) \leq C. \end{aligned}$$

Therefore the sequences $\{F(x_k)\}$ and $\{R(x_k)\}$ are bounded. Just like in the proof of the previous theorem, we can deduce that Assumption 4.2.2 yields a $\tau$ convergent subsequence $\{x_n\}$ with the following properties: $x_n \xrightarrow{\tau} \bar{x}$, $x_n \rightharpoonup \bar{x}$ and $F(x_n) \rightharpoonup F(\bar{x})$. The weak lower semicontinuity of the norm and the penalty then allow the following estimate

$$\begin{aligned}\|F(\bar{x}) - y^\delta\|^2 + \alpha R(\bar{x}) &\le \liminf_{n\to\infty} \|F(x_n) - y_n\|^2 + \alpha R(x_n) \\ &\le \limsup_{n\to\infty} \|F(x_n) - y_n\|^2 + \alpha R(x_n) \\ &\le \lim_{n\to\infty} \|F(x) - y_n\|^2 + \alpha R(x) \\ &= \|F(x) - y^\delta\|^2 + \alpha R(x) \qquad \forall x \in \mathcal{D}. \end{aligned} \tag{4.3}$$

Hence, $\bar{x}$ is a minimizer of the Tikhonov functional. Further, it follows from (4.3) that

$$\|F(\bar{x}) - y^\delta\|^2 + \alpha R(\bar{x}) = \lim_{n\to\infty} \|F(x_n) - y_n\|^2 + \alpha R(x_n).$$

If we now assume that $R(x_n)$ does not converge to $R(\bar{x})$ and define

$$c := \limsup R(x_n) > R(\bar{x}),$$

we can find a subsequence $\{x_l\} \subset \{x_n\}$, such that $x_l \rightharpoonup \bar{x}$. Then we estimate

$$\lim_{l\to\infty} \|F(x_l) - y_l\|^2 = \|F(\bar{x}) - y^\delta\|^2 + \alpha(R(\bar{x}) - c) < \|F(\bar{x}) - y^\delta\|^2,$$

which is a contradiction to the weak lower semicontinuity of the norm. Hence, $R(x_n) \to R(x)$. □

The most important property to proof is the regularization property, i.e. if $\delta \to 0$ and $\alpha$ is chosen appropriately, then the minimizer approaches a true solution for the problem.

**Theorem 4.2.6.** *Let Assumption 4.2.2 hold. Let $x^\dagger$ be a $R$ minimizing solution of $F(x) = y$. Further assume, that the sequence $\delta_k$ converges monotonically to 0 and $y^{\delta_k}$ satisfies $\|y - y^{\delta_k}\| \le \delta_k$. Then, if $\alpha = \alpha(\delta)$ is chosen such that*

$$\alpha(\delta) \to 0 \text{ and } \frac{\delta^2}{\alpha(\delta)} \to 0 \qquad \text{as } \delta \to 0$$

*and $\alpha_k = \alpha(\delta_k)$, every sequence of minimizers*

$$x_{\alpha_k}^{\delta_k} \in \operatorname*{argmin}_{x\in\mathcal{D}(F)} \|F(x) - y^{\delta_k}\|^2 + \alpha_k R(x)$$

*has a $\tau$ convergent subsequence $\{x_n\}$, that converges to a $R$-minimizing solution. Additionally it holds $R(x_n) \to R(x)$. If the $R$ minimizing solution $x^\dagger$ is unique, then $x_n \xrightarrow{\tau} x^\dagger$.*

*Proof.* The definition of $x_{\alpha_k}^{\delta_k}$ implies that

$$\|F(x_{\alpha_k}^{\delta_k}) - y^{\delta_k}\|^2 + \alpha_k R(x_{\alpha_k}^{\delta_k}) \le \delta_k^2 + \alpha_k R(x^\dagger)$$

and therefore $\lim_{k\to\infty} F(x_{\alpha_k}^{\delta_k}) = y$ and $\limsup_{k\to\infty} R(x_{\alpha_k}^{\delta_k}) \leq R(x^\dagger) \leq C$. By Assumption 4.2.2 there exists a $\tau$ convergent subsequence $\{x_n\}$ that converges to $\bar{x} \in \mathcal{D}$. By the fact that $\tau$ convergence implies weak convergence, we deduce that $\bar{x}$ is also the weak limit of $\{x_n\}$. Since strong convergence implies weak convergence and the weak limit is unique, the $\tau$-weak sequential closedness of $F$ implies $F(\bar{x}) = y$. The weak lower semicontinuity of the penalty gives

$$R(\bar{x}) \leq \liminf_{n\to\infty} R(x_n) \leq \limsup_{n\to\infty} R(x_n) \leq R(x^\dagger) \leq R(\bar{x}). \tag{4.4}$$

Hence, $\bar{x}$ is also an $R$ minimizing solution. From (4.4) it further follows that $\lim_{n\to\infty} R(x_n) = R(\bar{x})$. If the $R$ minimizing solution is unique, the convergence $x_n \xrightarrow{\tau} x^\dagger$ follows from the fact that every subsequence has a subsequence, that converges to $x^\dagger$ with respect to $\tau$. □

**Remark 4.2.7.** If one assumes Assumption 4.2.2 $(vii)'$ instead of $(vii)$ one obtains a $\tau$ convergent subsequence in the proofs of theorems 4.2.4, 4.2.5 and 4.2.6 directly by the fact that this sequence is in $\mathcal{D}$. An even stronger assumption would be to have a compact domain of $F$, in this case continuity of $F$ is enough to prove the above statements and a weak closedness statement on $F$ is not needed (note that the case of a compact domain is basically included in Assumption 4.2.2). This becomes relevant, when we discuss regularization properties for nonlinear partial differential equations.

**Remark 4.2.8.** If $\{x_k\} \subset X$ converges to $x \in X$ with respect to $R$, i.e. $R(x_k - x) \to 0$, one automatically gets convergence of $\{x_k\}$ with respect to the norm if $R$ is coercive due to $\|x_k - x\| \leq CR(x_k - x) \to 0$.

Last but not least, one wants to know a direct estimate between true and regularized solution. This can only be derived under very special assumptions, so called *source conditions*. While there are several general formulations of source conditions, mostly given through variational inequalities, see [28] for an overview, in our work we only want to look at the more classical setting. In this case, an element $\xi \in \partial R(x^\dagger)$ has to exist, such that $\xi$ is an element of the range of $F'(x^\dagger)^*$ to ensure a convergence rate.

**Theorem 4.2.9** ([40, Theorem 3.5]). *Let Assumption 4.2.2 be fulfilled. Further assume*

*(i) $F$ is Gâteaux differentiable,*

*(ii) $x^\dagger$ fulfills a source condition, i.e. there exist a $w \in Y$ and $\xi \in \partial R(x^\dagger)$ with*

$$\xi = F'(x^\dagger)^* w \in \partial R(x^\dagger), \tag{4.5}$$

*(iii) there exists a $\gamma > 0$, such that $\|F(x) - F(x^\dagger) - F'(x^\dagger)(x - x^\dagger)\| \leq \gamma d_\xi(x, x^\dagger)$ in a sufficiently large ball around $x^\dagger$,*

*(iv)* $\gamma\|w\| < 1$.

*Then, for a parameter choice* $\alpha \sim \delta$ *the minimizer* $x_\alpha^\delta$ *of* $J_\alpha$ *fulfills*

$$d_\xi(x_\alpha^\delta, x^\dagger) = \mathcal{O}(\delta).$$

**Remark 4.2.10.** The nonlinearity conditions $(i)$, $(iii)$ and $(iv)$ can be replaced by the condition $\|F(x) - F(x^\dagger) - F'(x^\dagger)(x - x^\dagger)\| \leq \gamma_2 \|F(x) - F(x^\dagger)\|^{c_1} \|x - x^\dagger\|^{c_2}$, $0 < c_1 \leq 1, 0 \leq c_2 \leq 1$, see [34]. In fact it is not completely clear if and how different nonlinearity conditions influence the convergence behaviour for $\delta \to 0$ and to which degree they are necessary for a convergence rate to hold.

A relaxation to source conditions are so called approximate source conditions, introduced in [35] and for general inverse problems investigated in [28, 34], which in our case are very interesting to look at. First of all we introduce the following distance function for $\xi \in \partial R(x^\dagger)$

$$d(r) := \inf\{\|\xi - F'(x^\dagger)^* w \mid w \in Y, \|w\| \leq r\}, r \geq 0 \tag{4.6}$$

This is a convex function and only zero, if a $x^\dagger$ fulfills (4.5), see [28]. One now can define the concept of an approximate source condition:

**Definition 4.2.11** ([28, Definition 12.6])**.** *The exact solution* $x^\dagger$ *satisfies an approximate source condition with respect to the stabilizing functional* $R$ *and the operator* $F'(x^\dagger)$ *if there is a subgradient* $\xi \in \partial R(x^\dagger)$ *such that the associated distance function defined by* (4.6) *decays to zero at infinity.*

Now one can indeed show a convergence rate result if such an approximate source condition is fulfilled:

**Theorem 4.2.12** ([34, Theorem 4.3])**.** *Let Assumption 4.2.2 be fulfilled. Assume that* $x^\dagger$ *satisfies an approximate source condition for* $\xi \in \partial R(x^\dagger)$*. Further let* $0 < c_1 \leq 1$, $0 \leq c_2 \leq 1$ *with* $c_1 + c_2 \leq 1$ *and let* $F$ *be differentiable satisfying the nonlinearity condition* $\|F(x) - F(x^\dagger) - F'(x^\dagger)(x - x^\dagger)\| \leq \gamma_2 \|F(x) - F(x^\dagger)\|^{c_1} \|x - x^\dagger\|^{c_2}$*. Moreover, we set* $\kappa = c_1/(1 - c_2)$ *and introduce for* $r > 0$ *the functions* $\Psi(r) := d(r)^{(2-\kappa)/\kappa} / r^{2/c_1}$ *and* $\Phi(r) := d(r)^{1/\kappa} / r^{1/c_1}$*. Then, for a parameter choice* $\alpha = \alpha(\delta)$*, where* $\alpha$ *satisfies the equation* $\delta \sim \sqrt{\alpha d(\Psi^{-1}(\alpha))}$*, the minimizer* $x_\alpha^\delta$ *of* $J_\alpha$ *fulfills*

$$d_\xi(x_\alpha^\delta - x^\dagger) = \mathcal{O}(d(\Phi^{-1}(\delta))).$$

**Remark 4.2.13.** The convergence rate in Theorem 4.2.12 depends on the decay of the distance function $d$, since $\Phi^{-1}(\delta) \to \infty$ as $\delta \to 0$. It is always lower than the archievable rate that is granted by a source condition and the discrepancy in rates becomes greater, the slower the distance function $d$ decays to zero as $R \to \infty$, cf. [34, Remark 4.5].

For parameter identification problems, the source condition $x^\dagger = F(x^\dagger)^* w$ is usually interpretable in some way [22, 38, 40]. In particular that means we can directly establish properties that the true solution $x^\dagger$ must fulfill for a source condition to hold. From an applicational point of view, this means we can directly motivate if a source condition is likely to hold or if it cannot hold at all because the solutions generated by the application do not fit into this setting. For a detailed discussion for semilinear reaction diffusion systems we refer to Section 6.8.

**Remark 4.2.14.** Although we assumed $X$ and $Y$ to be Hilbert spaces, all the above results can be easily transferred to the case where $X$ and $Y$ are Banach spaces, see for example [28, 34, 36, 40, 56].

### 4.2.1 Regularization with sparsity constraints

We already mentioned several times before that the prior $R$ in the Tikhonov functional can be used to highlight certain features of the solution. One very important feature that many applicational problems have in common is *sparsity* of the solution in a certain basis. Sparsity means that the solution can be expanded into a sum with only finitely many coefficients in that basis. So if we assume that the true solution is sparse in a basis or frame $\{\varphi_i\}_{i\in\mathbb{N}}$, the idea is to penalize the number of coefficients of the expansion of the true solution into this basis, which would lead to a penalty

$$R(x) = \|x\|_{\ell_0} := \#\{i \mid \langle x, \varphi_i \rangle \neq 0\}. \tag{4.7}$$

However, the this choice of a penalty does not fulfill the requirements of Assumption 4.2.2. In fact, the minimization of a Tikhonov type functional with an $\ell_0$ penalty is not even a regularization in the general case [46] and can therefore not be considered for our problem. Hence, instead one replaces this penalty by

$$\mathcal{R}(x) = \|x\|_{\ell_1} = \sum_{n\in\mathbb{N}} |\langle x, \varphi_i \rangle|. \tag{4.8}$$

This penalty now is well suited for Tikhonov regularization:

**Proposition 4.2.15** ([31, Chapter 3])**.** *$R(x) = \|x\|_{\ell_1}$ is convex, weakly lower semicontinuous and coercive. Further, for $\|x_k\|_{\ell_1} \to \|x\|_{\ell_1}$ and $x_k \rightharpoonup x$, it holds $\|x_k - x\|_{\ell_1} \to 0$.*

An immediate consequence from this proposition is the fact that Tikhonov regularization is applicable and all stability results hold with respect to the $\ell_1$-norm.

Note that the $\ell_1$ penalty term indeed produces sparse minimizers:

**Proposition 4.2.16** ([40, Theorem 3.2])**.** *Let $F$ be differentiable, then every minimizer of the Tikhonov functional with the penalty from* (4.8) *has a finite expansion in the basis $\{\varphi_i\}_{i\in\mathbb{N}}$.*

Finally, one can obtain better convergence rates as in the general case, if the right assumptions are matched:

**Theorem 4.2.17** ([40, Theorem 3.7]). *Let (i) – (iv) from Theorem 4.2.9 be fulfilled. Further assume*

*(v) $F'(x^\dagger)$ fulfills the FBI property, i.e. for every finite set $J \subset \mathbb{N}$ the restriction of its derivative $F'(x^\dagger)$ to $\{\varphi_j \mid j \in J\}$ is injective.*

*Then, for a parameter choice $\alpha \sim \delta$ the minimizer $x_\alpha^\delta$ of the $\ell_1$ penalized Tikhonov functional fulfills*

$$\|x - x^\dagger\| = \mathcal{O}(\delta).$$

**Remark 4.2.18.** If only assumption $(v)$ from 4.2.17 is not fulfilled, but $(i) - (iv)$ do hold, then one only obtains a convergence rate $\mathcal{O}(\delta)$ in the Bregman distance derived in Theorem 4.2.9.

Again, as stated already above, these source-conditions are unlikely to hold for practical problems, since they enforce a special structure (usually some kind of smoothness, cf. for example [23])of the true solution, which usually cannot be verified, because the true solution is unknown.

**Remark 4.2.19.** Even if a source condition can be verified, the results of Theorem 4.2.9, Theorem 4.2.12 and Theorem 4.2.17 are still just theoretical, because the convergence rate only holds for $\delta \to 0$ and with an optimal parameter choice for $\alpha$. In applications, $\delta$ often is a good quantity away from zero and a good choice of a regularization parameter is always a problem, especially if $\delta$ is not known. So one might think that even if a convergence rate can be verified, it has very little practical impact. This however is not always true. It can be observed in experiments that the reconstructions behave very well if a source condition holds, see [22] for example. This is even more true in the case of sparsity constraints, where (at least for linear problems) a source condition always holds if the solution is sparse [31, 46]. Thus, the study of source conditions might also be of interest for practical problems.

### 4.2.2 Minimization of Tikhonov type functionals

To apply Tikhonov regularization to a concrete problem, one must possess a practical way to determine a minimizer of the Tikhonov functional. This usually is done iteratively. For the classical Hilbert space penalty $\|x - x^*\|_X^2$ this is easily done, since the Tikhonov-functional is differentiable (as long as $F$ is differentiable) in this case. Its derivative can be computed as

$$J'_\alpha(x) = 2(F'(x)^*(F(x) - y^\delta) + \alpha(x - x^*)),$$

where the first summand is the derivative of the discrepancy term and the second summand is the derivative of the penalty term. For a sparsity promoting penalty term, the minimization of the Tikhonov functional becomes more complicated. In this chapter we study the functional

$$J(x) = \tilde{F}(x) + \tilde{R}(x), \tag{4.9}$$

where $\tilde{F} : X \to \mathbb{R}$ is differentiable but not necessarily convex and $\tilde{R} : X \to (-\infty, \infty]$ is convex but not necessarily differentiable. One approach in that case is, that instead of choosing a descent direction as the negative gradient, one makes the approach to choose a descent direction as $\min_{v \in X} \langle \tilde{F}'(x), v\rangle + \tilde{R}(v)$. This leads to

**Algorithm 4.2.20.**

1. Choose $x_0$ with $\tilde{R}(x) < \infty$, set $n = 0$ and determine a stopping rule.
2. Determine a descent direction $v_n$ as solution of
$$\min_{v \in X} \langle \tilde{F}'(x), v\rangle + \tilde{R}(v).$$
3. Determine a step size $s_n$ as solution of
$$\min_{s \in [0,1]} \tilde{F}(x_n + s(v_n - x_n)) + \alpha \tilde{R}(x_n + s(v_n - x_n)).$$
4. Perform a descent step $x_{n+1} = x_n + s_n(v_n - x_n)$.
5. Check if the stopping rule is met, if not set $n = n + 1$ and go to step 2.

To show convergence of this algorithm, one has to make some assumptions.

**Assumption 4.2.21.**

*(i) A stationary point of $J(x)$ exists.*

*(ii) There exists $x \in X$ with $\tilde{R}(x) < \infty$.*

*(iii) $\tilde{R}$ is convex and lower semicontinuous.*

*(iv) $\tilde{R}$ is coercive, i.e. $\frac{\|\tilde{R}(x)\|}{\|x\|} \to \infty$ if $\|x\| \to \infty$.*

*(v) $\tilde{F}$ is a continuously differentiable functional which is bounded on bounded sets.*

*(vi) $\tilde{F} + \tilde{R}$ is coercive.*

For functionals of type (4.9) the following convergence statement holds:

**Theorem 4.2.22** ([10, Theorem 1]). *Let $\tilde{R}$ satisfy Assumption 4.2.21 and assume $E_t = \{x \in X \mid \tilde{R}(x) \leq t\}$ to be compact for every $t \in \mathbb{R}$. Then there exists a subsequence of the sequence $\{x_n\}$ generated by Algorithm 4.2.20 that converges to a stationary point of the functional* (4.9).

Remember that the main goal was to minimize the Tikhonov functional with an $\ell_1$ penalty term. This fits into the above framework in the following way. If we define

$$J(x) := \underbrace{\frac{1}{2}\|F(x) - y^\delta\|^2 - \frac{\lambda}{2}\|x\|^2}_{=:\tilde{F}(x)} + \underbrace{\frac{\lambda}{2}\|x\|^2 + \alpha\|x\|_{\ell_1}}_{=:\tilde{R}(x)}$$

then the $\ell_1$ penalized Tikhonov functional can be fit into the framework of the generalized conditional gradient method and as a result we get the well known iterative soft shrinkage method from [17], where we utilize the proximity operator of the absolute value function, which can be expressed through the shrinkage function

$$S_\alpha := \operatorname{sgn}(x)\max\{|x| - \alpha, 0\}.$$

Algorithm 4.2.20 now becomes:

**Algorithm 4.2.23.**

1. Choose $x_0$ with $\tilde{R}(x) < \infty$, set $n = 0$ and determine a stopping rule.
2. Determine a descent direction $v_n$ via
$$v_n = \sum_{i\in\mathbb{N}} S_{\alpha/\lambda}(\langle x_n - \lambda^{-1}F'(x_n)^*(F(x_n) - y^\delta), \varphi_i\rangle)\varphi_i$$
3. Determine a step size $s_n$ as solution of
$$\min_{s\in[0,1]} \|F(x_n + s(v_n - x_n)) - y^\delta\|^2 + \sum_{i\in\mathbb{N}} |\langle x_n + s(x_n - v_n), \varphi_i\rangle|$$
4. Update the iterate $x_n = x_n + s_n(v_n - x_n)$.
5. Check if the stopping rule is met, if not set $n = n + 1$ and go to step 2.

In [65] it is furthermore shown, that this sequence converges for constant step size $s = 1$, if the parameter $\lambda$ is chosen big enough. So the line search in algorithm 4.2.23 can be omitted. Moreover, in [57] this method was generalized to Banach spaces.

The iterative shrinkage method proposed in Algorithm 4.2.23 converges rather slow in practice, especially if one uses a constant step size. Therefore it is desirable to find faster methods or to speed up the iteration. In [47] the authors therefore considered a quadratic approximation approach of the functional at the current iterate $x_n$, where one choses a step size $\lambda_n$ and determines the next iterate as the minimizer of

$$J_{\lambda_n}(x, x_n) = \tilde{F}(x_n) + \langle \tilde{F}'(x_n), x - x_n \rangle + \frac{\lambda_n}{2}\|x - x_n\|^2 + \tilde{R}(x)$$

A descent direction then can be computed as

$$\underset{x \in X}{\operatorname{argmin}}\, J_{\lambda_n}(x, x_k) = \operatorname{prox}_{\tilde{R}(x_k)}(x)$$

For the moment, we only consider the case $\tilde{R} = \alpha\| \cdot \|_{\ell_1}$, in that case the proximity operator is given as

$$\operatorname{prox}_{\|\cdot\|_{\ell_1}}(x) := \sum_{i \in \mathbb{N}} S_\alpha(\langle x, \varphi_i \rangle)\varphi_i,$$

The trick is now to choose a clever step size that ensures the decay condition

$$J(x_{n+1}) \leq J_{\lambda_n}(x_{n+1}, x_n). \tag{4.10}$$

A good approximation on a step size satisfying this condition can be done by the so called Barzilai-Borwein rule introduced in [8]. The idea is to chose the step size as

$$s_n = \frac{\langle x_n - x_{n-1}, \tilde{F}'(x_n) - \tilde{F}'(x_{n-1})\rangle}{\langle \tilde{F}'(x_n) - \tilde{F}'(x_{n-1}), \tilde{F}'(x_n) - \tilde{F}'(x_{n-1})\rangle}$$

Nevertheless the condition (4.10) still has to be verified. The algorithm proposed in [47] then is

**Algorithm 4.2.24.**

1. Choose $x_0$ with $\tilde{R}(x) < \infty$, $q \in (0, 1)$, set $n = 0$ and determine a stopping rule.
2. Compute $\tilde{F}'(x_n)$
3. Compute the step size via the Barzilai-Borwein rule.
4. Determine a candidate for the next iterate via
$$v_n = \sum_{i \in \mathbb{N}} S_{s_n\alpha}(\langle x_n - s_n\tilde{F}'(x_n), \varphi_i \rangle)\varphi_i$$
5. Check if $v_n$ is a valid update, i.e. condition (4.10) is fulfilled, otherwise decrease the step size via $s_n = qs_n$ and go to step 4.
6. Check if the stopping rule is met, if not set $n = n + 1$ and go to step 2.

Note that in the case of a constant step size $s = s_n$ this algorithm resembles the generalized conditional gradient method from Algorithm 4.2.23.

To show convergence of this algorithm, the following assumption is needed:

**Assumption 4.2.25.**

*(i) A minimizer of $J(x)$ exists.*

*(ii) $\tilde{R}$ is convex, proper, weakly lower semicontinuous and weakly coercive, i.e. $\tilde{R}(x) \to \infty$ for $\|x\| \to \infty$.*

*(iii) $\tilde{F}$ is a continuously differentiable functional with Lipschitz continuous derivative, i.e.*

$$\|\tilde{F}'(x) - \tilde{F}'(y)\|_{L(X,Y)} \leq L\|x - y\|_X$$

*(iv) If $x_n$ converges weakly to $x$, so that $J(x_n)$ is monotonically decreasing, then there exists a subsequence $\{x_m\} \subset \{x_n\}$ such that*

$$\tilde{F}'(x_m) \rightharpoonup \tilde{F}'(x)$$

Note that the assumptions on $\tilde{F}$ are stronger than the one made in Assumption 4.2.25, while the coercivity assumption on $\tilde{R}$ is weakened. Under this assumption, one is able to prove

**Theorem 4.2.26.** *Let Assumption 4.2.25 be fulfilled. Assume that the sequence of step sizes $\{\lambda_n\}$ satisfies $\lambda_n \in [\lambda_u, \lambda^o]$ with $0 < \lambda_u \leq L \leq \lambda^o < \infty$, such that*

$$J(x_{n+1}) \leq J_{\lambda_n}(x_{n+1}, x_n)$$

*Then the sequence $\{x_n\}$ generated by Algorithm 4.2.24 is bounded and therefore has a weakly convergent subsequence $\{x_m\}$. This subsequence converges to a stationary point of* (4.9). *If $\tilde{F}'(x_m) \to \tilde{F}(x_m)$ in the norm topology, then the sequence $\{x_m\}$ converges strongly to a stationary point.*

Often, the operator $\tilde{F}$ is not defined on the whole space $X$, but only on a subset $\mathcal{D}(F)$. To work around this, one can check if the next iteration step stays in $\mathcal{D}(F)$ and only continues if this is the case. If it is not the case, one then just has restart the iteration with a different starting value and hope for better results. It is to be expected that if the starting value $x_0$ is chosen well enough and there is at least one stationary point in $X$ this is always possible. In our numerical experiments (see Chapter 8), the restricted domain of the forward operator was never a problem. Also, instead of a weak continuity result we use a $\tau$-weak continuity result (see Assumption 4.2.2, which makes Tikhonov-regularization applicable for a broader class of problems. Theorem 4.2.26 is thus not directly applicable, since the boundedness of the sequence $\{x_n\}$ does not necessarily yield a $\tau$ convergent subsequence. So we propose the following generalization of Theorem 4.2.26.

**Theorem 4.2.27.** *Let condition (i),(ii) and (vii′) of Assumption 4.2.2 and (i)-(iii) of Assumption 4.2.25 hold. Assume that if a sequence $\{x_k\} \subset X$ converges to $x$ in the $\tau$-topology, so that $J(x_k)$ is monotonically decreasing, there exists a subsequence $\{x_l\} \subset \{x_k\}$ such that $\tilde{F}'(x_l) \rightharpoonup \tilde{F}(x)$. Further assume that the sequence of step sizes $\lambda_n$ satisfies $\lambda_n \in [\lambda_u, \lambda^o]$ with $0 < \lambda_u \leq L \leq \lambda^o < \infty$, such that*

$$J(x_{n+1}) \leq J_{\lambda_n}(x_{n+1}, x_n)$$

*and that for sequence $\{x_n\}$ generated by Algorithm 4.2.24 it holds $\{x_n\} \subset \mathcal{D}(F)$. Then the sequence $x_n$ generated by Algorithm 4.2.24 has a weakly convergent subsequence that converges to a stationary point of* (4.9)*. If $\tilde{F}'(x_m) \to \tilde{F}(x_m)$ in the norm topology, then the sequence $\{x_m\}$ converges strongly to a stationary point.*

*Proof.* The fact that the sequence generated by Algorithm 4.2.24 stays in $\mathcal{D}(F)$ and that $\mathcal{D}(F)$ is $\tau$-sequentially compact ensures the existence of a subsequence that converges in the $\tau$-topology. Since this sequence also converges weakly in $X$, the rest the proof can be carried out exactly as in [47]. □

**Remark 4.2.28.** Another approach to ensure that the iteration stays in the set $\mathcal{D}(F)$ is to extend the penalty via an additional indicator function of a convex set $C \subset \mathcal{D}(F)$.

$$\iota_C(x) := \begin{cases} 0 & x \in C \\ \infty & x \notin C \end{cases}$$

If the set $C$ is closed, convex and bounded, so the indicator function fulfills condition 4.2.21 and so does

$$\tilde{R}(x) = \|x\|^2 + \alpha\|x\|_{\ell_1} + \iota_{\mathcal{D}(F)}$$

So in principle, Algorithm 4.2.20 is applicable. The challenge now is to compute a valid descent direction, which is to solve the minimization problem

$$\min_{v \in C} \langle F'(x), v\rangle + \tilde{R}(v)$$

which is surprisingly highly nontrivial.

If wants to use the quadratic approximation approach one has to compute the proximity operator of the penalty

$$\tilde{R}(x) := \|x\|_{\ell_1} + \iota_{\mathcal{D}(F)}$$

For a general convex set $C$ it holds $\operatorname{prox}_{\iota_C + \|\cdot\|_{\ell_1}} \neq \operatorname{prox}_{\iota_C} \circ \operatorname{prox}_{\|\cdot\|_{\ell_1}} \neq \operatorname{prox}_{\|\cdot\|_{\ell_1}} \circ \operatorname{prox}_{\iota_C}$. This can for example be seen with $f \in L_2([0, 2\pi])$, $f(x) = 1.1\pi \sin(x)$, where the convex set is given as $C := \{f \in L_2([0, 2\pi]) \mid 0 \leq f(x) < \infty\}$ and the basis is the Fourier basis. Nevertheless, at least the computation is possible numerically as one has to basically compute a sum of proximity operators, which can be done as proposed in [14]. Note that the sequence generated by the quadratic approximation approach still has a convergent subsequence [47]. The challenge in this case is to show that this subsequence converges to a stationary point of $J$.

# CHAPTER 5

# A general solution theory

In Section 4.2, we have seen, that the forward operator of the inverse problem has to fulfill some kind of weak closedness to guarantee the regularization properties of Tikhonov regularization or even the existence of a minimizer of the Tikhonov functional in appropriate function spaces. Further, the forward operator of the problem must have a uniformly continuous derivative if we want to apply numerical minimization schemes. So, the first thing that we have to address if we want to perform parameter identification for the problem (1.3) is to find a solution space. That means, that one searches for a function space, where problem (1.3) has a unique solution for all parameters and in which the above properties can hold. In this section we will define general solution spaces and make some assumptions that we will need, when we discuss the parameter-to-state map later on. All in all, this gives a rather complex model of general function spaces that interact with each other.

## 5.1 Weak solutions and solution spaces

Classical solutions of a PDE-system like (1.3) are solutions that are located in $C^1([0,T], C^2(\overline{\Omega})^N)$. It turns out, that these spaces are not well suited when dealing with inverse problems. Often, if one wants to show the existence of a classical solution of a PDE like (1.3), one needs some regularity or smoothness assumptions on the parameters involved, as well as onto the boundary, boundary conditions and the nonlinear function $g$ that are usually not given in real world applications. So we need a weaker approach to a solution which we will establish in this section. This approach will also be useful for numerical comparisons later on.

### 5.1.1 A motivation of the weak solution theory

In this chapter, we will start with a classical solution of the PDE and motivate a weak formulation as well as the appropriate spaces suitable for this formulation. Note that this motivation is much easier to understand, if the reader is familiar with the weak solution theory of elliptic equations. An excellent introduction is for example given in the lecture notes [37]. For simplicity reasons, we restrict ourselves to the case of a linear equation and $N = 1$. The generalization of this motivation to higher order systems is straightforward as we will see in the next section. So let us assume that $u$ is a classical solution of the PDE

$$\begin{aligned} u_t(x,t) - \Delta u(x,t) + \lambda u(x,t) = f(x,t) \qquad &\text{in } \Omega_T \\ u(x,t) = 0 \qquad &\text{on } \partial\Omega \times [0,T] \\ u(x,0) = u_0 \qquad &\text{on } \Omega \times \{0\} \end{aligned}$$

i.e. $u \in C^1([0,T], C^2(\overline{\Omega}))$. For every time instance, we can multiply the equation with a test function $\varphi \in C_0^\infty(\Omega)$ and integrate over $\Omega$ afterwards.

$$\int_\Omega u'(t)\varphi \; dx + \int \nabla u(t) \cdot \nabla v + \lambda uv \; dx = \int f\varphi \; dx. \tag{5.1}$$

We will use this integral equation to define a weak formulation for the problem. First, we look at the part, where no time derivative is involved. Similar to elliptic problems, we can handle this, if we define a solution space for the space variable and a space of test functions. In our simple example, $H_0^1(\Omega)$ is a well suited space for this task.

Now, one has to think about a solution space for the time dependent problem. For this, we will fall back to the Bochner spaces defined in Section 3.1 as well as to the definition of the weak time derivative. From many points of view, it makes sense to interpret the variational formulation (5.1) as a differential equation again (especially from a numerical point of view). By knowing $u \in H_0^1(\Omega)$, it holds $\nabla u \in L_2(\Omega)$. If we now iterate that process, i.e. differentiate $u$ again, we arrive at $\Delta u \in H^{-1}(\Omega)$. Now we consider the time derivative. For this, we look at the the variational inequality that represents the weak derivative of $u$ with respect to the time component:

$$\int_0^T u'\varphi \; dt = -\int_0^T u\varphi' \; dt.$$

If we want to test this inequality with a test function in $H^1(\Omega)$, this is only well defined if $u$ and $u'$ are elements $H^{-1}(\Omega)$. This fact is dictated by properties of the Bochner Integral, since we want to use the Hölder like estimates in Proposition

3.1.5 as well as Proposition 3.1.7. By these properties it holds for $\rho \in C_0^\infty([0,T])$:

$$\begin{aligned}\int_0^T \langle u', v\rangle_{(H^{-1},H_0^1)}\rho\, dt &= \langle \int_0^T u'\rho\, dt, v\rangle_{(H^{-1},H_0^1)}\\ &= -\langle \int_0^T u\rho'\, dt, v\rangle_{(H^{-1},H_0^1)}\\ &= -\int_0^T \langle u, v\rangle_{(H^{-1},H_0^1)}\rho'\, dt,\end{aligned}$$

hence the weak derivative is compatible with multiplication with a test function from $H^{-1}$ and the weak derivative of $\langle u, v\rangle_{(H^{-1},H_0^1)}$ is exactly $\langle u', v\rangle_{(H^{-1},H^1)}$. So we replace the weak formulation (5.1) by the following one:

$$\langle u'(t), \varphi\rangle_{(H^{-1},H_0^1)} + \int \nabla u(t)\cdot\nabla v\, dx = \int u(t)\varphi\, dx \qquad \forall \varphi \in H_0^1(\Omega). \tag{5.2}$$

We can now define a solution space for weak solutions:

$$\mathbb{W}_2^1 := \{u \in L_2(0,T,H_0^1(\Omega)) \mid u' \in L_2(0,T,H^{-1}(\Omega))\}. \tag{5.3}$$

Based on this, we can define a weak solution of problem (1.3):

**Definition 5.1.1.** *A function $u \in \mathbb{W}_2^1$ is called a weak solution of* (1.3)*, if* (5.2) *is fulfilled for almost every $t \in [0,T]$ and the initial condition $u(0) = u_0$ is fulfilled for almost every $x \in \Omega$.*

For this definition to make sense, the function $u$ has to be continuous in time. This is indeed the case, as the embedding $\mathbb{W}_2^1 \hookrightarrow C([0,T], L_2(\Omega))$ is continuous, see for example [25].

### 5.1.2 General solution spaces

In the previous section, we have dealt with a rather simple example. In this section we generalize the above theory to systems of semilinear equations and more general function spaces. The generalization to the system case is very simple. One just chooses vector-versions of the above function spaces and treats the solution of each equation in the system in the above manner. We also want to include (in addition to the classical Hilbert space theory) recent results concerning maximal parabolic regularity [32] that allow more general function spaces which then allow showing existence and uniqueness results for a more general class of semilinear parabolic equations. An example for such an equation is given in [48]. Also, the existence of solutions for the embryogenesis equation from Section 2.4 was shown in the general setting discussed in this section. In this case, instead of the spaces $H^1(\Omega)$ or $H^1_0(\Omega)$ one adapts the solution space for the space variable to $H^{1,q}(\Omega)$, i.e. a space of more regular functions. We will see later on that this more general approach is also well suited for the analysis of the inverse problem and the exponent $q$ does barely influence its analysis at all, as long as some embeddings of the solution space are met and the non-linearity $g$ is well behaved in the sense of continuity and differentiability of its superposition operator.

**Definition 5.1.2.** *Let $q \in [\tau_1, \tau_2)$ and $1/q + 1/q' = 1$, $2 \leq \tau_1 < \tau_2 \leq \infty$. Depending on the type of boundary conditions, we set*

$$\begin{aligned} Y &:= Y_q := H^{1,q}(\Omega)^N \\ \tilde{Y} &:= \tilde{Y}_{q'} := H^{1,q'}(\Omega)^N \end{aligned} \tag{5.4}$$

*in the case of Neumann type boundary conditions and*

$$\begin{aligned} Y &:= Y_q := H^{1,q}_0(\Omega)^N \\ \tilde{Y} &:= \tilde{Y}_{q'} := H^{1,q'}_0(\Omega)^N \end{aligned} \tag{5.5}$$

*in the case of Dirichlet type boundary conditions.*

For the spaces $Y$ and $\tilde{Y}^*$, we get an analogon to the classical Gelfand-triple [25]:

**Lemma 5.1.3.** *For $Y$, $\tilde{Y}$ as in definition 5.1.2 the embeddings*

$$Y \hookrightarrow L_q(\Omega)^N \hookrightarrow \tilde{Y}^* \tag{5.6}$$

*are continuous. Further, if $q' \in (\max\{1, 2d/(d+2)\}, 2]$, the embeddings*

$$\tilde{Y} \hookrightarrow L_2(\Omega)^N \hookrightarrow \tilde{Y}^* \tag{5.7}$$

*are continuous.*

*Proof.* This lemma is a direct consequence of Proposition 3.4.4 and Corollary 3.4.5. □

One can now define a solution space in the same way as we did in (5.3):

$$\mathcal{W} := \mathcal{W}_{s,q} := \{u \in L_s([0,T], Y_q) \mid u' \in L_s([0,T], (\tilde{Y}_{q'})^*)\}, \qquad 2 \leq s < \infty.$$

We collect some basic properties of $\mathcal{W}$:

**Proposition 5.1.4.** *For $q, s \geq 2$, the space $\mathcal{W}$ equipped with the norm*

$$\|u\|_{\mathcal{W}_{f,\mathrm{II}}} := \|u\|_{L_s([0,T],Y)} + \|u'\|_{L_s([0,T],\tilde{Y}^*)}$$

*is a reflexive Banach space.*

*Proof.* Let $\{u_k\}$ be a Cauchy sequence in $\mathcal{W}$. Then, $\{u_k\}$ and $\{u_k'\}$ are Cauchy sequences in the spaces $L_s([0,T],Y)$ and $L_s([0,T],\tilde{Y}^*)$. These are Banach spaces by Proposition 3.1.4, so there exist $z$ and $z_2$ with $u_k \to z$ in $L_s([0,T],Y)$ and $u_k' \to z_2$ in $L_s([0,T],\tilde{Y}^*)$. All we have to show now is that $z' = z_2$. Because of the embedding $Y \hookrightarrow \tilde{Y}^*$ and Proposition 3.1.9 it is clear that $u_k \in L_s([0,T],\tilde{Y}^*)$ and because of Proposition 3.1.8 the following holds for all $\rho \in C_0^\infty([0,T])$:

$$\begin{aligned}\int_0^T z_2(t)\rho(t)\ dt &= \lim_{k\to\infty} \int_0^T u_k'(t)\rho(t)\ dt \\ &= \lim_{k\to\infty} \int_0^T u_k(t)\rho'(t)\ dt \\ &= \int_0^T z(t)\rho'(t)\ dt.\end{aligned}$$

Hence, $z_2$ is the weak derivative of $z$ in $L_s([0,T],\tilde{Y}^*)$ and therefore the limit is in $\mathcal{W}$ as desired. For the reflexivity, we define the operator

$$\begin{aligned}T : \mathcal{W} &\to L_s([0,T],Y) \times L_s([0,T],\tilde{Y}^*) \\ u &\mapsto (u, u'),\end{aligned}$$

which obviously is an isometry. By the reflexivity of $Y$ and $\tilde{Y}^*$ it follows, that $L_s([0,T],Y)$ and $L_s([0,T],\tilde{Y}^*)$ are reflexive spaces and thus the product (note that our definition of the norm is exactly the product one norm) is a reflexive space as well. Hence, $T(\mathcal{W})$ is a closed subset of a reflexive Banach space and therefore has to be reflexive [19, Satz 3.31]. This concludes the proof. □

For functions in $\mathcal{W}$ the following rule of integration holds:

**Theorem 5.1.5.** *Let $u, v \in \mathcal{W}$, $q' \in (\max\{1, 2d/(d+2)\}, 2]$ and $s \geq 2$. Then $\mathcal{W} \hookrightarrow C([0,T], L_2(\Omega)^N)$ continuously and the following rule of integration holds*

$$\langle u(T), v(T)\rangle_{(L_2,L_2)} - \langle u(0), v(0)\rangle_{(L_2,L_2)} = \langle u', v\rangle_{(\tilde{Y}^*,\tilde{Y})} + \langle v', u\rangle_{(\tilde{Y}^*,\tilde{Y})} \tag{5.8}$$

*Proof.* We only sketch parts the proof, for a detailed version see [61, Lemma 7.3]. Let $\tilde{W} := \{u \in L_s([0,T],\tilde{Y}) \mid u' \in L_s([0,T],\tilde{Y}^*)\}$. For $u, v \in C^1([0,T],\tilde{Y})$, the formula (5.8) is valid by classical calculus. This is a direct consequence of the embeddings from (5.7) as we get

$$\langle u, v\rangle_{(L_2,L_2)} = \langle u', v\rangle_{(L_2,L_2)} + \langle v', u\rangle_{(L_2,L_2)} = \langle u', v\rangle_{(\tilde{Y}^*,\tilde{Y})} + \langle v', u\rangle_{(\tilde{Y}^*,\tilde{Y})}.$$

Further, it holds $C^1([0,T],\tilde{Y}) \hookrightarrow \tilde{W}$ dense, cf. [61, Lemma 7.2]. Thus the formula also holds for $u, v \in \tilde{W}_{s,q}$. Further, by [61, Lemma 7.3] the embedding $\tilde{W} \hookrightarrow C([0,T], L_2(\Omega)^N)$ is continuous. Clearly $\mathcal{W} \hookrightarrow \tilde{W}$ continuous by the continuous embedding $H^{1,q}(\Omega)^N \hookrightarrow H^{1,q'}(\Omega)^N$ for $q' \leq 2$, so the assertion also follows for $u, v \in \mathcal{W}$. □

If $q$ is greater than the space dimension and $s$ is chosen appropriately, we get stronger embeddings for the solution space:

**Proposition 5.1.6.** *Let $2 < s \leq q$ and $q > d$ such that $1 - 2/s - d/q > 0$, then the embeddings*

$$\mathcal{W} \hookrightarrow C([0,T], C(\overline{\Omega})^N) \hookrightarrow L_p([0,T], L_p(\Omega)^N) \tag{5.9}$$

*for $p \geq 1$ are continuous.*

*Proof.* The assertion is a combination of the statements from [44, Corollary A.28] and [2, Theorem 4.10.2]. □

**Remark 5.1.7.** The embedding from Proposition 5.1.6 will be important, when we are analyzing the inverse problem in certain concrete situations, since it guarantees that the solution of the equation is an $L_\infty$ function in space and time simultaneously, which we later on will use for various estimates. Note that if $s = q$, then $1 - 2/q - d/q > 0$ is equivalent to $q > d + 2$.

One obtains a weak formulation for the general semilinear problem as follows

$$\sum_{i=1}^{N} \langle u_i'(t), \varphi_i \rangle_{(\tilde{Y}^*, \tilde{Y})} + \sum_{i=1}^{N} \int_\Omega D \nabla u_i(t) \cdot \nabla \varphi_i \, dx$$
$$= \sum_{i=1}^{N} \int_\Omega (f(t) - g_i(p(t), u_i(t)))\varphi_i \, dx, \qquad \text{a.e. in } [0,T] \qquad \forall \varphi \in \tilde{Y} \tag{5.10}$$

From now on we will often omit the summation in all appearing weak formulations and define $uv := \sum_{i=1}^N u_i v_i$ as well as $D\nabla u \cdot \nabla v := \sum_{i=1}^N D_i \nabla u_i \cdot \nabla v_i$ for $u \in Y$, $v \in \tilde{Y}$. For the rest of the work, we assume for given $p \in L_\infty(\Omega_T)^M$ and $u \in \mathcal{W}$ that $g(p,u) \in L_s(\Omega_T)^N$ (note that this restricts the growth of $g$, see Theorem 3.7.2). In this case for $v \in L_{s'}([0,T], \tilde{Y})$ it holds

$$\int_0^T \langle g(p,u), v \rangle (L_q([0,T], \tilde{Y}^*), L_{q'}([0,T], \tilde{Y})) \, dt = \int_0^T \int_\Omega g(p,u) v \, dx \, dt.$$

This directly follows from Proposition 3.4.4. For derivatives of $g$ that will occur later on we make the same assumption. Note that this assumption is just technical in order to work with the weak formulation in an integral sense, which we will need for numerical discretezation, but it is not necessary in the functional analytic part of analyzing the parameter identification problem. Depending on a concrete problem, one may be able to omit this assumption.

Before we can now utilize this weak formulation generalize weak solutions to our abstract setting, we introduce another function space for the initial values.

**Definition 5.1.8.** *Let $Z$ be a function space with the following properties:*

*(i) The embedding*

$$\mathcal{W} \hookrightarrow C([0,T], Z) \tag{5.11}$$

*is continuous.*

*(ii) The embedding $Z \hookrightarrow L_2(\Omega)^N$ is continuous.*

*(iii) The embedding $Y \hookrightarrow Z^*$ is continuous and for $u \in \mathcal{W}, v \in Z$ it holds*

$$\langle u(t), v(t) \rangle_{(Z^*,Z)} = \int_\Omega u \cdot v \; dx.$$

**Remark 5.1.9.** Such a space $Z$ exists, since $Z = L_2(\Omega)^N$ fulfills all wanted properties. However, depending on the differential equation, $Z = L_2(\Omega)^N$ may not have enough regularity to ensure existence of solutions. Especially in the $H^{1,q}$ setting, more regularity of the initial values is needed, which we will see in the next section. At this point, we just assume properties on $Z$ that we need later on to analyze the parameter identification problem.

The definition for a weak solution then generalizes to:

**Definition 5.1.10.** *A function $u \in \mathcal{W}$ is called a (weak) solution of* (1.3)*, if* (5.10) *is fulfilled for almost every $t \in [0,T]$ and $u(0) = u_0$ in $Z$.*

A weak solution of (1.3) can indeed be interpreted as a solution of a Cauchy problem in the Banach space $L_2([0,T], \tilde{Y}^*)$.

**Proposition 5.1.11.** *$u \in \mathcal{W}$ is a weak solution of* (1.3)*, if and only if*

$$u_t - \nabla \cdot D\nabla u + g(p,u) = f \text{ in } L_s([0,T], \tilde{Y}^*), \tag{5.12}$$

*i.e for all $v \in L_{s'}([0,T], \tilde{Y})$ it holds*

$$\int_0^T \langle u', v \rangle_{(\tilde{Y}^*,\tilde{Y})} \; dt + \int_0^T \int_\Omega D\nabla u \cdot \nabla v + g(p,u)v \; dx \; dt = \int_0^T \int_\Omega fv \; dx \; dt, \tag{5.13}$$

*and $u(0) = u_0$ in $Z$.*

*Proof.* If (5.13) holds, it holds especially for all functions of the form $v(x)\varphi(t)$ with $v \in \tilde{Y}$, $\varphi \in C_0^\infty(0,T)$ and thus the assertion follows from the Fundamental Lemma of Calculus of Variations, cf. [19, Satz 5.1]. If $u \in \mathcal{W}$ is a weak solution, all the integrals in (5.13) are well defined and the integrand is zero by the definition of a weak solution. Thus (5.13) holds. □

**Remark 5.1.12.** If $g$ is well behaved in $u$, the above proposition allows us to define a differential operator that describes the partial differential equation for a given parameter $p$, that is:

$$\begin{aligned} A(u) : \mathcal{W} &\to Z \times L_q([0,T], \tilde{Y}^*) \\ u &\mapsto (u(0) - u_0, u_t - \nabla \cdot D\nabla u + g(p,u) - f) \end{aligned}$$

It is easy to see, that $A$ is injective, if the weak solution is unique. If a weak solution exists for every initial condition and every right hand side, this operator is surjective. To see this one picks $(v_0, h) \in Z \times L_2([0,T], \tilde{Y}^*)$ and solves the differential equation with initial condition $v_0$ and right hand side $\tilde{f} = f + h$.

Now, we make the following central assumption

**Assumption 5.1.13.** *There exists a* $q \in [2, \min\{\frac{2d}{d-2}, \infty\})$ *and* $s \geq 2$ *such that the equation* (1.3) *has a unique weak solution in* $\mathcal{W}$*.*

### 5.1.3 Existence of solutions

While we introduced a general solution theory in the previous section, the question remains if solutions in this setting even exists and if so, under which conditions, i.e. how reasonable Assumption 5.1.13 really is. In this section we will give a short insight into results concerning weak solutions of parabolic partial differential equations without going to much into detail. While there are different approaches to the topic of showing existence of solutions, we focus one one approach that involves the so called maximal parabolic regularity property, which utilizes semigroup theory to show the existence of solutions.

In this section let $1 < s < \infty$, $X$ be a Banach space, $A : D(A) \subset X$ be a closed and densely defined, but not necessarily bounded operator with dense domain $D(A)$ (which we assume to be equipped with the graph norm). Let $W^{1,s}([0,T], X) := \{u \in L_s([0,T], X) \mid u' \in L_s([0,T], X)\}$. Further we denote the *maximal regularity space*

$$MR(0,T) = W^{1,s}([0,T], X) \cap L_s([0,T], D(A)),$$

which is a Banach space for the norm

$$\|u\|_{MR} = \|u\|_{W^{1,s}([0,T],X)} + \|u\|_{L_s([0,T],D(A))}.$$

Often in parabolic equations, the time derivative $u_t$ is less regular than the right hand side $f$. This is a problem for us, since we want to be able to interpret the differential operator that describes the differential equations as an invertible mapping between two function spaces, So, one wants to find function spaces, where this is possible. This leads to the following

**Definition 5.1.14.** *Let $1 < s < \infty$. Then $A : D(A) \to X$ satisfies maximal parabolic $L_s$ regularity if for any $f \in L_s([0,T],X)$ there exists a unique function $u \in MR(0,T)$ with*

$$u'(t) + Au(t) = f(t) \quad a.e.\ in\ (0,T], \qquad u(0) = 0 \quad a.e.\ in\ \Omega,$$

*where the time derivative is taken in the sense of $X$-valued distributions.*

**Remark 5.1.15.** If $A$ satisfies maximal parabolic $L_s$ regularity for an $s \in (1,\infty)$, it satisfies maximal parabolic $L_s$ regularity for all $s \in (1,\infty)$ and the maximal regularity property is independent of $T$, see [32, Remark 5.2].

This regularity property can now be utilized to show the existence of solutions for very general parabolic partial differential equations. For this let

$$X_0 := (\mathcal{D}(A), X)_{1-\frac{1}{s},s}$$

the real interpolation space of order $1 - 1/s, s$ between $D(A)$ and $X$, see [68] for an introduction to interpolation spaces and their properties. Then we have the following two existence results:

**Theorem 5.1.16** ([6, Proposition 1.3])**.** *Assume that $A$ fulfills maximal parabolic $L_s$-regularity. Let and $B : (0,T) \to L(D(A),X)$ be Bochner measurable for each $t \in (0,T)$. Assume that $M$ is a constant such that for the operator $L_A := u_t + Au$ mapping from the space $\{u \in MR(0,T) \mid u(0) = 0\}$ to $X$ the estimate*

$$\|(\lambda + L_A)^{-1}\|_{L(L_s([0,T],X),MR(0,T))} \leq M \ and\ \|(1+\lambda)(\lambda - L_A)^{-1}\|_{L(L_s([0,T],X)} \leq M$$

*holds for all $\lambda \geq 0$. Further suppose that there exists an $\eta > 0$ such that for all $x \in D(A)$*

$$\|B(t)x\|_X \leq \frac{1}{2M}\|x\|_{D(A)} + \eta\|X\|_X. \tag{5.14}$$

*Then for all $f \in L_s([0,T],X)$ and $u_0 \in X_0$ there exists a unique $u \in MR(0,T)$ satisfying*

$$u_t(t) + Au(t) + B(t)u(t) = f(t) \quad a.e.\ in\ (0,T], \qquad u(0) = u_0\ in\ X_0.$$

**Remark 5.1.17.** If $A$ fulfills maximal parabolic regularity, a constant $M$ as needed in Theorem 5.1.16 always exists, see [6, Lemma 1.2].

**Theorem 5.1.18** ([54, Theorem 3.1])**.** *Assume that $A$ fulfills maximal parabolic $L_s$ regularity and $B : [0,T] \times X_0 \to X$ is a Caratheodory function. Further assume the following Lipschitz condition for $B$:*
*For each $R > 0$ there is a function $\phi_R \in L_s([0,T])$ such that*

$$\|B(t,u) - B(t,\tilde{u})\|_X \leq \phi_R(t)\|u - \tilde{u}\|_{X_0} \tag{5.15}$$

*for almost all* $t \in [0, T]$ *and* $u, \tilde{u} \in X_0$ *with* $\|u\|_{X_0}, \|\tilde{u}\|_{X_0} \leq R$.
*Then there exists* $\tilde{T} < T$ *such that the equation*

$$u_t(t) + Au(t) + B(t, u(t)) = f(t) \quad a.e. \ in \ (0, \tilde{T}], \qquad u(0) = u_0 \ in \ X_0$$

*has a unique solution* $u \in MR(0, \tilde{T})$.

Note that the previous results all are given for scalar equations, but it is highlighted in [32, Remark 8.3] that all results carry over in a straightforward way to diagonal systems. With this in mind, we can set $D(A) = Y$ and $X = \tilde{Y}^*$ and then the space $MR(0, T)$ becomes the space $\mathcal{W}$ from the previous section. For $D \in L_\infty(\Omega)^N$ with $0 < C_1 < D < C_2$, we can define a bilinearform $a(u, v)$ : $H^{1,q}(\Omega)^N \times H^{1,q'}(\Omega)^N$ via

$$a(u, v) = \int_\Omega D\nabla u \cdot \nabla v \, dx$$

and an operator $A : Y \to \tilde{Y}^*, u \mapsto -\nabla \cdot D\nabla u$ via

$$\langle Au, v \rangle_{(\tilde{Y}^*, \tilde{Y})} := a(u, v). \tag{5.16}$$

For this operator, the following result holds:

**Theorem 5.1.19** ([32, Section 5]). *Let* $A : Y \to \tilde{Y}^*$ *be as in* (5.16) *and* $\partial\Omega$ *be sufficiently smooth. Then the operator* $A$ *has maximal parabolic regularity on* $H^{1,q'}(\Omega)^N$ *for all* $q \in [2, \infty)$ *if* $d = 2$ *and* $q \in [2, 6]$ *if* $d = 3$, *i.e. problem*

$$u'(t) + Au(t) = f(t) \quad a.e. \ in \ (0, T], \qquad u(0) = 0,$$

*has a solution* $u \in \mathcal{W}$ *for all* $f \in \tilde{Y}^*$.

By combining Theorems 5.1.18 and 5.1.19 we get:

**Corollary 5.1.20.** *Let* $s > 1$, $A$ *be as in* (5.16) *and* $u_0 \in (\tilde{Y}^*, Y)_{1-1/s,s}$. *Assume that* $g : [0, T] \times (\tilde{Y}^*, Y)_{1-1/s,s} \to \tilde{Y}^*, (t, u) \mapsto g(p(t), u)$ *is a Caratheodory function and fulfills the condition* (5.15). *Then* (1.3) *has a unique (local in time) solution* $u \in \mathcal{W}$.

The condition (5.15) is very abstract. But if we utilize the right Lipschitz-condition on $g$ between Lebesgue spaces, we are still able to show the existence of solutions:

**Corollary 5.1.21.** *Let* $b > 1$, $a \geq b$ *and* $s > 1$ *be given in a way that the embeddings* $L_b(\Omega)^N \hookrightarrow \tilde{Y}^*$ *and* $X_0 \hookrightarrow L_a(\Omega_T)^N$ *are continuous. Let* $A$ *be as in* (5.16) *and* $u_0 \in (\tilde{Y}^*, Y)_{1-1/s,s}$. *Further assume that there exists* $h \in L_s([0, T], L_{\frac{ab}{a-b}}(\Omega))$ *such that each component* $g_i : \Omega_T \times L_a(\Omega_T)^N \to L_b(\Omega_T)^N, (x, t, u) \mapsto g_i(p(x, t), u)$

*of $g$ is a Caratheodory function that fulfills the condition*

$$|g_i(x,t,u) - g_i(x,t,\tilde{u})| \leq h(x,t) \sum_{j=1}^{N} |u_j - \tilde{u}_j| \tag{5.17}$$

*for a given parameter $p$. Then the equation* (1.3) *has a unique (local in time) solution $u \in \mathcal{W}$.*

*Proof.* By taking the $a$th power of (5.17), integrating over $\Omega$ and applying the Hölder inequality we get

$$\begin{aligned}
\|g_i(x,t,u) - g_i(x,t,\tilde{u})\|_{L_b(\Omega)}^b &\leq \int_\Omega h(x,t)^b \Big(\sum_{i=1}^{N} |u_i - \tilde{u}_i|\Big)^b \, dx \\
&\leq \left(\int_\Omega h(x,t)^{\frac{ab}{a-b}} \, dx\right)^{\frac{a-b}{a}} \left(\int_\Omega \Big(\sum_{i=1}^{N} |u_i - \tilde{u}_i|\Big)^a\right)^{b/a} \\
&\leq C\|h(t)\|_{L_{\frac{ab}{a-b}}(\Omega)^N}^b \|u - \tilde{u}\|_{L_a(\Omega)^N}^b,
\end{aligned}$$

where the last inequality follows from the equivalence of norms in finite dimensions. With the help of the continuous embeddings $L_b(\Omega)^N \hookrightarrow \tilde{Y}^*$ and $X_0 \hookrightarrow L_a(\Omega_T)^N$ the summation over $i = 1, ..., N$ yields

$$\begin{aligned}
\|g(p,u) - g(p,\tilde{u})\|_{\tilde{Y}^*} &\leq C\|g(p,u) - g(\tilde{p},\tilde{u})\|_{L_b(\Omega)^N} \\
&\leq C\|h(t)\|_{L_{\frac{ab}{a-b}}(\Omega)^N} \|u - \tilde{u}\|_{L_a(\Omega)^N} \\
&\leq C\|h(t)\|_{L_{\frac{ab}{a-b}}(\Omega)^N} \|u - \tilde{u}\|_{X_0},
\end{aligned}$$

where $C$ is a generic constant that may change in each line.
With $\|h(t)\|_{L_{ab/(a-b)}(\Omega)^N} \in L_s([0,T])$, condition (5.15) is fulfilled. The claim now follows from Theorem 5.1.18. □

**Example 5.1.22.** Let us assume the most general case from Section 2.1, that is

$$g_i(p,u) = \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i \left( \sum_{k=L}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right),$$

Further let us assume that all $\psi_i : \mathbb{R} \to \mathbb{R}$ and all $\phi_{ik} : \mathbb{R}^N \to \mathbb{R}$ are globally Lipschitz-continuous and it holds $C_1 \leq p_{ij} \leq C_2$ uniformly for each $k = L, ..., \tilde{M}$, $i = 1, ..., N$ and $j = 1, ...\tilde{M}$, then condition (5.17) if fulfilled, as the following estimate shows:

$$
\begin{aligned}
|g_i(p,u) - g_i(p,\tilde{u})| &= \left| \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i \left( \sum_{k=L}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1 - \tilde{u}_1, ..., u_N - \tilde{u}_N) \right) \right| \\
&\leq C \sum_{l=1}^{L} \left| \psi_i \left( \sum_{k=L}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1 - \tilde{u}_1, ..., u_N - \tilde{u}_N) \right) \right| \\
&\leq 2CL_{\psi_i} |\phi_{ik}(u_1 - \tilde{u}_1, ..., u_N - \tilde{u}_N)| \\
&\leq \underbrace{2CL_{\psi_i} \max_{k \in \{L,...,\tilde{M}\}} \{L_{\phi_{ik}}\}}_{=:h(x,t)} \sum_{j=1}^{N} |u_j - \tilde{u}_j|,
\end{aligned}
$$

where $C = \max\{C_1, C_2\}$. If further each $p_{ij}$ is a measurable function, then each $g_i$ is a Caratheodory function in the sense of Corollary 5.1.21. Note that this example especially includes the embryogenesis equation from Section 2.4.

**Remark 5.1.23.** The embedding $\mathcal{W} \hookrightarrow C([0,T], X_0)$ is continuous by interpolation theory, see [2, Theorem 4.10.2]. By [44, Corollary A.28], the embedding $(\tilde{Y}^*, Y)_{\tilde{s},q}$ into the (fractional) Sobolev space $H^{2\tilde{s}-1,q}(\Omega)^N$ is continuous for $\tilde{s} > 1/2$ (which then continuosly embeds into spaces of Hölder continuous functions if $q$ is sufficiently large). Further by interpolation theory $(\tilde{Y}^*, Y)_{1-1/s,s} \hookrightarrow (\tilde{Y}^*, Y)_{1-1/s,q}$ for $s \leq q$. Also note that for $s = 2, q \geq 2$ it holds $(\tilde{Y}^*, Y)_{1/2,q} \cong L_q(\Omega)^N$. Thus the space $Z = (\tilde{Y}^*, Y)_{1-1/s,s}$ fulfills the wanted properties on the space for the initial value from Definition 5.1.8 for $2 \leq s \leq q$.

Theorem 5.1.19 can be generalized further, i.e. existence can be shown for example for time dependent diffusion coefficients, see [6, Chapter 2] and [32, Chapter 6] for an outline. Also global solutions, i.e. solutions on the whole interval $[0,T]$ are possible, see [54, Chapter 3]. Note that a global solution under the assumptions of Theorem 5.1.19 always exists if $q$ and $s$ are chosen large enough, for example if $s = q > d + 2$, which is a consequence from [54, Corollary 3.2] combined with [48, Theorem 3.1.2]. It is also a consequence from [54, Corollary 3.2] that global solutions are always possible if it holds $|g_i(p,u)| \leq C$ uniformly for $u \in \mathcal{W}$ and a given set of parameters. This is for example the case in the embryogenesis equation (2.4), as the function $\phi$ is globally bounded.

Maximal parabolic regularity can further be used to derive solutions for very general quasilinear equations, as long as the involved nonlinear functions are Caratheodory-functions that satisfy the right Lipschitz-conditions, see [32, Chapter 6, Chapter 7]. Note that the Lipschitz-conditions given in Theorem 5.1.18 (and in the Theorems in [6, 32] if the diffusion is also time dependent) are very general. For more specific problems weaker or different Lipschitz conditions on the nonlinear function $g$ along with the right fixed point theorems might be sufficient to show the existence of solutions. Examples for such an approach can be found in [48, 49] and [57, 58]. In both examples it is required that $q > d+2$ to arrive at an existence result. Important for the upcoming chapters is the following result concerning the embryogenesis equation:

**Theorem 5.1.24** ([57, Theorem 3.3.4]). *There exists $\tau > 0$ and $q \in (d+2, d+2+\tau)$ such that equation (2.4) has a unique weak solution in $\mathcal{W}_{q,q}$ for a given set of parameters $(D, \lambda, R, W) \in L_\infty(\Omega_T)^{3N+N^2}$.*

**Remark 5.1.25.** Another approach to show existence of solutions is to construct a sequence of finite dimensional subspaces $X_h$, where the finite dimensional problem has a solution $u_h$. Then one shows convergence of these sequences by using the right compactness arguments. These methods are known as Galerkin method and Rothe method, see [25, 37, 61] for a detailed explanation and they are especially attractive in the case of space and time dependent parameters and more general diffusion coefficients, since less regularity on the parameters is demanded compared to the semigroup approach.

# CHAPTER 6

## The parameter-to-state map

In this chapter we investigate the parameter-to-state map of the partial differential equation (1.3). We discuss the properties needed to ensure the existence of a minimizer of the Tikhonov functional, as well as to ensure the stabilizing properties of Tikhonov regularization. These properties are the continuity and some kind of weak closedness of the forward operator, depending on the involved function spaces. Additionally, for numerical minimization, the derivative of the Tikhonov functional must fulfill at least a uniform continuity property to guarantee convergence of iterative algorithms. Additionally, we look at certain types of measurements and source conditions for our parameter identification problem. Spaces and notations appearing in this chapter, that are not explicitly introduced, are the ones from the previous chapter.

## 6.1 Definition

As we have seen in the sections before, there are various function spaces involved in the process of regularization. Formally the parameter-to-state map maps a function from a set of parameter spaces into the solution space, which are Banach spaces in our case. However, for the inverse problem it is better to have a parameter-to-state map mapping between Hilbert spaces, because they are easier to handle. This is, at least concerning the topology of the parameter space, not always possible. To verify the sufficient properties for Tikhonov regularization to admit a solution, we have to restrict the domain of the parameter identification problem in the following way.

$$\mathcal{D}(F) := \{p \in L_2(\Omega_T)^M \mid C_1 \leq \ p_i \leq C_2, 0 \leq C_1 < C_2 < \infty\}.$$

This domain restriction is primarily needed to ensure the well definedness of the weak formulation for the partial differential equation, but it is also useful in various estimates and some of them crucially depend on having a restricted domain like this. Note especially, that $\mathcal{D}(F)$ is obviously a convex, closed and bounded subset of $L_r(\Omega_T)^M, 1 \leq r \leq \infty$, but it is not compact as a subset of $L_r(\Omega_T)^M$, since for example if we consider $M = d = 1$, the sequence $x_n = \sin(nx)$ possesses no convergent subsequence on this set with respect to the $L_r$ topology if $r < \infty$. In fact the introduction of pointwise bounds for the parameters is done in many parameter identification problems and thus not a strong assumption. Often at least one of the constants $C_1$ or $C_2$ is defined as an arbitrary constant. Depending on the situation, we will restrict this domain even further to verify needed properties from Section 4.2.

Now we define the parameter-to-state map:

$$\begin{aligned} F : \mathcal{D}(F) \subset L_2(\Omega_T)^M &\to L_2(\Omega_T)^N \\ p &\mapsto u(p), \end{aligned} \tag{6.1}$$

where $u(p)$ is the weak solution of (1.3). Further we define $\mathcal{P} := L_r(\Omega_T)^M$, where $2 \leq r < \infty$ will be adapted to specific situations. We equip this space with the product one norm, i.e.

$$\|p\|_{\mathcal{P}} = \|p_1\|_{L_r} + \ldots + \|p_m\|_{L_r}.$$

Note that $\mathcal{D}(F) \subset \mathcal{P}$ for all $r \geq 2$. Further note that the range of $F$ is a subset of the solution space $\mathcal{W}$ of the parameter identification problem. This will be important, when we compute the derivative of $F$ and its adjoint.

**Remark 6.1.1.** The set $\mathcal{D}(F)$ does not contain open subsets with respect to the $L_r$ topology for $r < \infty$. To circumvent this problem, one can try to enlarge the domain in the following way to achieve a nonempty interior of $\mathcal{D}(F)$:

$$\tilde{\mathcal{D}}(F) := \{p \in L_r(\Omega_T)^M \mid \exists \tilde{p} \in \mathcal{D}(F) : \|p - \tilde{p}\|_{L_r} \leq \beta\},$$

where $\beta > 0$ is sufficiently small. This technique has been widely used for parameter identification problems, see for example [59]. Usually simple continuity arguments are enough to justify such an extension of the domain. However, such an extension is not always possible depending on the form of $g$ and the concrete application, where certain pointwise bounds on the parameters are required. In that case, one can only hope to show differentiability in the sense of Definition 3.5.2. For example, this technique has been used in [39] to show differentiability of the forward operator for a parameter identification problem arising electrical impedance tomography with respect to an $L_r$ topology.

## 6.2 $\tau$ - weak sequential closedness

A weak sequential closedness property of the forward operator of the inverse problem is the key ingredient to show the existence of a minimizer of the Tikhonov-functional as well as its regularization properties (cf. Section 4.2). For parameter identification problems, this is usually done by combining weak continuity properties of the operator with compact embeddings. We make the following assumptions:

**Assumption 6.2.1.**

*i) For a bounded sequence $\{p_n\} \subset \mathcal{D}(F)$, the sequence $F(\{p_n\})$ is bounded in $\mathcal{W}$.*

*ii) For $p_n \rightharpoonup p$ in $\mathcal{P}$ and $u_n \to u$ in $L_s([0,T], L_q(\Omega)^N)$, it holds*

$$\int_0^T \int_\Omega g(p_n, u_n) v \; dx \; dt \to \int_0^T \int_\Omega g(p,u) v \; dx \; dt \qquad \forall v \in L_{s'}([0,T], \tilde{Y}).$$

We will see, that this assumption is all we need to show the weak sequential closedness of the forward operator. In fact, it turns out that this assumption can be fulfilled for general equations, at least on a subdomain of $\mathcal{D}(F)$. For this one has to choose the subspace $\tilde{X}$ with topology $\tau$ introduced in Assumption 4.2.2 in the right way. A detailed discussion of some examples will follow in Section 6.4.

**Theorem 6.2.2.** *Let the Assumptions 5.1.13 and 6.2.1 hold and $\mathcal{D}(F) \subset \tilde{\mathcal{P}} \subset \mathcal{P}$. Further assume that $\tau$ is a topology on $\tilde{\mathcal{P}}$ and convergence with respect to $\tau$ implies weak convergence in $\mathcal{P}$. Then the forward operator $F : \mathcal{D}(F) \subset \mathcal{P} \to L_2(\Omega_T)^N$ given through* (6.1) *is $\tau$-weakly sequentially closed.*

*Proof.* We start with a sequence $\{p_n\}$ that converges in the $\tau$ topology in $\tilde{\mathcal{P}}$, i.e. there exists $p \in \tilde{\mathcal{P}}$ with $p_n \stackrel{\tau}{\to} p$. This sequence converges weakly in $\mathcal{P}$ by assumption and is therefore bounded in $\mathcal{P}$. By assumption $F(\{p_n\})$ is bounded in $\mathcal{W}$, and hence the sequence $\{u_n\}$ is bounded in the Banach space $\mathcal{W}$. By Proposition 5.1.4 the space $\mathcal{W}$ is reflexive and therefore applying the Banach-Alaoglu Theorem yields a weak convergent subsequence that we again denote by $\{u_n\}$ with $u_n \rightharpoonup z$. Further, the sequence $\{u_n\}$ is bounded in $L_s([0,T], \tilde{Y})$ and the sequence $\{(u_n)_t\}$ in $L_s([0,T], \tilde{Y}^*)$ by the definition of the $\mathcal{W}$-norm. Hence, there exists a subsequence of this sequence that we again denote by $\{u_n\}$ with $u_n \rightharpoonup z$ in $L_s([0,T], Y)$ and $(u_n)_t \rightharpoonup z'$ in $L_s([0,T], \tilde{Y}^*)$. Also this sequence converges strongly in $L_s([0,T], L_q(\Omega)^N)$ by the Lions-Aubin Theorem. Hence, we get

$$\int_0^T \langle (u_n)_t, \varphi \rangle_{(\tilde{Y}^*, \tilde{Y})} \; dt + \int_0^T \int_\Omega D \nabla u_n \nabla v \; dx \; dt$$
$$+ \int_0^T \int_\Omega g(p_n, u_n) v \; dx \; dt = \int_0^T \int_\Omega f v \; dx \; dt \quad \forall \in L_{s'}([0,T], \tilde{Y}).$$

Passing this to the limit, we get

$$\int_0^T \langle z_t, \varphi \rangle_{(\tilde{Y}^*, \tilde{Y})} \, dt + \int_0^T \int_\Omega D \nabla u \nabla v \, dx \, dt + \int_0^T \int_\Omega g(p,z) v \, dx \, dt = \int_0^T \int_\Omega f v \, dx \, dt \quad \forall v \in L_{s'}([0,T], \tilde{Y}),$$

where the first summand converges by the weak convergence of $(u_n)_t$ in $L_s([0,T], \tilde{Y}^*)$, the second by the weak convergence of $u_n$ in $L_s([0,T], Y)$ and the third by Assumption 6.2.1. Further, it can be shown that $\lim_{n\to\infty} u_n(0) = z_0$ in $Z$ (see [57, Lemma 2.3.12]) and hence $z(0) = \lim_{n\to\infty} u_n(0) = u_0$ in $Z$. Hence, by Proposition 5.1.11 $z$ is a weak solution for the differential equation for $p$ and since the solution is unique, it holds $F(p) = u$. Therefore, the forward operator is $\tau$-weakly sequentially closed. □

**Remark 6.2.3.** Since $u_n$ converges strongly in $L_s([0,T], L_q(\Omega)^N)$, it also converges strongly in $L_2(\Omega_T)^N$. This means that the forward operator is even $\tau$-strong sequentially continuous.

**Remark 6.2.4.** Weak convergence $g(p_n, u_n) \rightharpoonup g(p,u)$ in $L_s([0,T], \tilde{Y}^*)$ is a necessary condition for $\tau$-weak sequential closedness to hold for the forward operator. This can easily be seen by substracting the weak formulations for $(p_n, u_n)$ and $(p,u)$ and passing to the limit.

## 6.3 Differentiability

For any parameter identification problem, one can easily find a candidate for the derivative just by formal differentiation of the equation. For this we look at the implicit formulation of (1.3), that can be written as

$$A(p,u) = A(p, F(p)) = 0.$$

Formal differentiation with respect to $p$ in direction $h$ of this equation now yields:

$$A_u(p,u) \circ F'(p)h + A_p(p,u)h = 0$$

and therefore

$$F'(p)h = -(A_u(p,u))^{-1} A_p(p,u)h. \tag{6.2}$$

However, to show that this candidate is the actual derivative is a bit more complex, since existence and continuity properties have to be verified. One elegant way to show the differentiability of the forward operator is the implicit function theorem, which seems a natural choice due to the implicit definition of the forward operator $F$. To apply the implicit function theorem it is necessary to show that the involved partial derivatives fulfill some continuity properties, as well as that the operator $A_u$ is continuously invertible. In our case the differential operator $A$ has the following form

$$\begin{aligned} A : \mathcal{P} \times \mathcal{W} &\to Z \times L_s([0,T], \tilde{Y}^*) \\ (p,u) &\mapsto (u(0) - u_0, u_t + \nabla \cdot D\nabla u + g(p,u) - f). \end{aligned}$$

The partial derivatives in (6.2) then take the form

$$A_u v = (v(0), v_t - \nabla \cdot D\nabla v + g_u(p,u)v), \qquad v \in \mathcal{W},$$

and

$$A_p h = (0, g_p(p,u)h), \qquad h \in \mathcal{P},$$

where

$$(g_p(p,u)h)_i = \sum_{k=1}^{M} (g_i)_{p_k}(p,u)h_k \tag{6.3}$$

and

$$(g_u(p,u)v)_j = \sum_{k=1}^{N} (g_j)_{u_k}(p,u)v_k \tag{6.4}$$

with $i = 1, ..., M$, $j = 1, ..., N$. The existence and continuity of the derivatives $g_u(p,u)$ and $g_p(p,u)$ strongly depends on the form of $g$. Also, one has to ensure enough regularity on the parameter space, as discussed in Section 3.7. All in all continuity and differentiability properties of the parameter-to-state map mainly depend on the properties of the superposition operator

$$\begin{aligned} G : \mathcal{P} \times \mathcal{W} &\to L_s([0,T], \tilde{Y}^*) \\ (p,u) &\mapsto g(p,u) \end{aligned}$$

So, for an analysis that can provide the needed properties for Tikhonov regularization, we have to make the following assumptions

**Assumption 6.3.1.**

*(i) For given $r \geq 2$ and $s, q \geq 2$ the (partial) derivatives $g_{p_i}(p,u)$ and $g_{u_j}(p,u)$, $i = 1, ..., M$, $j = 1, ..., N$ of the operator $G$ (in terms of the respective superposition operators associated with the mappings $p_j \mapsto g(p_j, \cdot)$, $u_i \mapsto g(\cdot, u_i)$) exist and are continuous.*

(ii) *For every $p \in \mathcal{D}(F)$ and every $y \in L_s([0,T], \tilde{Y}^*)$ , the (linear) differential equation $A_u(p,u) = y$ has a unique weak solution in $\mathcal{W}$.*

**Remark 6.3.2.** Assumption 6.3.1 (i) is enough to ensure the differentiability of the operator $G$ with respect to $u$ and $p$, because we compute the derivative of the associated superposition operator with the help of partial derivatives anyways. Partial continuous differentiability implies total differentiability and the derivatives $g_p(p,u)$ and $g_u(p,u)$ are then computed as in (6.3) and (6.4). Assumption 6.3.1 (ii) ensures the invertibility of $A_u$ and hence the well-definedness of the operator proposed in (6.2).

Now, with Assumption 6.3.1 at hand, it is easy to show the differentiability of the parameter-to-state map via the implicit function theorem. The proofs are mostly straightforward and almost the same as in [57]:

**Proposition 6.3.3.** *Let the Assumptions 5.1.13 and 6.3.1 hold for given $r, s, q \geq 2$. Then, the operator*

$$A : \mathcal{P} \to Z \times L_s([0,T], \tilde{Y}^*)$$
$$p \mapsto (u(0) - u_0, u_t + \nabla \cdot D\nabla u + g(p,u) - f)$$

*is continuously differentiable and its derivative is given through*

$$A_p(p)h = (0, g_p(p,u)h).$$

*Proof.* The only part that depends on $p$ is the nonlinear function $g(p,u)$. The superposition operator $G(p)$ is differentiable by Assumption 6.3.1 with derivative $g_p(p,u)h$. □

**Proposition 6.3.4.** *Let the Assumptions 5.1.13 and 6.3.1 holds for given $r, s, q \geq 2$. Then, the operator*

$$A : \mathcal{W} \to Z \times L_s([0,T], \tilde{Y}^*)$$
$$u \mapsto (u(0) - u_0, u_t + \nabla \cdot D\nabla u + g(p,u) - f)$$

*is continuously differentiable with derivative*

$$A_u(u)v = (v(0), v_t - \nabla \cdot D\nabla v + g_u(p,u)v).$$

*Further, for $p \in \mathcal{D}(F)$ the derivative is invertible.*

*Proof.* The first component of the map $A$ is affine linear in $u$ and because of the embedding from (5.11), it is of course continuous. Hence, it is differentiable in $u$. The first part of the second component, that is $u_t + \nabla \cdot D\nabla u$, is just linear in $u$. The continuity follows directly from the definition of the respective norms. Hence, the first part of the second component is continuously differentiable. The differentiability of the superposition operator $(p,u) \mapsto g(p,u)$ is given via Assumption

6.3.1. Hence, the second component is continuously differentiable as well. Now we look at the invertibility of the derivative. Let $y \in L_2([0,T], \tilde{Y}^*)$ be arbitrary, we now define the differential equation

$$v_t - \nabla \cdot D\nabla v + g_u(p,u)v = y.$$

This is a linear parabolic partial differential equation. This equation has a unique weak solution by Assumption 6.3.1. Hence, there exists a $v \in \mathcal{W}$ with $A_u(u)v = y$. It follows that the operator $A_u$ is surjective. Now assume $A_u(u)v = A_u(u)w = y$. Since the solution of the differential equation is unique, it must hold $v = w$ and therefore, the operator $A_u$ is injective. So it is invertible. □

**Theorem 6.3.5.** *Let the Assumptions 5.1.13 and 6.3.1 hold for given $r, s, q \geq 2$. Then the operator $F : \mathcal{D}(F) \subset \mathcal{P} \to \mathcal{W}$ is continuously differentiable. The derivative is given through*

$$F'(p)h = -(A_u)^{-1} A_p h,$$

*which corresponds to the weak solution of the differential equation*

$$v_t - \nabla \cdot D\nabla v + g_u(p,u)v = -g_p(p,u)h$$

*with initial condition $v(0) = 0$.*

*Proof.* The existence of a unique weak solution of the forward problem ensures a solution of the equation $A(p,u) = 0$. With the help of Propositions 6.3.3 and 6.3.4 the claim follows directly from the implicit function theorem. □

**Corollary 6.3.6.** *Let the Assumptions 5.1.13 and 6.3.1 hold for given $r, s, q \geq 2$. Then the operator $F : \mathcal{D}(F) \subset \mathcal{P} \to L_2(\Omega_T)^N$ is continuously differentiable and the derivative is the same as in Theorem 6.3.5.*

*Proof.* Clear by the continuous embeddings from (5.9), since
$\mathcal{W} \hookrightarrow C([0,T], L_2(\Omega)^N) \hookrightarrow L_2(\Omega_T)^N$. □

**Remark 6.3.7.** Due to the restriction of the domain $\mathcal{D}(F)$, the differentiability results derived in this section have to be understood as strong derivatives, i.e. as derivatives with respect to the relative topology. Note that differentiation of $A$ with respect to $p$ is possible on the whole space $\mathcal{P}$ if $u$ is regular enough (i.e. an $L_\infty$ function). On the other hand, differentiability (and invertibility) of $A$ and $A_u$ can only be guaranteed on a subset of the parameters (which ideally is a bounded subset of $L_\infty(\Omega_T)^M$), especially if one wants to utilize differentiability of $G$ in Lebesgue spaces (see also Remark 6.3.10 below).

Finally, we want to analyze conditions onto $r$, $q$ and $g(p,u)$ that are sufficient to guarantee differentiability in the case that $g$ is a nonlinear function. For this we apply our findings from Section 5.1.3:

**Proposition 6.3.8.** *Let $2 < s \leq q$ and $q > d$ such that $1 - 2/s - 1/q > 0$. Let $Z = (Y, \tilde{Y}^*)_{1-1/s,s}$ and let $D, g(p,u)$ fulfill the assumptions from Corollary 5.1.20 for all $p \in \mathcal{D}(F)$. Further let the operator*

$$\begin{aligned} G(p) : L_r(\Omega_T)^M &\to L_s(\Omega_T)^N \\ p &\mapsto g(p,u) \end{aligned}$$

*be differentiable for $r \geq s$. Additionally assume that there exists $a \in \mathbb{R}$ with $s < a < \infty$ such that the operator*

$$\begin{aligned} G(u) : L_a(\Omega_T)^N &\to L_s(\Omega_T)^N \\ u &\mapsto g(p,u) \end{aligned}$$

*is differentiable and for every $p \in \mathcal{D}(F)$, $u \in \mathcal{W}$ and $g_u(p,u)$ fulfills condition (5.14). Then $u \in L_\infty(\Omega_T)^N$ and $F : \mathcal{P} \to \mathcal{W}$ is differentiable.*

*Proof.* The existence of a solution $u \in L_\infty(\Omega_T)^N$ of the partial differential equation is guaranteed by Corollary 5.1.20. By the continuous embeddings $\mathcal{W} \hookrightarrow L_a(\Omega_T)^N$ from Proposition 5.1.6 and $L_s(\Omega_T)^N \hookrightarrow L_s([0,T], \tilde{Y}^*)$, the first part of Assumption 6.3.1 is fulfilled. The existence of a solution for the differential equation $A_u v = 0$ follows from Theorem 5.1.16. □

The advantage of the Proposition 6.3.8 over the approach of showing differentiability of $G$ directly between $\mathcal{P}$ (respectively $\mathcal{W}$) and $L_s([0,T], \tilde{Y}^*)$ is that differentiability of superposition operators between Lebesgue spaces is well understood and concrete conditions for differentiability to hold are given in Theorem 3.7.4. In the next remark, we take a closer look at these conditions.

**Remark 6.3.9.** To verify differentiability of $G$ with respect to $p$ between $L_r(\Omega_T)^M$ and $L_s(\Omega_T)^N$ one has to check certain conditions for each $p \in \mathcal{P}$ and $u \in \mathcal{W}$. At first one has to verify that each of the functions

$$\begin{aligned} g_{ij} : \Omega_T \times L_r(\Omega_T) &\to L_s(\Omega_T) \\ (x,t,p_j) &\mapsto g_i(p_1(x,t), ..., p_j, ..., p_M(x,t), u(x,t)) \end{aligned}$$

is a Caratheodory function. Additionally the limits

$$(g_i)_{p_j}(x,t) := \lim_{z \to 0} \frac{g_{ij}(x,t,p_j(x,t)+z) - f(x,t,p_j(x,t))}{z}$$

have to be an element from $L_{\frac{rs}{r-s}}(\Omega_T)$ and a growth condition of the form

$$|g_i(x,t,p_j(x,t)+h) - g_i(x,t,p_j(x,t)) - (g_i)_{p_j}(x,t)h|^s \leq \lambda^{-s} b_{\lambda_{ij}}(x,t) + \lambda^{r-s}|h|^r.$$

has to be fulfilled for any given $\lambda_{ij} > 0$ and $i = 1, ..., N$, $j = 1, ..., M$ with $b_{\lambda_{ij}} \in L_1(\Omega_T)$. Finally one has to verify that the mappings

$$\begin{aligned} L_r(\Omega_T) &\to L(L_r(\Omega_T), L_s(\Omega_T)) \\ p_j &\mapsto (h \mapsto (g_i)_{p_j} h) \end{aligned}$$

are continuous for each $i, j$. In analogue fashion one verifies differentiability of $G$ with respect to $u$ between $L_a(\Omega_T)^N$ and $L_s(\Omega_T)^N$.

**Remark 6.3.10.** One might ask, if an exponents $2 < s \leq q$ and $q > d$ such that $1 - 2/s - 1/q > 0$ and $r > s > 2$ are really necessary in the nonlinear case.

For one part of this question, let us take a look at the second component of $g$. Here we made the restriction $1 - 2/s - 1/q > 0$. However, this is not necessary. From computations in [61, Section 8.6] it follows that there exists a continuous embedding from $\mathcal{W}_{q,q} \hookrightarrow L_b(\Omega_T)^N$, where $q < b \leq (d+2)q/d$. So if $g$ is differentiable between $L_b(\Omega_T)^N$ and $L_q(\Omega_T)^N$, we have the continuous embedding $\mathcal{W}_{q,q} \hookrightarrow L_b([0,T], L_b(\Omega)^N)$. This ensures enough regularity so that $L_b(\Omega_T)^N$-$L_q(\Omega_T)^N$ differentiability guarantees differentiability between $\mathcal{W}$ and $L_q([0,T], \tilde{Y}^*)$. This especially is possible for $q = 2$. However in this situation, one loses that $u \in L_\infty(\Omega_T)^N$ which will be important in some estimates later on.

We now proceed to answer the second part of the question in two steps. If we want a solution $u \in L_\infty(\Omega_T)^N$ and want to utilize the maximal parabolic regularity approach, we need an exponent $r > s > 2$. The reason for this is the time axis, where at least $L_s$ regularity on the parameters is demanded in time and thus by Theorem 3.7.5, differentiability can not hold if $r = 2$ and $s > 2$. Instead we need an exponent exponent $r > s$. We further require $g_p(p, u)$ to be in $L_s([0,T], \tilde{Y}^*)$, where $s > 2$ to utilize the continuous embedding from Proposition 5.1.6. While a continuous embedding $L_2(\Omega)^N \hookrightarrow \tilde{Y}^*$ does exist, we can not guarantee the existence of a continuous embedding $L_2([0,T], L_2(\Omega)^N) \hookrightarrow L_s([0,T], \tilde{Y}^*)$ for $s > 2$ and therefore we have to choose $r > s > 2$.

If now $u$ is not needed to be in $L_\infty(\Omega_T)^N$ and each $g_i(p, u)$ is linear in each $p_j$, we can have better results. In this case we may be able to choose an exponent $r = 2$ for the parameter space, if one utilizes the embedding $\mathcal{W}_{q,q} \hookrightarrow L_{(d+2)q/d}(\Omega_T)^N$.

An approach to get an exponent $r = 2$ even in the nonlinear case would be to show differentiability of the operator $G(p) : L_2(\Omega_T)^M \to L_s(\Omega_T)^N$, $G(p) = g(p, u)$ where $s \in (\max\{1, dq/(d-q)\}, 2)$. Then by Proposition 3.4.4 one has the continuous embedding $L_s(\Omega_T)^N \hookrightarrow L_s([0,T], \tilde{Y}^*)$. One then can interpret $F$ as mapping from $L_2(\Omega_T)^M \to \mathcal{W}_{s,q}$ and deduce differentiability of the parameter to state map again with the help of the implicit function theorem (existence of solutions is ensured by $\mathcal{W} \hookrightarrow \mathcal{W}_{s,q}$ and invertibility of the equation $A_u v = g_p(p, u)$ can be deduced with the help of maximal parabolic regularity results). But in this case a continuous embedding $\mathcal{W}_{s,q} \to L_2(\Omega_T)^N$ does not exist without any further restrictions on $u$. Thus we are only shifting the problem of not having a Hilbert space to the data site.

Note that stronger growth conditions on $g$ or certain equations arising from applications might yield solutions that have more regularity. That allows greater flexiblility on the parameter space as long as each $g_i$ is at least linear in every involved component of the parameter $p$. Also note that for only space dependent parameters, differentiability with respect to $L_2(\Omega)^M$ should possible to achieve with the help of Sobolev embeddings, since in this case $g(p)$ can be viewed as constant in time.

## 6.4 The reaction term $g$ and the parameter space

As we have seen in the two sections before, we have to make certain assumptions to get weak sequential closedness and differentiability of the forward operator. For this, we will investigate the function $g$. As we have seen in Section 3.7 truly nonlinear functions have to fulfill certain requirements to ensure continuity and differentiability of the associated superposition operators. These are required to verify the $\tau$-weak sequential closedness and the differentiability of the parameter-to-state map, which is expressed in Assumption 6.3.1 and Assumption 6.2.1. Together with conditions on $g$ there are also conditions onto the parameter space that have to be fulfilled. Hence, the parameter space $\mathcal{P}$ has to be chosen wisely and the limitations on that parameter space are given through the restrictions in Section 3.7. We take a look what this means in the concrete examples from Section 2.1. So let $\tilde{M}$, $\lambda_{ik}$, $\phi_{ik}$ be as in Section 2.1. Further, we assume the involved functions $\phi_{ik} : \mathbb{R}^N \to \mathbb{R}, \psi_{il} : \mathbb{R} \to \mathbb{R}$ to be continuously differentiable and to fulfill a growth estimate of the form (3.8) with respect to the exponents $b > q$ and $a > b$ so that we can deduce differentiability of the superposition operator as a map from $L_a(\Omega_T) \to L_b(\Omega_T)$, which is sufficient for differentiability of the forward operator by Proposition 6.3.8, where $a$ is sufficiently large. Note that by our restrictions on $\mathcal{D}(F)$ and the fact that $u \in L_\infty([0,T], L_\infty(\Omega)^N)$ by embedding (5.9) (at least if exponents $q > d$ and $s > 2$ sufficiently large are chosen for the solution space, which we assume at this point), it holds in all of the upcoming cases that $g(p,u) \in L_\infty([0,T], L_\infty(\Omega)^N)$, since the pointwise application of a continuous function to an $L_\infty$ function is again an $L_\infty$ function (see also Remark 6.4.2 at the end of this section).

1. First we look at linear combinations of the form

$$g_i(p,u) = \sum_{k=1}^{N} \lambda_{ik} p_{ik} u_k.$$

In this case it is possible to choose $\mathcal{P} = L_2(\Omega_T)^M$. For this let $q = ab$, where $2 > a > 2d/(d+2)$ and $2 \leq b < \infty$ such that $ab' \leq 2$. Further we assume $u \in \mathcal{W}_{2,q}$. Then we can estimate (with the help of the Hölder-inequality in space and $\mathcal{W}_{2,q} \hookrightarrow C([0,T], L_q(\Omega)^N)$ continuous)

$$\begin{aligned}\|g(p,u)\|_{L_2([0,T],\tilde{Y}^*)} &\le C \sum_{i=1}^{N} \|g_i(p,u)\|_{L_2([0,T],L_a(\Omega))} \\ &\le C \sum_{i=1}^{N}\sum_{k=1}^{N} \|p_{ik}u_k\|_{L_2([0,T],L_a(\Omega))} \\ &\le C \sum_{i=1}^{N}\sum_{k=1}^{N} \|p_{ik}\|_{L_2([0,T],L_{ab'}(\Omega))} \|u_k\|_{L_\infty([0,T],L_{ab}(\Omega)^N)} \\ &\le C\|p\|_{\mathcal{P}}\|u\|_{\mathcal{W}},\end{aligned}$$

where $C$ is a generic constant and hence, the map $(p,u) \to g(p,u)$ is bilinear and (Lipschitz)-continuous and therefore continuously differentiable with respect to $p$ and $u$ (which directly coincides with the findings of Theorem 3.7.4 concerning superposition operators). The partial derivatives from (6.3) and (6.4) are then given as

$$(g_i)_{p_{ij}} h_{ij} = \lambda_{ij} u_j h_{ij}$$

and

$$(g_i)_{u_j} v_j = \lambda_{ij} p_{ij} v_j.$$

One can now directly deduce, that Assumption 6.3.1 is fulfilled. For Assumption 6.2.1 to be fulfilled, we choose the $L_2$ topology as $\tau$-topology on $\mathcal{D}(F)$. It is well known that for $p_n \rightharpoonup p$ in $L_2$, $u_n \to u$ in $L_2$ with $u_n \in L_\infty$, it directly follows $p_n u \rightharpoonup pu$ in $L_2$. Since the sum of weakly convergent sequences converges weakly, we can directly deduce, that Assumption 6.2.1 is fulfilled as well.

2. For functions that are a linear combinations in $p$ and nonlinear in $u$, i.e.

$$g_i(p,u) = \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N),$$

we can assume the existence of a solution, where $q, s \ge 2$ and then utilize Proposition 6.3.8 (with possible addition of Remark 6.3.10) to show differentiability of $F$. Differentiability with respect to $p$ (again with $\mathcal{P} = L_2(\Omega_T)^M$) directly follows from its linearity along with continuity and can be deduced as in the last example. For the differentiability with respect to $u$ we refer to the assumption that the with $\phi_{ik}$ associated superposition operator is differentiable as an operator from $L_a(\Omega_T) \to L_b(\Omega_T)$, which then implies differentiability of the forward operator as stated in Proposition 6.3.8. The respective partial derivatives are then given as

$$(g_i)_{p_{ij}} h_{ij} = \lambda_{ij} \phi_{ik}(u_1, ..., u_N) h_{ij}$$

and

$$(g_i)_{u_j} v_j = \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} (\phi_{ik})_{u_j} (u_1, ..., u_N) v_j,$$

as (3.5) dictates. Since we assumed a continuous derivative for $\phi$, we find that at least $(g_i)_{u_j} \in L_\infty(\Omega)$, so that the linear partial differential equation has a solution for all $f \in \tilde{Y}^*$ by standard solution theory. Hence, Assumption 6.3.1 is fulfilled. Assumption 6.2.1 can be deduced as before.

3. In the case, where general nonlinear functions $\psi_i : \mathbb{R} \to \mathbb{R}$ are involved additionally, i.e.

$$g_i(p, u) = \psi_i \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right),$$

the situation gets a lot more complicated. Now the parameter $p$ itself is an argument of a nonlinear function. Differentiability of $g$ with respect to $p$ can be ensured by the properties of the functions $\psi_i$. In case of exponents $q, s \geq 2$, we have to restrict the parameter space to $L_r(\Omega_T)^M$ for some $r > s$, so that we have $L_s$-regularity in time for the derivative $g_p(p, u)$. So in this case the parameter space (formally) becomes a Banach space. The differentiability with respect to $u$ can be handled as in the previous case. Even more difficult to handle is the fact that establishing a weak continuity result with respect to the $L_2$ topology (or with respect to any $L_r$ topology with $r \geq 2$) is not possible due to Theorem 3.7.8.

Again we can compute the derivatives of the superposition operators via (3.5)

$$(g_i)_{p_{ij}} h_{ij} = \psi_i' \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right) \lambda_{ij} \phi_{ij}(u_1, ..., u_N) h_{ij}$$

and

$$(g_i)_{u_j} v_j = \psi_i' \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right) \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} (\phi_{ik})_{u_j} (u_1, ..., u_N) v_j.$$

As stated before, we cannot directly show the weak closedness property on the original domain $\mathcal{D}(F)$ for this example. The goal would be to find a topology $\tau$ as in Assumption 4.2.2, such that Assumption 6.2.1 can be verified. It is highly unlikely that such a topology $\tau$ exists, because if we assume for example a $L_r$ weak topology or the $L_\infty$ weak star topology on $\mathcal{D}(F)$, it can be shown that $g_i(p_n, u_n)$ has a subsequence with $g_i(p, u) \overset{\star}{\rightharpoonup} y$

in $L_\infty$, but $y \neq g_i(p,u)$ in general (see Remark 6.4.2 below). So if one wants to ensure the existence of a minimizer, we have to choose a parameter space $\tilde{\mathcal{P}}$ and a topology $\tau$ on $\tilde{\mathcal{P}}$, such that $p_n \xrightarrow{\tau} p$ in $\mathcal{P}$ implies the existence of a strongly convergent subsequence $p_n \to p$ in $L_r(\Omega)$. Then we can use the continuity of $\psi_i$ to verify Assumption 6.2.1. An example of such a domain would be

$$\tilde{\mathcal{D}}(F) = \{p \in \mathcal{D}(F) \mid \|p\|_{\tilde{\mathcal{P}}} < \tilde{C}\}, \tag{6.5}$$

A first idea to choose $\tilde{\mathcal{P}}$ could be

$$\tilde{\mathcal{P}} := \{p \in L_2([0,T], H^{1,r}(\Omega)^M), p' \in L_2([0,T], (H^{1,r'}(\Omega)^M)^*)\}. \tag{6.6}$$

Then the $\tau$-topology would be the weak topology on $\tilde{\mathcal{P}}$. Since $\tilde{\mathcal{P}}$ is reflexive, a sequence in $\tilde{\mathcal{D}}(F)$ has a weakly convergent subsequence (by the almost everywhere bound on the $\tilde{\mathcal{P}}$-norm combined with the Banach-Alaoglu theorem). A weak convergent sequence in $\tilde{\mathcal{P}}$ converges strongly in $L_r(\Omega_T)^M$ by Theorem 3.3.4. But of course, this is not optimal in terms of parameter identification since it basically excludes all non continuous functions.

A much better idea in fact is to choose

$$\tilde{\mathcal{P}} := BV(\Omega_T)^M, \tag{6.7}$$

the space of functions of bounded variation, see [3] for the definition and properties of $BV$. The advantage of (6.7) in comparison with (6.6) is, that the space of bounded variation includes much more functions than the space from (6.6), especially functions that have jumps and most likely any parameter $p^\dagger$ that appears in practical applications. For showing regularization properties on $\tilde{\mathcal{D}}(F)$, one now chooses the $\tau$-topology as the weak$^*$ topology in $BV(\Omega_T)^M$. Note that the Banach-Alaoglu Theorem is not directly applicable in this case, since $BV(\Omega_T)^M$ is not a separable space and thus weak$^*$ compactness is not necessarily equivalent to sequential weak$^*$ compactness. But there exists a generalization, the so called sequential Banach-Alaoglu Theorem [62, Lemma 4.10], which, combined with (6.5), yields a weakly star convergent subsequence in $BV(\Omega_T)$. It is known that a $BV$ weakly star convergent sequence converges strongly in $L_1(\Omega_T)^M$ and by the Dominated Convergence Theorem combined with the almost everywhere bound on $\mathcal{D}(F)$ this sequence even converges strongly in $L_r(\Omega_T)^M$. If the penalty appears to have sequentially compact level sets with respect to the topology of $\tilde{\mathcal{P}}$ (i.e. $R(p) = \|p\|^2_{\tilde{\mathcal{P}}}$), the restriction $\|p\|_{\tilde{\mathcal{P}}} < \tilde{C}$ can be omitted. Another way to secure the existence of a minimizer of the Tikhonov functional would be the restriction of $\mathcal{D}(F)$ to any compact subset of $L_2(\Omega)^M$, as explained in Remark 4.2.7.

4. Our last example are combinations of the above, where multiplications of different parameters are allowed, i.e.

$$g_i(p,u) = \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i \left( \sum_{k=L}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right).$$

Here, parameter space and solution space can be chosen as in the last example. To verify a weak closedness property, one has to basically restrict the domain as in the last example. We just show, how the derivatives are computed in this case. It holds for $j \leq L$,

$$(g_i)_{p_{ij}} h_{ij} = \lambda_{ij} h_{ij} \psi_i \left( \sum_{k=L+1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right)$$

and for $j > L$

$$(g_i)_{p_{ij}} h_{ij} = \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i' \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right) \lambda_{ij} \phi_{ij}(u_1, ..., u_N) h_{ij}.$$

The derivative for $u$ can basically be computed as in the example before, i.e.

$$(g_i)_{u_j} v_j = \sum_{l=1}^{L} \lambda_{il} p_{il} \psi_i' \left( \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} \phi_{ik}(u_1, ..., u_N) \right) \sum_{k=1}^{\tilde{M}} \lambda_{ik} p_{ik} (\phi_{ik})_{u_j}(u_1, ..., u_N) v_j.$$

The above calculations are still very abstract, so we now look at our primary example from Section 2.4

**Example 6.4.1.** Let us consider the nonlinear reaction part

$$g_i((\lambda, R, W), u) = \lambda_i u_i + R_i \phi(W_{i1} u_1 + ... + W_{i_n} u_N),$$

so we are in the fourth of the above situations. Continuity and differentiability of the involved superposition operators have been shown in [57]. For the partial derivatives we find

$$\begin{aligned} (g_i)_{\lambda_j} \bar{\lambda}_j &= \bar{\lambda}_j u_j, \\ (g_i)_{R_j} \bar{R}_j &= \bar{R}_j \phi(W_{i1} u_1 + ... + W_{i_n} u_N), \\ (g_i)_{W_{ij}} \bar{W}_{ij} &= R_i \phi'(W_{i1} u_1 + ... + W_{i_n} u_N) \bar{W}_{ij} u_j \end{aligned}$$

and

$$(g_i)_{u_j} v_j = R_i \phi'(W_{i1} u_1 + ... + W_{i_n} u_N) W_{ij} v_j.$$

So in total we get

$$g_p((\lambda, R, W), u)(\bar{\lambda}, \bar{R}, \bar{W}) = \bar{\lambda} u + \bar{R}\phi(Wu) + R\phi'(Wu)\bar{W}u \tag{6.8}$$

and

$$g_u((\lambda, R, W), u)v = \lambda v + R\phi'(Wu)Wv. \tag{6.9}$$

Again, $\tau$-weak sequential continuity cannot be shown for weak $L_r$ topologies, so we cannot guarantee the existence of a minimizer of the Tikhonov-functional on $\mathcal{D}(F)$ at the moment. To ensure the existence of minimizer of the Tikhonov functional on a subset of $\mathcal{D}(F)$, one can formally restrict the domain as in (6.7). In our numerical experiments, we just utilize parameters that are elements of $BV(\Omega_T)$, so that we do not have to worry too much about domain restrictions. But in numerical experiments the situation is a lot easier anyways, since all computations are done in finite dimensional subspaces, where weak convergence is equivalent to strong convergence.

**Remark 6.4.2.** Let $\phi : \mathbb{R} \to \mathbb{R}$ be continuous and $u_n \in L_\infty(\Omega)$ be a $L_\infty$ weakly$^*$ convergent sequence with limit $u \in L_\infty(\Omega)$. Since $u_n$ is bounded in $L_\infty$, it especially holds $|u_n(x)| \leq C$ almost everywhere and therefore $\sup|\phi(u_n(x))| \leq C_2$ almost everywhere by continuity of $\phi$. So $\{\phi(u_n)\}$ is uniformly bounded in $L_\infty$ and therefore has a weakly$^*$ convergent subsequence by the Banach-Alaoglu Theorem, i.e. $\phi(u_n) \overset{\star}{\rightharpoonup} z$. But usually, $z \neq \phi(u)$. For this consider the sequence $u_n := \sin(nx)$ on $L_2(0, 2\pi)$ and $\phi(\cdot) = (\cdot)^2$. The sequence $\{u_n\}$ converges weakly with respect to the $L_r$ topology for $1 \leq r < \infty$ and weakly$^*$ in $L_\infty(0, 2\pi)$. However, it holds

$$\int_0^{2\pi} \phi(u_n)\ dx = \pi,$$

Therefore $z \neq 0 = \phi(u)$.

## 6.5 The adjoint of the derivative

For the computation of the gradient of the Tikhonov functional, it is necessary to know the adjoint of the derivative of the parameter-to-state map. Since we assume our data to be in $L_2(\Omega_T)^N$, we need to compute the adjoint of the operator $F'(p) : \mathcal{P} \to L_2(\Omega_T)^N$, where the exponent of $\mathcal{P}$ is determined by the shape of $g$, see Proposition 6.3.8. We have seen, that we can write the derivative as the concatenation of two linear operators, i.e. $F'(p)h = (A_u)^{-1}(A_p h)$. Hence, we can compute its adjoint by computing the adjoint of the two involved linear operators (note that these are mapping between Banach spaces) and it holds

$$F'(p)^* w = -(A_p)^* \circ \left((A_u)^{-1}\right)^* w$$

For the rest of the work let $g_p(p,u)^*$ and $g_u(p,u)^*$ be the adjoints of the respective multiplication operators

$$\begin{aligned} \mathcal{W} &\to L_s([0,T],\tilde{Y}^*) \\ v &\mapsto g_u(p,u)v \end{aligned}$$

and

$$\begin{aligned} L_r(\Omega_T)^M &\to L_s([0,T],\tilde{Y}^*) \\ h &\mapsto g_p(p,u)h. \end{aligned}$$

Then, we can get an explicit expression for the adjoint

**Theorem 6.5.1.** *Let Assumption 6.3.1 hold. Then, for fixed $p$ in $\mathcal{P}$ the adjoint of $F'(p)$ is given as*

$$\begin{aligned} F'(p)^* : L_2(\Omega_T)^N &\to \mathcal{P}^* \\ w &\mapsto -g_p(p,u)^* v(w), \end{aligned}$$

*where $v(w)$ is given as the unique solution of the differential equation*

$$-v_t - \nabla \cdot D\nabla v + g_u(p,u)^* v = w, \qquad v(T) = 0 \tag{6.10}$$

*Proof.* The claim follows immediately from Corollary 6.5.5 and Lemma 6.5.7 below. □

**Remark 6.5.2.** The adjoint $g_u(p,u)^*w$ of the multiplication operator $g_u(p,u)v$ can be computed via

$$\begin{aligned} \langle g_u(p,u)v, w\rangle_{\mathbb{R}^N} &= \sum_{k=1}^N \sum_{j=1}^N (g_{u_j}(p,u)v_j)_k w_k \\ &= \sum_{j=1}^N \sum_{k=1}^N (g_{u_j}(p,u)w_k)_j v_j \\ &= \langle g_u(p,u)^* w, v\rangle_{\mathbb{R}^N} \end{aligned}$$

and the adjoint $g_p(p,u)^*m$ of the multiplication operator $g_p(p,u)h$ via

$$\begin{aligned} \langle g_u(p,u)h, m\rangle_{\mathbb{R}^N} &= \sum_{k=1}^N \sum_{j=1}^M (g_{p_j}(p,u)h_j)_k m_k \\ &= \sum_{j=1}^M \sum_{k=1}^N (g_{p_j}(p,u)m_k)_j h_j \\ &=: \langle g_p(p,u)^* m, h\rangle_{\mathbb{R}^M}. \end{aligned} \tag{6.11}$$

Basically we transpose the Jacobi matrices $g_p$ and $g_u$, which is nothing else reordering the brackets and the summation to compute the respective adjoints. Especially note that it holds pointwise $g_p(p(x,t),u(x,t))^*m(x,t) \in \mathbb{R}^M$.

Before we proof Theorem 6.5.1 successively in the next two parts of this section, we want to look more closely to the computation of the adjoints of the multiplication operator with the help of a concrete example.

**Example 6.5.3.**

- In the no system / one parameter case, i.e. $M = N = 1$, the operators $g_u(p, u)$ and $g_p(p, u)$ are basically self adjoint (if one pays no attention to the topology).
- Now we consider the embryogenesis example from Section 2.4. Here, the respective derivatives are given via (6.8) and (6.9). Let $s_i := W_{i1}u_1 + \ldots + W_{iN}u_N$. For the parameter part (note that we have $M = 2N + N^2$ in this case), we have by reordering summands

$$\begin{aligned} g_p((\lambda, R, W), u)(\bar{\lambda}, \bar{R}, \bar{W})m &= \sum_{i=1}^{N}\sum_{j=1}^{N}(\bar{\lambda}_i u_i + \bar{R}_i \phi(s_i) + R_i \phi'(s_i)\bar{W}_{ij}u_j)m_i \\ &= \sum_{i=1}^{N} m_i u_i \lambda_i + \sum_{i=1}^{N} m_i \phi(s_i)\bar{R}_i \\ &\quad + \sum_{i=1}^{N}\sum_{j=1}^{N} R_i \phi'(s_i) m_i u_j \bar{W}_{ij}. \end{aligned}$$

So it holds

$$g_p((\lambda, R, W), u)^* m = \begin{pmatrix} m_1 u_1 & \ldots & m_N u_N \\ m_1 \phi(s_i) & \ldots & m_N \phi(s_i) \\ R_1 \phi'(s_i) m_1 u_1 & \ldots & R_1 \phi'(s_i) m_1 u_N \\ \vdots & \ddots & \vdots \\ R_N \phi'(s_i) m_N u_1 & \ldots & R_N \phi'(s_i) m_N u_N \end{pmatrix},$$

where the first row denotes the adjoint with respect to $\lambda$, the second row the adjoint with respect to $R$ and the last $N$ rows the adjoint with respect to $W$. For the multiplication operator with respect to $u$ we find

$$\begin{aligned} g_u((\lambda, R, W), u)v &= \sum_{i=1}^{N}\sum_{j=1}^{N}(\lambda_i u_i + R_i \phi'(s_i) W_{ij} u_j) v_i \\ &= \sum_{j=1}^{N}\sum_{i=1}^{N}(\lambda_i v_i + R_i \phi'(s_i) W_{ij} v_i) u_j, \end{aligned}$$

so we deduce

$$g_u((\lambda, R, W), u)^* v = \begin{pmatrix} \lambda_1 v_1 + R_1 \phi'(s_1) W_{11} v_1 + \ldots + R_N \phi'(s_N) W_{N1} v_N \\ \vdots \\ \lambda_N v_N + R_1 \phi'(s_1) W_{1N} v_1 + \ldots + R_N \phi'(s_N) W_{NN} v_N \end{pmatrix}.$$

### 6.5.1 The adjoint of $(A_u)^{-1}$

In this subsection we derive the adjoint of $(A_u)^{-1}$, which is the more difficult part, since $(A_u)^{-1}$ is only implicitly known. First note, that this part of the computation is more or less independent of the parameter space and therefore can be done in a general fashion. Note that our approach of computing the adjoint as well as proof ideas are inspired by [57]. Since

$$(A_u)^{-1} : Z \times L_s([0,T], \tilde{Y}^*) \to L_2(\Omega_T)^N$$

is bounded the adjoint maps

$$\left((A_u)^{-1}\right)^* : L_2(\Omega_T)^N \to Z^* \times L_{s'}([0,T], \tilde{Y}).$$

Because of the implicit definition of the operator it is not possible to compute its adjoint directly. Instead we take the indirect route via computing the adjoint of the operator $A_u$. First of all note that

$$A_u : \mathcal{W} \subset L_2(\Omega_T)^N \to Z \times L_s([0,T], \tilde{Y}^*)$$

is an unbounded operator. This operator is densely defined because of the inclusions

$$C_0^\infty(\Omega_T)^N \cap \mathcal{W} \subset \mathcal{W} \subset L_2(\Omega_T)^N$$

and the fact that $C_0^\infty(\Omega_T) \subset L_s(\Omega_T)$ is dense with respect to the $L_s$ topology. Therefore, we can still compute an adjoint operator

$$(A_u)^* : Z^* \times L_{s'}([0,T], \tilde{Y}) \to L_2(\Omega_T)^N,$$

which follows from Theorem 3.8.2. Furthermore, the operator $A_u$ is closed. For this take a sequence $\{u_n\} \subset \mathcal{W}$ with $u_n \to u$ in $L_2(\Omega_T)^N$ and $A_u u_n \to v$. Since $A_u^{-1} : L_s([0,T], \tilde{Y}^*) \to L_2(\Omega_T)^N$ is bounded, it follows $u_n \to A_u^{-1} v$ and hence $u \in \mathcal{D}(F)$ with $Au = v$. So we can make use of the fact that for invertible operators that are densely defined, closed and have a dense range, it holds that the inverse of the adjoint is the adjoint of the inverse, see Theorem 3.8.3. Thus we can compute $((A_u)^{-1})^*$ as $((A_u)^*)^{-1}$.

**Lemma 6.5.4.** *The adjoint of the operator $A_u$ is given by*

$$\begin{aligned}(A_u)^* : \mathcal{D}((A_u)^*) \subset Z^* \times L_{s'}([0,T], \tilde{Y}) &\to L_2(\Omega_T)^N \\ (r, w) &\mapsto -w_t - \nabla \cdot D\nabla w + g_u(p,u)^* w,\end{aligned}$$

*with domain*

$$\begin{aligned}\mathcal{D}((A_u)^*) := \big\{ &(r,w) \in Z^* \times L_{s'}([0,T], \tilde{Y}) \mid w \in \mathcal{W}_{2,q},\ \exists z \in L_2(\Omega_T)^N : \\ &\langle (A_u)^* w, v \rangle = \langle z, v \rangle\ \forall v \in \mathcal{W}, w(T) = 0, r = w(0) \big\},\end{aligned}$$

*Proof.* Let $v \in \mathcal{W}$ and $(r, w) \in Z^* \times L_{s'}([0,T], \tilde{Y})$, then it must hold

$$\begin{aligned}
&\langle A_u v, (r,w)\rangle_{(Z\times L_s([0,T],\tilde{Y}^*), Z^*\times L_{s'}([0,T],\tilde{Y}))} \\
&= \int_0^T \langle v' - \nabla\cdot D\nabla v + g_u(u)v, w\rangle_{\tilde{Y}^*,\tilde{Y}}\ dt + \int_\Omega v(0)r\ dx \\
&= \int_0^T \langle v', w\rangle_{(\tilde{Y}^*,\tilde{Y})}\ dt + \int_0^T\int_\Omega D\nabla v\cdot\nabla w + g_u(u)v\cdot w\ dx\ dt + \int_\Omega v(0)r\ dx.
\end{aligned}$$

We can now use Theorem 5.1.5 and get

$$\begin{aligned}
\langle A_u v, (r,w)\rangle = &\int_0^T \langle -w', v\rangle_{(\tilde{Y}^*,\tilde{Y})}\ dt - \int_0^T\int_\Omega D\nabla w\cdot\nabla v + g_u(p,u)^* w\cdot v\ dx\ dt \\
&+ \int_\Omega v(T)w(T)\ dx + \int_\Omega v(0)(r - w(0))\ dx.
\end{aligned}$$

We define an operator (that has to be interpreted in the weak sense)

$$\begin{aligned}
(A_u)^* : \mathcal{D}((A_u)^*) \subset Z^* \times L_{s'}([0,T],\tilde{Y}) &\to L_2(\Omega_T)^N \\
(r,w) &\mapsto -w' - \nabla\cdot D\nabla w + g_u(p,u)^* w
\end{aligned}$$

with domain of definition

$$\begin{aligned}
\mathcal{D}((A_u)^*) := \big\{(r,w) \in Z^* \times L_{s'}([0,T],\tilde{Y}) \mid w \in \mathcal{W},\ \exists z \in L_2(\Omega_T)^N :& \\
\langle (A_u)^* w, v\rangle = \langle z, v\rangle\ \forall v \in \mathcal{W}, w(T) = 0, r = w(0)\big\}&.
\end{aligned}$$

By our assumptions $\mathcal{D}((A_u)^*)$ is nonempty, because the equation

$$-w' - \nabla\cdot D\nabla w + g_u(p,u)^* w = z, \qquad w(T) = 0 \tag{6.12}$$

has a unique weak solution in the solution space $\mathcal{W}$ for any $z \in L_2(\Omega_T)^N$. This is a direct consequence of the solution theory, the embedding $L_2(\Omega_T)^N \hookrightarrow L_2([0,T],\tilde{Y}^*)$ and the fact that $g_u(p,u)^*$ is sufficiently regular by Assumption 6.3.1. Since $\mathcal{W}_{2,q} \hookrightarrow C([0,T], L_q(\Omega)^N)$, the point evaluation $r = w(0)$ is possible as well. It follows

$$\begin{aligned}
\langle A_u v, (r,w)\rangle = &\int_0^T \langle -w', v\rangle_{\tilde{Y}^*,\tilde{Y}}\ dt - \int_0^T\int_\Omega D\nabla w\cdot\nabla v + g_u(p,u)^* w\cdot v\ dx\ dt \\
&+ \int_\Omega v(T)w(T)\ dx + \int_\Omega v(0)(r - w(0))\ dx \\
= &\langle (A_u)^* w, v\rangle_{(L_2(\Omega_T)^N, L_2(\Omega_T)^N)}
\end{aligned}$$

From this computation it is obvious, that the restrictions $r = w(0)$ and $w(T) = 0$ are necessary. Since the equation (6.12) has a unique solution in $\mathcal{W}_{2,q}$ for all $f \in L_2(\Omega_T)^N$, so that any domain, where $(A_u)^*$ can be defined is already part of $\mathcal{D}((A_u)^*)$. Hence, by Theorem 3.8.2 $(A_u)^*$ is the adjoint of $A_u$. □

Now we can compute the adjoint of $(A_u)^{-1}$:

**Corollary 6.5.5.** *The adjoint of $(A_u)^{-1}$ is given by the operator*

$$\begin{aligned} ((A_u)^{-1})^* : L_2(\Omega_T)^N &\to Z^* \times L_{s'}([0,T], \tilde{Y}) \\ z &\mapsto (w(0), w), \end{aligned}$$

*where $w$ is the unique weak solution of the differential equation*

$$-w' - \nabla \cdot D\nabla w + g_u(p,u)^* w = z, \qquad w(T) = 0.$$

*Proof.* By Theorem 3.8.3 we can compute $((A_u)^{-1})^*$ as $((A_u)^*)^{-1}$, which directly proves the claim. □

We can derive the following regularity result for the adjoint:

**Lemma 6.5.6.** *Let $g_u(p,u)^*$ be sufficiently regular and assume that $z \in L_s([0,T])^N$ with $s > 2$ then $(A_u)^{-1})^* z \in \mathcal{W}_{s,q}$.*

*Proof.* Under sufficient regularity assumptions on $g_u(p,u)^*$ and $z$, the adjoint equation has a solution in $\mathcal{W}_{s,q}$ by Theorem 5.1.16. The claim follows with $\mathcal{W}_{s,q} \hookrightarrow \mathcal{W}_{2,q}$ and by uniqueness of the solution. □

### 6.5.2 The adjoint of $A_p$

In this section we will compute the adjoint of the operator $A_p$. The computation of the adjoint of this operator itself is indeed very simple, because it is just a multiplication operator. We only have to ensure that the adjoint maps between the right spaces:

**Lemma 6.5.7.** *The adjoint of $A_p$ is given by*

$$\begin{aligned} (A_p)^* : Z^* \times L_{s'}([0,T], \tilde{Y}) &\to \mathcal{P} \\ (z,h) &\mapsto g_p(p,u)^* h. \end{aligned}$$

*Proof.* It holds

$$\begin{aligned} &\langle A_p(p,u)h, v\rangle_{(L_s([0,T],\tilde{Y}^*)\times Z, L_{s'}([0,T],\tilde{Y})\times Z^*))} \\ =&\langle g_p(p,u)v, w\rangle_{((L_s([0,T],\tilde{Y}^*), L_{s'}([0,T],\tilde{Y}))} + 0 \\ =&\langle g_p(p,u)^* w, v\rangle_{(\mathcal{P}^*,\mathcal{P})}, \end{aligned}$$

where the last equality follows directly from the fact that the derivative of the superposition operator is a linear operator that maps $\mathcal{P} \to L_s([0,T], \tilde{Y}^*)$ and thus its adjoint maps from $L_{s'}([0,T], \tilde{Y}) \to \mathcal{P}^*$. □

## 6.6 Application of gradient descent methods

In the previous section, we derived an expression for the adjoint of the derivative. Formally, the adjoint of the derivative is just an element of the dual pace of an $L_r$ space. As explained in Remark 6.3.10 the choice $r = 2$ is not always possible. In fact has to assume $r > 2$ if $g$ is truly nonlinear to ensure differentiability of the parameter to state map. Hence, by $r > 2$ the dual of $L_r$ is $L_{r'}$ with $r' < 2$. In this case, it might be difficult to show convergence of the minimization algorithms discussed in Section 4.2.2 and thus one may have to fall back to minimization schemes between Banach spaces or other minimization algorithms that are not directly depending on continuity properties of the derivative. Also the quadratic expansion approach that we discussed in Section 4.2.2 to speed up the minimization of the Tikhonov functional is not directly applicable in this case, since $\mathcal{P}$ is not a Hilbert space. But in our case we have more information, namely regularity for the solution of the adjoint equation from Lemma 6.5.6 as well as a restricted domain of definition for $F$. This allows us to justify the Hilbert space $L_2$ as parameter space for the problem, since we are only working with strong derivatives and all involved functions have enough regularity to still make this approach work, even though differentiability of the forward operator possibly can only be established with respect to the $L_r$ topology, where $r > 2$.

We make the following assumptions:

**Assumption 6.6.1.**

*(i)* *The forward operator $F$ is Lipschitz continuous with respect to the topology of $\mathcal{P} = L_r(\Omega_T)^M$,*

*(ii)* $u^\delta \in L_\infty(\Omega_T)^N$,

*(iii)* *It holds for $p_1, p_2 \in \mathcal{P}$*

$$\|g_p(p_1, \cdot)^* - g_p(p_2, \cdot)^*\|_{L_{r'}} \leq C_p \|p_1 - p_2\|_{L_r}$$

*and for $u_1, u_2 \in \mathcal{W}$*

$$\|g_p(\cdot, u_1)^* - g_p(\cdot, u_2)^*\|_{L_{r'}} \leq C_u \|u_1 - u_2\|_{\mathcal{W}},$$

*i.e. $g_p$ is Lipschitz-continuous in both arguments.*

*(iv)* *It holds for $1 - 2/s - d/q > 0$, $g_u(p, u)^*$ fulfills* (5.14) *and the adjoint equation $w \mapsto v(w)$ fulfills an energy estimate of the form*

$$\|v\|_{\mathcal{W}} \leq C_v \|w\|_{L_2([0,T], \tilde{Y}^*)}.$$

**Remark 6.6.2.** To show that the forward operator $F$ is Lipschitz-continuous is a difficult task and has to be done individually in dependence of $g$. If it can be shown, that the derivatives $g_p(p, u)$ and $g_u(p, u)$ are uniformly bounded on $\mathcal{P}$, then one can easily show, that $F' : \mathcal{P} \to L(\mathcal{P}, L_2(\Omega_T)^N)$ is uniformly bounded with the help of an energy estimate for the differential equation that describes the derivative (cf. [58, Lemma 3.4]). Lipschitz continuity of $F$ then follows from the Mean Value Theorem (cf. [58, Lemma 3.5]).

Now we can show Lipschitz continuity of the derivative of the Tikhonov functional (at least with respect to the topology of $\mathcal{P}$):

**Theorem 6.6.3.** *Let Assumption 6.3.1 and Assumption 6.6.1 hold and $1-2/s-1/q>0$. Then the derivative $\tilde{F}'$ of the discrepancy term $\tilde{F} := \|F(p)-u^\delta\|^2$*

$$\begin{aligned}\tilde{F}'(p) : \mathcal{P} &\to L(\mathcal{P}, \mathbb{R})\\ p &\mapsto F'(p)^*(F(p)-u^\delta)\end{aligned}$$

*is Lipschitz continuous with respect to the topology of $\mathcal{P}$.*

*Proof.* Let $u_1 = F(p_1)$ and $u_2 = F(p_2)$. By the restriction of the domain and the Lipschitz-continuity of $u$ there exists $\tilde{C} > 0$ such that

$$\|u(p)\|_{\mathcal{W}} \leq \tilde{C}$$

uniformly for all $p \in \mathcal{D}(F)$. Further it holds

$$\begin{aligned}&\|g(p_1,u_1)^* - g(p_2,u_2)^*\|\\ \leq&\|g(p_1,u_1)^* - g(p_2,u_1)^*\| + \|g(p_2,u_1)^* - g(p_2,u_2)\|\\ \leq&C_p\|p_1-p_2\|_{L_r} + C_u\|u_1-u_2\|_{\mathcal{W}})\\ \leq&C_g(\|p_1-p_2\|_{\mathcal{P}})\end{aligned}$$

where the last inequality follows with the Lipschitz-continuity of $F$. Hence, again by the restriction of the domain, there exists $\hat{C}$ with

$$\|g_p(p,u(p)\|_{L_{r'}} \leq \hat{C}$$

uniformly for all $p \in \mathcal{D}(F)$. Finally we estimate (with the help of Proposition 3.4.4 and Proposition 3.1.9 and the fact that the adjoint equation is linear)

$$\begin{aligned}\tilde{F}'(p_1)h - \tilde{F}'(p_2)h &= \langle F'(p_1)^*(u_1-u^\delta) - F'(p_2)^*(u_2-u^\delta), h\rangle_{(\mathcal{P}^*,\mathcal{P})}\\ &\leq \|F'(p_1)^*(u_1-u^\delta) - F'(p_2)^*(u_2-u^\delta)\|_{L_{r'}}\|h\|_{L_r}\\ &= \big\|g_p\big(p_1,u_1\big)^* v\big(u_1-u^\delta\big) - g_p\big(p_2,u_2\big)^* v\big(u_2-u^\delta\big)\big\|_{L_{r'}}\|h\|_{L_r}\\ &= \|g_p\big(p_1,u_1\big)^*\big[v(u_1-u_2)\big)\big]\\ &\qquad + \big[g_p\big(p_1,u_1\big)^* - g_p\big(p_2,u_2\big)^*\big)\big]\big(v(u_2-u^\delta)\big)\big\|_{L_{r'}}\|h\|_{L_r}\\ &\leq \|g_p\big(p_1,u_1\big)^*\|_{L_{r'}}\|v(u_1-u_2)\|_{L_\infty}\\ &\qquad + \|g_p\big(p_1,u_1\big)^* - g_p\big(p_2,u_2\big)^*\|_{L_{r'}}\|v(u_2-u^\delta)\|_{L_\infty}\\ &\leq (\hat{C}\|v(u_1-u_2)\|_{\mathcal{W}} + \tilde{C}C_g\|p_1-p_2\|_{\mathcal{P}})\|h\|_{L_r}\\ &\leq C\|p_1-p_2\|_{\mathcal{P}}\|h\|_{L_r}\end{aligned}$$

So the Lipschitz continuity is established. □

**Remark 6.6.4.** It is in fact much easier to derive Lipschitz continuity of the derivative of the Tikhonov-functional than of the derivative of the forward operator, if one already knows that $F$ is Lipschitz continuous. The reason for this is that we can directly use the a priori energy estimate for the solution of the adjoint equation and do not have to care about further occurences of parameters in this equation. Nevertheless, a Lipschitz-estimate for the derivative of the forward operator is also possible under the right conditions on $g$ and can be derived as in [58, Chapter 3.4].

**Remark 6.6.5.** The fact that we only get a Lipschitz estimate with respect to the $L_r$-topology does barely influence the applicability of Theorem 4.2.27. The reason for this is that we only work on the set $\mathcal{D}(F)$ instead of the whole space. On this subset convergence with respect to $L_r$ is equivalent to convergence with respect $L_2$, which follows from the Dominated Convergence Theorem. Also, the minimizer of the Tikhonov-functional is not dependent on the exponent $r \geq 2$. As one can easily deduce from the proof of the convergence result in the original paper [47], a Lipschitz result with respect to the $L_r$ topology is enough to ensure the convergence of the quadratic approximation method under these circumstances if it can be ensured that the iteration generated by Algorithm 4.2.24 stays in $\mathcal{D}(F)$.

Finally we need to show, that the derivative of the Tikhonov functional is $\tau$-strongly closed.

**Theorem 6.6.6.** *Let Assumption 5.1.13, Assumption 6.2.1 and Assumption 6.6.1 hold. For $p_n \xrightarrow{\tau} p$ in $\tilde{\mathcal{P}} \subset \mathcal{P}, u_n \rightharpoonup u$ in $\mathcal{W}$ assume that $g_p(p_n, u_n)^* \rightharpoonup g_p(p, u)^*$ in $\mathcal{P}^*$. Then*

$$F'(p_n)^*(F(p_n) - u^\delta) \rightharpoonup F'(p)^*(F(p) - u^\delta)$$

*in $\mathcal{P}^*$. Additionally, if $g_p(p_n, u_n)^* \to g_p(p, u)^*$ in $\mathcal{P}^*$, then*

$$F'(p_n)^*(F(p_n) - u^\delta) \to F'(p)^*(F(p) - u^\delta).$$

*Proof.* Let $p_n \stackrel{\tau}{\rightharpoonup} p$ in $\tilde{\mathcal{P}}$. Since $F$ is $\tau$-strongly closed, it holds $u(p_n) \to u$ in $L_2(\Omega_T)^N$. Thus

$$\begin{aligned}\|v(F(p_n) - u^\delta)) - v(F(p) - u^\delta)\|_{\mathcal{W}} &= \|v(F(p_n) - F(p))\|_{\mathcal{W}} \\ &\leq C\|F(p_n) - F(p)\|_{L_2(\Omega_T)} \\ &\to 0 \text{ as } n \to \infty.\end{aligned}$$

In the next two estimates, let $v_n := v(F(p_n) - u^\delta)$ and $v := v(F(p) - u^\delta)$, so that we get

$$\begin{aligned}&|\langle F'(p_n)^*(F(p_n) - u^\delta) - F'(p)^*(F(p) - u^\delta), w\rangle_{(\mathcal{P}^*,\mathcal{P})}| \\ =&|\langle g_p(p_n, u_n)^* v_n - g_p(p, u)^* v, w\rangle| \\ =&|\langle g_p(p_n, u_n)^* - g_p(p, u)^*, wv\rangle| \\ &\quad + C\|v_n - v\|_{\mathcal{W}}\|g_p(p_n, u_n)^*\|_{\mathcal{P}^*} \\ &\to 0 \text{ as } n \to \infty,\end{aligned}$$

where we utilized $\mathcal{P} = L_r(\Omega)^N$, $v(F(p) - u^\delta) \in L_\infty([0,T], L_\infty(\Omega)^N)$ and the uniform boundness from the sequence $\{g_p(p_n, u_n)^*\}$ that follows from the Banach-Steinhaus Theorem. If $g_p(p_n, u_n)^* \to g_p(p,u)^*$ in $\mathcal{P}^*$ we can estimate in similar fashion

$$\begin{aligned}
&\|F'(p_n)^*(F(p_n) - u^\delta) - F'(p)^*(F(p) - u^\delta)\|_{\mathcal{P}^*} \\
=&\|g_p(p_n, u_n)^* v_n - g_p(p,u)^* v\|_{\mathcal{P}^*} \\
\leq&\|(g_p(p_n, u_n)^* - g_p(p,u)^*)v_n\|_{\mathcal{P}^*} + \|g_p(p,u)^*(v_n - v))\|_{\mathcal{P}^*} \\
\leq&C\|v_n\|_{\mathcal{W}}\|(g_p(p_n, u_n)^* - g_p(p,u)^*)\|_{\mathcal{P}^*} + C\|g_p(p,u)^*\|_{\mathcal{P}^*}\|v_n - v)\|_{\mathcal{W}} \\
\leq&C(\|(g_p(p_n, u_n)^* - g_p(p,u)^*)\|_{\mathcal{P}^*} + \|v_n - v\|_{\mathcal{W}}) \\
&\quad \to 0 \text{ as } n \to \infty,
\end{aligned}$$

which proves the claim. □

**Remark 6.6.7.** Items *(ii)* and *(iii)* of Assumption 6.6.1 as well as the restriction $1 - 2/s - d/q > 0$ are not needed in the linear case if $r = s = 2$, since $\tau$-strong-closedness of $u$ together with Lipschitz-continuity already yield the claim.

**Remark 6.6.8.** Another needed condition in Theorem 4.2.27 is that the iteration stays in $\mathcal{D}(F)$, which in the case of a truly nonlinear function could be a bounded subset of the space $BV(\Omega_T) \cap L_\infty(\Omega)$ restricted functions that satisfy an almost everywhere bound. In all of the situations explained in Section 6.4, if we start the algorithm with a smooth parameter $p_0 \in \mathcal{D}(F)$ and assume that that the data is $L_\infty$, we will at least have that the gradient $F'(p_0)^*(F(p_0) - u^\delta)$ is a continuous function in the case $1-2/s-1/q > 0$ (or a reasonably smooth function in the case $q = 2$), because $g_p(p_0, u)^* v(w)$ is just a sum of products of continuous functions. Depending on the penalty, the sequence $\{p_n\}$ generated by Algorithm 4.2.24 is then sequence of continuous functions that converge with respect to the $L_r$ norm to an $L_\infty$ function, which indicates that at least an arbitrary almost everywhere bound should be fulfilled for this sequence. Also, since all of the ongoing processes are rather smooth, one can most likely expect this sequence to stay in $BV(\Omega_T)$ as well.

## 6.7 Restricted measurements

As mentioned before, in practical applications, one does not have access to measurements on the whole set $\Omega_T$ but only on a subset of this set. In this section, we consider three types of measurements, which seem to make sense in the biological context of our key applications and should give a good insight into the problem of restricted measurements. For this section we consider

- measurements on an interior subset of positive measure,
- measurements of Dirichlet data on the boundary,

- measurements at certain timesteps, so called snapshots.

In all these cases, the measurement operator $O$ turns out to be a linear and bounded operator between function spaces. So all (weak) continuity and differentiability properties directly carry over to the operator $\tilde{F} := O \circ F$. For computing the gradient of the Tikhonov functional, we thus only have to compute the adjoint of the observation operator and how its concatenation with the adjoint of $F'$ interacts. Of course, there are a lot more possibilities for measurements. For example in [16] measurements at a single point over time are considered for the equation from Section 2.3.

### 6.7.1 Measurements on an interior subset of positive measure

This is probably the easiest case of measurements to occur. So let $\Omega_{T_1} \subset \Omega_T$ be of positive measure. Then we can define the measurement operator via

$$\begin{aligned} O : L_2(\Omega_T) &\to L_2(\Omega_{T_1}) \\ u &\mapsto u_{|\Omega_{T_1}}. \end{aligned}$$

It can easily be seen that the adjoint of $O$ is the operator

$$\begin{aligned} O^* : L_2(\Omega_{T_1}) &\to L_2(\Omega_T) \\ v(x,t) &\mapsto \begin{cases} v(x,t) & \text{on } \Omega_{T_1}, \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

since it clearly holds

$$\int\limits_{\Omega_{T_1}} u_{|\Omega_{T_1}} v \; d(x,t) = \int\limits_{\Omega_T} u O^* v \; d(x,t) \qquad \forall v \in L_2(\Omega_{T_1}).$$

### 6.7.2 Measurements of Dirichlet data on the boundary

In this case we do not assume zero boundary values, but instead the Dirichlet boundary condition

$$u = b \text{ on } \partial\Omega \times [0,T].$$

In this case, we can utilize the measurement operator:

$$\begin{aligned} O : L_2([0,T], H_0^{1,2}(\Omega)^N) &\to L_2([0,T], L_2(\partial\Omega)^N), \\ u &\mapsto u_{|\partial\Omega}. \end{aligned}$$

which certainly can be applied to every $u \in \mathcal{W}$. The operator $O$ is linear and bounded, which follows immediately from the definition of the trace operator for

Sobolev functions [19, Satz 6.15] and Proposition 3.1.9. Note that if we want to compute an adjoint of this operator, it is only located in $L_2([0,T], H^{-1}(\Omega)^N)$ so we cannot directly apply the adjoint of $F'$ to $O^*$. Nevertheless, an explicit expression for the adjoint of the combined operator $((\mathcal{A}_u)^{-1})^* \circ O^* w$ can be derived analogously to the computations from Section 6.5 and is given via $(v(0), v)$, where $v$ is the solution of the partial differential equation

$$\begin{aligned} -v_t - \nabla \cdot D \nabla v + g_u(p,u)v &= 0 && \text{in } \Omega_T \\ v &= w && \text{on } \partial\Omega \times [0,T] \\ v(x,T) &= 0 && \text{on } \Omega \times \{T\} \end{aligned}$$

### 6.7.3 Measurements at certain points in time

This case is rather difficult and not as easy as the ones before. Here, we have the measurement operator

$$\begin{aligned} O : C([0,T], L_2(\Omega)^N) &\to L_2(\Omega)^{N \times K} \\ u &\mapsto (u(t_1), ..., u(t_K)). \end{aligned}$$

This operator is obviously bounded and linear, but it is not a bounded operator from $L_2(\Omega_T)^N \to L_2(\Omega)^{N\times K}$ and even though it is densely defined, the explicit computation of an adjoint in the $L_2$ sense fails, since the operator $O$ is not closed. So we have to compute an adjoint for the bounded linear operator mapping into the dual space of continuous functions and thus its adjoint is only an atomic measure. The computation of the adjoint itself is rather easy, and it turns out to be the well known Dirac-Delta Function (with respect to the time axis). A detailed discussion of such a situation can be found in [57]. In this case one splits the adjoint equation (6.10) into several partial differential equations of the form

$$-(v^{(k)})_t - \nabla \cdot D \nabla v^{(k)} + g_u(p,u) v^{(k)} = \begin{cases} v^{(k+1)} + w^{(k)} & k < K, \\ w(K) & k = K. \end{cases}$$

If we extend each function $v^{(k)}$ with zero, so that it is defined on the whole interval $[0,T]$, we can define

$$v(w) = \sum_{k=1}^{K} v^{(k)}(w(k))$$

and then express the adjoint of the combined operator via

$$((\mathcal{A}_u)^{-1})^* \circ O^* = v(w).$$

A much easier approach is just to assume that we do have a little bit more information, so instead of point evaluations as measurement, we could assume to have measurements at a small interval around these as proposed in [57]. In this case we are back in the situation of Section 6.7.1.

A third way to deal with this data would just be to interpolate the data on the time axis, so that we get an approximation $u^{\delta_2}$ of $u^\delta$ in $\Omega_T$. So, in this case one just adds additional noise to the data. Since $u$ is continuous, and assuming the variance of the noise is not to high, we would get a reasonably good approximation of $u^\delta$, if the number of measurements $K$ is big enough. The drawback is of course that the noiselevel $\delta_2$ is unknown, even if $\delta$ can be estimated.

## 6.8 Source conditions and restriction of nonlinearity for semilinear reaction-diffusion equations

Since we have derived the adjoint of the derivative, we now can discuss how source conditions can be interpreted for a parabolic parameter identification problem. The approach we are using is inspired by a similar approach for linear elliptic equations proposed in [22, 24]. We will see that a similar result as in [22, 24] also holds for our parameter identification problem defined through (6.1). That means that the fulfillment of a source condition mainly depends on smoothness of the true solution and its boundary and initial conditions. In the system case, also the structure of the system itself is important. Moreover an interesting relation between controllability of the adjoint equation (6.10) and approximate source conditions is highlighted in this section.

### 6.8.1 An interpretation of the source condition

If we directly write down the source condition (note that we can do this independently of topologies), we get

$$\exists w \in L_2(\Omega_T)^N : \; F'(p^\dagger)^* w = g_p(p^\dagger, u(p^\dagger))^* v(w) \in \partial R(p^\dagger). \tag{6.13}$$

The goal is to find conditions under which such a $w$ exists. First we take a look at the scalar case, where only one parameter has to be identified, i.e. $N = M = 1$. In this case (6.13) becomes

$$v(w) g_p(p^\dagger, u(p^\dagger)) \in \partial R(p^\dagger), \tag{6.14}$$

where we use that $g_p(p^\dagger, u(p^\dagger)) = g_p(p^\dagger, u(p^\dagger))^*$ in the scalar case. From (6.14) it follows that there exists a $\xi \in \partial R(p^\dagger)$ with

$$\xi = v(w) g_p(p^\dagger, u(p^\dagger)).$$

We can formally divide by $g_p(p^\dagger, u(p^\dagger)$ and get

$$\begin{aligned} & \frac{\xi}{g_p(p^\dagger, u(p^\dagger))} = v(w) \\ \iff \quad & \frac{\xi}{g_p(p^\dagger, u(p^\dagger))} = ((A_u)^{-1})^* w \\ \iff \quad & (A_u)^* \left( \frac{\xi}{g_p(p^\dagger, u(p^\dagger))} \right) = w. \end{aligned} \tag{6.15}$$

We arrive at the abstract condition

$$z := \frac{\xi}{g_p(p^\dagger, u(p^\dagger))} \in \mathcal{D}((A_u)^*), \tag{6.16}$$

which basically reduces to

$$z \in \mathcal{W}, \qquad z(T) = 0.$$

Two cases that we previously highlighted for the penalty term are $R(p) = \frac{1}{2}\|p - p^*\|^2$ and $R(p) = \|p - p^*\|_{\ell_1}$. We first consider the squared norm penalty. Condition (6.16) then becomes

$$z := \frac{p^\dagger - p^*}{g_p(p^\dagger, u(p^\dagger))} \in \mathcal{W}, \qquad z(T) = 0.$$

The condition $z \in \mathcal{W}$ implies that the function $z$ has to be at least continuous in time and weakly differentiable in space. This means especially that $z$ has to be an $L_\infty$ function, if we assume $1-2/s-d/q > 2$ and thus, if $g_p(p^\dagger(x,t), u(p^\dagger)(x,t)) = 0$ at a point $(x,t)$, the estimate $p^*$ has to be exact at this point (and possibly even in small neighbourhood of $(x,t)$). The same goes for the case if the function $z$ does not fulfill the needed smoothness conditions. Special attention has to be paid to the final and boundary conditions. The final condition immediately implies that the estimate $p^*$ at the point $T$ has to be exact on the whole domain $\Omega$. If either Dirichlet or Neumann boundary conditions are involved, we have either

$$u(x,t) = 0 \text{ or } \frac{\partial}{\partial \nu} u(x,t) = 0 \text{ on } \partial\Omega.$$

These properties of $u$ usually (but not necessarily) imply that

$$g_p(p(x,t), u(x,t)) = 0 \text{ or } \frac{\partial}{\partial \nu} g_p(p(x,t), u(x,t)) = 0 \text{ on } \partial\Omega.$$

Since the adjoint equation (6.10) fulfills the same boundary conditions as the original equation, an exact estimate of $p^\dagger$ is thus not enough at this point, since we do not only need that $z$ is continuous at these points but we have also to enforce a special value, i.e.

$$z(x,t) = 0 \text{ or } \frac{\partial}{\partial \nu} z(x,t) = 0 \text{ on } \partial\Omega.$$

Hence, in this case we need to find an exact estimate of $p^\dagger$ (or its derivatives) in a reasonably big neighbourhood of $\partial\Omega$.

**Example 6.8.1.** First we consider the easiest case, namely $g(p,u) = pu$ as well as Dirichlet boundary conditions. Further let us assume that $p$ is smooth in $\Omega_T$ and $u > 0$. Then identity (6.16) becomes

$$\frac{p^\dagger(x,t) - p^*(x,t)}{u(p^\dagger)(x,t)} \in \mathcal{W},$$

thus by assumption the knowledge of $p^\dagger$ in a small environment of the boundary as well as the knowledge of $p^\dagger$ at time $T$ is enough to ensure a source condition. Especially no further information on the source representer $w$ is needed. If we consider the embryogenesis example from Section 2.4 and restrict us to the parameter $W$ (so that we have $M = 1$ and $N = 1$) the identity (6.16) now becomes

$$\frac{W^\dagger - W^*}{R\phi'(W^\dagger u(W^\dagger))u(W^\dagger)} \in \mathcal{W}.$$

We can see that the parameter $W^\dagger$ appears in the denominator as an argument of $\phi$ as well as the parameter $R$. Again, if $W^\dagger$ is assumed to be smooth in the interior, $R > 0$ and $u > 0$, we can deduce a source condition under the same assumptions as before (note the $\phi'(W^\dagger(x,t)u(x,t))$ is differentiable by the chain rule for Sobolev functions [19, Lemma 5.14] and the fact that $\phi$ is a $C^\infty(\mathbb{R})$ function [57, Appendix 8.1]).

In the case of sparsity constraints, we can derive a similar result, the source condition now becomes

$$\exists \xi \in \sum_{i\in\mathbb{N}} \operatorname{Sgn}(\langle \varphi_i, p - p^* \rangle)\varphi_i : \qquad \xi = v(w) g_p(p^\dagger, u(p^\dagger))^*,$$

so we can perform the same computations as in the squared case and arrive at

$$z := \frac{\xi}{g_p(p^\dagger, u(p^\dagger))} \in \mathcal{W}, \qquad z(T) = 0.$$

In this situation however, we cannot control the smoothness of $z$ with the help of an a priori estimate. Instead one has to find a basis $\{\varphi_i\}$ such that $p^\dagger$ is sparse in this basis and $z \in \mathcal{W}$ fulfills $z(T) = 0$ and the respective boundary conditions.

**Remark 6.8.2.** We can conclude a source condition enforces strong restrictions onto the parameters. In the squared norm case, we need to basically know the true solution in a neighbourhood of all points, where it is non smooth. Additional information of the values of the true solution on the boundary and at the final point of the experiment is needed as well. In usual practical applications, none of this information is available. In the sparsity case, a basis has to be found in which the true solution is sparse. Furthermore the basis itself has to possess certain smoothness properties. While in applications, the true solution can often be assumed as sparse in a certain basis, this basis will usually not have the exact smoothness properties that are needed for a source condition to hold.

In the system case the interpretation of a source condition becomes more difficult. The reason for this is that the adjoint equation itself is a coupled system and we possibly have a different number of parameters and solutions. So we remind the reader, that we have three cases $M < N$, more equations than parameters, $M = N$ equal number of parameters and $M > N$, more parameters than equations. If we write down the source condition in the system case, we get

$$\exists \xi \in \partial R(p^\dagger): \ \xi_j = (g_p(p,u)^* v)_j, \quad j = 1, \ldots, M,$$

that is in particular (see (6.11))

$$\xi_j = \sum_{k=1}^{N} (g_{p_k}(p,u) v_k(w))_j. \tag{6.17}$$

If we further assume

$$g(p,u) = \begin{pmatrix} g_1(p_{11}, \ldots p_{1M_1}, u) \\ \vdots \\ g(p_{N1}, \ldots, p_{NM_N}, u) \end{pmatrix}, \qquad M_1, \ldots, M_N \geq 0,$$

equation (6.17) can be rewritten to

$$\xi_{ij} = (g_i)_{p_{ij}}(p,u) v_i(w), \qquad j = 1, \ldots, M_i.$$

This especially means that it holds pointwise

$$\sum_{j=1}^{M_i} \xi_{ij} = \underbrace{\left( \sum_{j=1}^{M_i} (g_i)_{p_{ij}} \right)}_{=:B_i} v_i(w) \tag{6.18}$$

and if we formally assume $B_i \neq 0$, we get

$$v_i(w) = \begin{cases} \frac{1}{B_i} \sum\limits_{i=1}^{M_i} \xi_{ij}, & M_i \neq 0, \\ 0 & M_i = 0. \end{cases} \tag{6.19}$$

Thus, a $w$ as in (6.19) exists, if

$$z := \begin{pmatrix} \frac{1}{B_1} \sum\limits_{i=1}^{M_1} \xi_{1j} \\ \vdots \\ \frac{1}{B_N} \sum\limits_{i=1}^{M_N} \xi_{Nj} \end{pmatrix} \in \mathcal{D}((A_u)^*).$$

A discussion on necessary conditions for $z$ can now be done as in the scalar case. If a sufficiently function $h$ exists, where each component of $h$ can be split in functions $\xi_{ij}$, such that $\xi \in \partial R(p^\dagger)$ and $(1/B_1h_1, ..., 1/B_Nh_n) \in \mathcal{D}((A_u)^*)$ then a source condition is fulfilled. Note that if the number of parameters $M$ is greater than the number of solutions $N$ this condition reflects the overdetermination of the system.

**Remark 6.8.3.** Equation (6.19) defines an operator

$$\tilde{B} : \mathbb{R}^M \to \mathbb{R}^N,$$
$$\xi_{ij}(x,t) \mapsto \begin{cases} \frac{1}{B_i}(x,t) \sum_{i=1}^{M_i} \xi_{ij}(x,t) & M_i > 0 \\ 0 & M_i = 0, \end{cases} \tag{6.20}$$

which will be used in the next section.

## 6.8.2 Approximate source conditions

In the section before we found that it is rather unlikely that a source condition can be fulfilled, especially for problems that are motivated by real world applications, since the exact knowledge of boundary and final values as well as smoothness for the true solution $p^\dagger$ is highly unrealistic. Approximate source conditions as introduced in Section 4.2 are way more likely to hold. Note that approximated source conditions are automatically fulfilled if the derivative $F'(p^\dagger)$ is injective (see [34, Remark 4.2]). But injectivity of the derivative of the forward operator cannot be guaranteed in our case. A slightly different assumption than injectivity of $F'(p^\dagger)$ can be given through approximate controllability of the adjoint equation by the right hand side (which is a property that at least can be shown for scalar semilinear equations, see [26]). With this, an approximate source condition can be verified under the assumption $A^{-1}\xi \in L_\infty(\Omega_T)$, where $\xi \in \partial R(p^\dagger)$. Smoothness assumptions on $p^\dagger$ can be dropped in this case. Note that this can and most likely will still mean that boundary and final conditions as well as zeros of this function have to be known exactly if we assume a quadratic penalty or that the solution has to be sparse and the basis functions have to be chosen accordingly in the case of sparsity constraints, depending on the shape of the function $A^{-1}(\xi)$.

**Theorem 6.8.4.** *Let the penalty $R$ be as in Assumption 4.2.2 and $\tilde{B}$ be as in* (6.20)*. Assume there exists $\xi \in \partial R(p^\dagger)$ with $\tilde{B}\xi \in L_\infty(\Omega_T)$ and let the adjoint equation* (6.10) *be approximately controllable by the right hand side. Then $p^\dagger$ fulfills an approximate source condition with respect to $R$.*

*Proof.* To verify an approximate source condition we have to secure, that the distance function $d$ in (4.6) decays to zero as $r \to \infty$. This is for example fulfilled, if for any $\varepsilon > 0$, we can find $w \in L_2(\Omega_T)$, such that

$$\|\xi - g_p(p^\dagger, u(p^\dagger))^* v(w)\|_{L_2} \le \varepsilon$$

or equivalently

$$\|\tilde{B}\xi - v(w)\|_{L_2} \leq \varepsilon.$$

Since $\mathcal{D}((A_u)^*)$ is dense in $L_2(\Omega_T)$ and $\tilde{B}\xi \in L_2(\Omega_T)$, for every $\varepsilon > 0$ we can find a function $\tilde{v}$, such that $\|\tilde{B}\xi - \tilde{v}\| \leq \varepsilon/2$. Further, since the adjoint equation is approximately controllable by the right hand side, we can find a $w$, such that $\|v(w) - \tilde{v}\|_{L_2} \leq \varepsilon/2$, so in total $\|\tilde{B}\xi - v(w)\|_{L_2} \leq \varepsilon$. Hence, an approximate source condition holds. □

In the situation of Theorem 6.8.4 the distance function $d$ is not known explicitly, so even though we get a convergence rate in terms of $d$, we cannot state how slow or fast this convergence is. In the case of $L_2$ functions that are approximated by smooth functions the convergence is usually very slow, so the knowledge of a fulfilled approximate source condition does most likely not give a huge advantage over the convergence induced by Theorem 4.2.6.

### 6.8.3 Nonlinearity conditions and smallness assumptions

Nonlinearity conditions are a property on the operator itself. In Chapter 4.2, we have introduced two different nonlinearity conditions (and a combination of those): One that relates the nonlinearity to the Bregman distance

$$\|F(p) - F(p^\dagger) - F'(p^\dagger)(p - p^\dagger)\| \leq \gamma d_\xi(p, p^\dagger), \tag{6.21}$$

and another condition that restricts the nonlinearity purely in the operator domain

$$\|F(p) - F(p^\dagger) - F'(p^\dagger)(p - p^\dagger)\| \leq c\|F(p) - F(p^\dagger)\|. \tag{6.22}$$

For many problems, the first condition is much more accessible, when it comes to source conditions. To see this, we look at the following example.

**Example 6.8.5.** Let the penalty be the classical squared Hilbert space norm of $X$. Then condition (6.21) follows directly from Lipschitz continuity of the derivative of $p$. On the other hand, if $F$ itself is (locally) Lipschitz-continuous (which is not a strong assumption as for example continuously differentiable functions are at least locally Lipschitz continuous), condition (6.22) implies (6.21). However, to verify the assumptions of Theorem 4.2.9, we would simultaneously have to estimate the constant $\gamma$ and the norm of the function $w$, if a source condition does hold to prove a possible convergence rate. If we write this down for our parameter identification problem in the case $N = M = 1$, we get by (6.15)

$$(A_u)^* \left( \frac{p^\dagger - p^*}{g_p(p^\dagger, u(p^\dagger))} \right) = w,$$

so theoretically, if the estimate $p^*$ on $p^\dagger$ is good enough (by the fact that $(A_u)^*$ is bounded on $\mathcal{D}((A_u)^*)$), the smallness condition can be fulfilled. Again, since $p^\dagger$ is unknown in practice, it is not likely to find an estimate that good (especially on the derivatives as it is needed here) and if one knows such an estimate, regularization is probably not needed anymore. In the tangential cone condition on the other hand, no estimate on the norm of $w$ is needed.

Hence, the condition (6.22) is way more practical, since it demands no information about the element $w$ and is also sufficient, when it comes to approximate source conditions. In fact, it is very difficult to verify. Nevertheless, in the case of a linear system, it is indeed possible to verify this condition on $\mathcal{D}(F)$.

**Proposition 6.8.6.** *Assume a general system of the form* (1.3). *Further let* $g(p,u)_i = \sum_{j=1}^{N} p_{ij} u_j$. *Then the forward operator $F$ fulfills condition* (6.22) *on* $\mathcal{D}(F)$.

*Proof.* First note, that $(g_p(p,u)h)_i = \sum_{j=1}^{N} h_{ij} u_j$ and $A_u = A$. Let $p, p^\dagger \in \mathcal{D}(F)$. Then for the difference we get

$$\begin{aligned}
&(A(p^\dagger)(u(p) - u(p^\dagger))_i \\
=&(u(p)_i)_t - (u(p^\dagger)_i)_t - \nabla \cdot D_i \nabla (u(p)_i - u(p^\dagger)_i) + \sum_{j=1}^{N} p^\dagger_{ij}(u(p)_j - u(p^\dagger)_j) \\
=&(u(p)_i)_t - \nabla \cdot D_i \nabla u(p)_i - f + \sum_{j=1}^{N} p^\dagger_{ij} u(p)_j \\
=&\sum_{j=1}^{N} (p^\dagger_{ij} - p_{ij}) u(p)_j
\end{aligned}$$

Thus we can estimate

$$\begin{aligned}
&\|F(p) - F(p^\dagger) - F'(p^\dagger)(p - p^\dagger)\|_{L_2(\Omega)^N} \\
=&\Big\| u(p) - u(p^\dagger) + (A_u)^{-1}\Big(\sum_{j=1}^{N} (p_{ij} - p^\dagger_{ij}) u(p^\dagger)_j\Big)\Big\|_{L_2(\Omega)^N} \\
=&\Big\| A(p^\dagger)^{-1}\Big(A(p^\dagger)(u(p) - u(p^\dagger)) + \sum_{j=1}^{N} (p_{ij} - p^\dagger_{ij}) u(p^\dagger)_j\Big)\Big\|_{L_2(\Omega_T)^N} \\
\leq&\|A(p^\dagger)^{-1}\|_{L(L_2,L_2)} \Big\| (A(p^\dagger)(u(p) - u(p^\dagger)) + \sum_{j=1}^{N} (p_{ij} - p^\dagger_{ij}) u(p^\dagger)_j \Big\|_{L_2(\Omega_T)^N} \\
=&\|A(p^\dagger)^{-1}\|_{L(L_2,L_2)} \Big\| \sum_{j=1}^{N} (p^\dagger_{ij} - p_{ij}) u(p)_j + \sum_{i=1}^{N} (p_{ij} - p^\dagger_{ij}) u(p^\dagger)_j \Big\|_{L_2(\Omega_T)^N}
\end{aligned}$$

$$
\begin{aligned}
=&\|A(p^\dagger)^{-1}\|_{L(L_2,L_2)}\Big\|\sum_{j=1}^{N}(p^\dagger_{ij}-p_{ij})(u(p)_j-u(p^\dagger)_j)\Big\|_{L_2(\Omega_T)^N}\\
\le&\|A(p^\dagger)^{-1}\|_{L(L_2,L_2)}\sum_{i=1}^{N}\sum_{j=1}^{N}\|(p^\dagger_{ij}-p_{ij})\|_{L_\infty(\Omega_T)}\|u(p)_j-u(p^\dagger)_j\|_{L_2(\Omega_T)}\\
\le&\|A(p^\dagger)^{-1}\|_{L(L_2,L_2)}2N\max\{C_1,C_2\}\|u(p)-u(p^\dagger)\|_{L_2(\Omega_T)^N}\\
=&C\|F(p)-F(p^\dagger)\|_{L_2(\Omega)^N},
\end{aligned}
$$

which establishes the claim. □

The derivation of a similar estimate in the nonlinear case is much more complicated, since a direct relation between $p$ and $u$ cannot be derived. However for special functions (especially for functions that are linear in $p$ and only nonlinear $u$) a similar estimate might be possible to achieve.

**Remark 6.8.7.** Besides the application to show source conditions, the condition (6.22) is also an assumption that appears in many iterative regularization schemes. Here, one additionally has to show that the constant $c$ in (6.22) is smaller then one to assure convergence or regularization properties of the iterative regularization schemes. In this case, condition (6.22) is also called tangential cone condition. However, the constant we derived in Proposition 6.8.6 is usually not good enough for these methods, because considering applications the bound on the functions $C_2$ is already much bigger than one. For more information about this topic we refer to [23, 59, 64].

## 6.9 Parameters that are only space dependent, only time dependent or neither space nor time dependent

Parameters not always have to be assumed to be space and time dependent. Nevertheless, the analysis from Chapter 5 still can be applied. This is just a straight forward result, since one can use the following parameter spaces

$$
\begin{aligned}
&\mathcal{P}_S = L_2(\Omega)^M && \text{(only space dependent)},\\
&\mathcal{P}_T = L_2([0,T])^M && \text{(only time dependent)},\\
&\mathcal{P}_I = \mathbb{R}^M && \text{(space time independent)}.
\end{aligned}
$$

All those spaces continuously embed into our initial parameter space $\mathcal{P}$. Therefore the computation of the derivative of the parameter-to-state map can be done in absolutely similar fashion as for space and time dependent parameters. Also the results concerning the $\tau$-weak closedness property carry over to this case, The adjoint of the derivative has to be computed for each case individually. This is again an easy task, since the adjoint of the respective embedding operators is just the integration over space or time respectively, so in each of the three cases we can simply compute the shape of the adjoint of the derivative of the parameter-to-state map via

$$F'(p)^*h = \int_0^T F'(I_{\mathcal{P}_T \hookrightarrow \mathcal{P}} p)^* h \; dt,$$
$$F'(p)^*h = \int_\Omega F'(I_{\mathcal{P}_S \hookrightarrow \mathcal{P}} p)^* h \; dx,$$
$$F'(p)^*h = \int_0^T \int_\Omega F'(I_{\mathcal{P}_I \hookrightarrow \mathcal{P}} p)^* h \; dx \; dt.$$

A discussion of source conditions can also be done in this case. While smoothness conditions remain the same, either the restriction on the boundary conditions in case of only time dependent parameters or the restriction on the final condition in case of only space dependent parameters can be dropped.

## 6.10 Identification of the diffusion coefficient

The simultaneous identification of a diffusion coefficient in addition to parameters appearing in the reaction term has been extensively discussed in [57]. Essentially, the results were that if the parameter space for the diffusion coefficient is chosen as $P_D = L_\infty(\Omega_T)^N$, an analysis like the above is possible. Note that again, the weak sequential closedness may give some trouble and probably requires a domain restriction for the diffusion parameter $D$. The overall parameter space then can be chosen as the product space $P_D \times \mathcal{P}$. Since the differential operator is linear with respect to the diffusion coefficient the derivative of this part is easy to compute. We then get the following differential equation for the derivative of the parameter-to-state map, i.e. $F'(D,p)h$ is the solution of the differential equation

$$v_t - \nabla \cdot D \nabla v + g_u(p,u)v = \nabla \cdot h \nabla u - g_p(p,u)h,$$

so we get an additional term in the right hand side of the partial differential equation for the derivative. The computation of the adjoint of the derivative is also straightforward, only one part for $D$ is added, it holds

$$F'(p^\dagger)^* = (\nabla v_i \cdot \nabla u_i, g_p(p,u)^* v),$$

where $v$ is the solution of the adjoint equation (6.10).

## 6.11 Some remarks on semilinear elliptic differential equations

To conclude this chapter, we want to add some final remarks concerning elliptic partial differential equations. As it is known, the weak solution theory, that we derived in Chapter 5 for parabolic partial differential equations is a generalization of the solution theory for elliptic partial differential equations. This means, that the results derived in the previous chapter can be transferred one to one to the case of elliptic equations under even slightly weaker assumptions, since there is no time derivative involved. In fact the only part that needs some attention is the nonlinear function $g$. Depending on $g$, similar restrictions onto the parameter space have to be made to show differentiability of $g$ with respect to the parameter $p$, depending on the superposition operator associated with $g$ and we face the same problems showing weak sequential closedness as in Chapter 6.4.

# CHAPTER 7

# Identifiability of solutions

Now, that we have adressed the regularization, the question whether the solutions are or are not identifiable from certain types of measurements (as discussed in Section 6.7 remains. In this section we will show identifiability of parameters in a semilinear parabolic PDE in the case $N = M = 1$ for certain types of measurements. Especially the case, where the measurements are given by snapshots at certain time instances, which is for example very relevant in the embryogenesis example from Section 2.4, is discussed. For this, we will use an adjoint approach proposed in [21] and generalize it to our model PDE (1.3).

## 7.1 Uniqueness in scalar reaction-diffusion equations

This section is split in two parts. First, we derive an adjoint equation for a semilinear PDE and introduce some technical conditions for the approach to work. Then we show uniqueness with the help of an approximate controllability assumption on an adjoint PDE for different kinds of measurements. The motivation behind this and the main idea of the paper [21] is the relation of the original partial differential equation to the above mentioned adjoint PDE with solution operator $F^*$, where one aims at an identity

$$\langle p_1 - p_2, F^*(f^*)\rangle_{L_2(\Omega_T)} = \langle F(p_1) - F(p_2), f^*\rangle_{L_2(\tilde{\Omega}_T)}, \qquad \tilde{\Omega}_T \subset \overline{\Omega_T} \tag{7.1}$$

for parameters $p_1, p_2 \in \mathcal{P}$ and $f^* \in L_2(\tilde{\Omega}_T)$. If now $F$ was a linear operator and its range was dense, it would immediately follow that $F$ is injective. However, since $F$ is not linear and $F^*$ is not the adjoint of $F$ in a strict sense, one can not directly derive injectivity. But something similar to injectivity is granted by approximate controllability, which we will indeed use to show uniqueness. In this section we consider the following types of measurements:

(i) On a subset $\tilde{\Omega} \subset \Omega$ over the whole time domain,

(ii) on the boundary $\partial\Omega$ over the whole time domain,

(iii) over the whole domain $\Omega$ via snapshots at times $\{t_0, ..., t_K\}$.

### 7.1.1 Derivation of an adjoint equation

So let $p_1, p_2 \in \mathcal{P}$ and $u(p_1)$, $u(p_2)$ the respective solution of (1.3). In the following, let $\Delta u = u(p_1) - u(p_2)$. Then for $\Delta u$ we get the differential equation.

$$\begin{aligned} \Delta u_t(x,t) - \nabla \cdot D(x,t)\nabla \Delta u(x,t) & \\ + g(p_1(x,t), u_1(x,t)) - g(p_2(x,t), u_2(x,t)) &= 0 \qquad \text{in } \Omega_T, \\ \Delta u(x,t) &= 0 \qquad \text{on } \partial\Omega \times [0,T], \\ \Delta u(x,0) &= 0 \qquad \text{on } \Omega \times \{0\}. \end{aligned}$$

We can multiply both sides of this equation with a test function $\varphi \in C_0^\infty(\Omega_T)$, add $g(p_1, u_2) - g(p_1, u_2)$ and integrate over space and time, so we get

$$\begin{aligned} \int_0^T \int_\Omega \Delta u_t \varphi - \nabla \cdot D \nabla \Delta u \varphi + (g(p_1, u_1) - g(p_1, u_2))\varphi \; dx \; dt & \\ = \int_0^T \int_\Omega (g(p_2, u_2) - g(p_1, u_2))\varphi \; dx \; dt & \end{aligned}$$

Partial integration with respect to space and time then yields

$$\begin{aligned} \int_0^T \int_\Omega \Delta u(-\varphi_t - \nabla \cdot D\nabla\varphi + (g(p_1, u_1) - g(p_2, u_2))\varphi) \; dx \; dt + \int_\Omega \Delta u \varphi|_{t=0}^{t=T} \; dx & \\ + \int_0^T \int_{\partial\Omega} \varphi \frac{\partial}{\partial n}\Delta u - \Delta u \frac{\partial}{\partial n}\varphi \; dS \; dt = \int_0^T \int_\Omega (g(p_2, u_2) - g(p_1, u_2))\varphi \; dx \; dt & \end{aligned} \tag{7.2}$$

Now we are facing a problem. In the paper [21] a direct relationship between the differences of parameters and solutions as in (7.1) can be derived. In our case, this is not directly possible, because the possibly nonlinear function $g$ is still involved. To generalize the results from [21], we need some conditions to get a relation between parameters and solutions. For this we define

$$\hat{g}(p_1, u_1, u_2) = \begin{cases} \frac{g(p_1,u_1) - g(p_1,u_2)}{\Delta u} & \Delta u \neq 0 \\ 0 & \Delta u = 0 \end{cases}$$

This definition however is not as great as it might seem. Because for $\Delta u \to 0$, $1/\Delta u \to \infty$ and therefore an adjoint equation with the reaction term $\hat{g}$ might not be solvable anymore, since the reaction term can not be considered as an element of $L_\infty$. Hence, we introduce a condition that handles this problem:

**Assumption 7.1.1.** *For all $u_1, u_2 \in F(\mathcal{P})$ and $p \in \mathcal{P}$ it holds*

$$|g(p, u_1) - g(p, u_2)| = \mathcal{O}(\Delta u). \tag{7.3}$$

This assumption is for example fulfilled if $g$ is Lipschitz continuous with respect to the second argument. Now, in the case of measurements of type (i), we can have $\varphi$ to fulfill the differential equation

$$\begin{aligned} -\varphi_t - \nabla \cdot D\nabla\varphi + \hat{g}(p_1, u_1, u_2) &= \begin{cases} f^* & \text{in } \tilde{\Omega} \times [0, T] \\ 0 & \text{elsewhere} \end{cases}, \\ \varphi(x, t) &= 0 \qquad \text{on } \partial\Omega \times [0, T], \\ \varphi(x, T) &= 0 \qquad \text{on } \Omega \times \{T\}, \end{aligned} \tag{7.4}$$

and in case of measurements of type (ii) the equation

$$\begin{aligned} -\varphi_t - \nabla \cdot D\nabla\varphi + \hat{g}(p_1, u_1, u_2) &= 0 \qquad \text{in } \Omega_T, \\ \varphi(x, t) &= f^* \qquad \text{on } \partial\Omega \times [0, T], \\ \varphi(x, T) &= 0 \qquad \text{on } \Omega \times \{T\}. \end{aligned}$$

If we now denote the map $f^* \mapsto \varphi$ via $F^*$ the identity (7.2) reduces to

$$\langle g(p_1, u_2) - g(p_2, u_2), F^*(f^*)\rangle_{L_2(\Omega_T)} = \langle f^*, F(p_1) - F(p_2)\rangle_{L_2(\tilde{\Omega}\times[0,T])}, \tag{7.5}$$

for interior measurements (i) and for boundary measurements (ii) to

$$\langle g(p_1, u_2) - g(p_2, u_2), F^*(f^*)\rangle_{L_2(\Omega_T)} = \langle f^*, F(p_1) - F(p_2)\rangle_{L_2(\partial\Omega\times[0,T])}. \tag{7.6}$$

As we can see, both these identities are of the form (7.1).

For measurements at certain points in time, we propose a slightly different approach. First, we split the original differential equation into $K$ equations and get:

$$\begin{aligned} \Delta(u_k)_t(x,t) - \nabla \cdot D(x,t)\nabla\Delta u_k(x,t) & \\ +g(p_1(x,t), (u_k)_1(x,t)) & \\ -g(p_2(x,t), (u_k)_2(x,t)) &= 0 \qquad \text{in } \Omega_T, \\ \Delta u_k(x,t) &= 0 \qquad \text{on } \partial\Omega \times [t_k, t_{k+1}], \\ \Delta u_k(x, t_k) &= \begin{cases} \Delta u_{k-1}(x, t_k) & k > 1 \\ 0 & k = 1 \end{cases} \qquad \text{on } \Omega \times \{0\}. \end{aligned}$$

Now, we treat each equation on its own. We multiply each equation by a function $\varphi_k$ and perform the same analysis as above, that means (7.2) holds for each equation separately. Now we can have each $\varphi_k$ to fulfill an adjoint differential equation of the form:

$$\begin{aligned} -(\varphi_k)_t - \nabla \cdot D\nabla\varphi_k + \hat{g}(p_1, u_1, u_2) &= 0 \qquad \text{in } \Omega \times [t_{k-1}, t_k], \\ \varphi_k(x,t) &= 0 \qquad \text{on } \partial\Omega \times [0,T], \\ \varphi_k(x,t_k) &= f_k^* \qquad \text{on } \Omega \times \{t_k\}. \end{aligned} \tag{7.7}$$

and thus, in the case of snapshots (iii) we get the identity.

$$\begin{aligned} \langle g(p_1,u_2) - g(p_2,u_2), F^*(f^*)\rangle_{L_2(\Omega_T)} = &\sum_{k=1}^{K} \langle f_k^*, F(p_1) - F(p_2)\rangle_{L_2(\Omega)} \\ &+ \sum_{k=2}^{K} \langle \varphi_k(t_k), F(p_1) - F(p_2)\rangle_{L_2(\Omega)}, \end{aligned} \tag{7.8}$$

if we define

$$F^*(f^*) := \varphi_k \text{ on } [t_{k-1}, t_k].$$

Based on the identities (7.5), (7.6) and (7.8), there is well-founded hope to show that if $g(p_1,u_2) - g(p_2,u_2)$ differ from each other, the solutions must as well. This is of course not enough to ensure the identifiability of the parameters. So on must impose a limited injectivity condition for the second argument of $g$, that is

**Assumption 7.1.2.** *For all $p_1, p_2 \in \mathcal{P}$, and almost all $(x,t) \in \Omega_{T_1} \subset \Omega_T$ it holds*

$$g(p_1, u(p_2)) = g(p_2, u(p_2)) \Longrightarrow p_1 = p_2.$$

**Remark 7.1.3.** This assumption is in fact necessary for the uniqueness of parameters, as one can easily imagine. For this consider the following example: Let $g(p,u) = pu$ and $u(x,t) = 0$ in $\Omega_{T_2} \subset \Omega_T$. Then Assumption 7.1.2 cannot hold on $\Omega_T$, since then for every parameter $p_1$ we can define

$$p_2 = \begin{cases} p_1 & \text{in } \Omega_{T_2}, \\ p_1 + 1 & \text{in } \Omega_T \setminus \Omega_{T_2}, \end{cases}$$

but clearly $u(p_1) = u(p_2)$. In other words, if $u$ is zero on a set with a positive measure, the parameter $p$ has no influence at that set on the evolution of $u$. Hence, the solution of the inverse problem cannot be unique in this case. However, if it for example can be ensured that $u > 0$ on a subset $\Omega_{T_1} \subset \Omega_T$, then Assumption 7.1.2 can be fulfilled on this subset.

**Remark 7.1.4.** If assumption 7.1.2 holds, uniqueness of the parameters can be directly deduced, if measurements on the whole set $\Omega_T$ are given. In this case, if we assume $u(p_1) = u(p_2)$, substracting the corresponding differential equations gives

$$g(p_1, u) - g(p_2, u) = 0,$$

and the uniqueness of the parameters directly follows from assumption 7.1.2.

### 7.1.2 Uniqueness via approximate controllability

Now we can show uniqueness of parameters under the right assumptions onto parameters and measurements. As stated before, the proof can mostly be carried out along the lines of [21, Theorem 2.1], one only has to pay attention to the fact that now space and time dependent parameters are involved. First, we start with the uniqueness result for interior and boundary measurements:

**Theorem 7.1.5.** *Let measurements of type* (i) *or* (ii) *be given and* $\Delta g := g(p_1(x,t), u_2(x,t)) - g(p_2(x,t), u_2(x,t))$ *be piecewise smooth in time with only finitely many jumps and assume that on a subset* $\Omega_0 \times [T_1, T_2] \subset \Omega_T$ *of positive measure* $\Delta g$ *is continuous in time and it holds* $\Delta g \geq g^* > 0$*. Then it holds* $F(p_1) \neq F(p_2)$*.*

*Proof.* Let $F(p_1) = F(P_2)$, then it follows from (7.5) that

$$I := \int_0^T \int_\Omega \Delta g(x,t)\varphi(x,t,f^*) \; dx \; dt = 0 \qquad \forall f^* \in L_2(\Omega_T).$$

Now we can find an equidistant partition $P := \{0 = t_0, \ldots, t_n = T\}$ of the time interval $[0, T]$ so that we can replace the time integration by a discrete sum

$$I = \sum_{i=0}^{n-1} \int_\Omega \Delta t \Delta g(x, t_i)\varphi(x, t_i, f^*) \; dx + C(\Delta t)^2,$$

where the error estimator is associated with the trapezoid rule (here the piecewiese continuity of $\Delta g$ comes into play). The last summand can be dropped because of the final condition for $\varphi$. For each timepoint $t_i \in [T_1, T_2]$, we can find a smooth function $r(x, t_i)$ with support contained in $\Omega_0$, such that

$$\int_\Omega \Delta g(x, t_i) r(x, t_i) \; dx = \int_{\Omega_0} \Delta g(x, t_i) r(x, t_i) \; dx := C_2 > 0,$$

since $\Delta g > 0$ on $\Omega_0$ and the point evaluation makes sense, because $\Delta g$ is continuous in time on $[T_1, T_2]$. Now we define the function

$$V_i(x) = \begin{cases} r(x, t_i) & (x, t_i) \in \Omega_0 \times [T_1, T_2], \\ 0 & \text{otherwise.} \end{cases}.$$

The linear parabolic equation of type (7.4) is approximately controllable by the right hand side multiplied with an indicator function of a subset as well as by the boundary data (see for example [26] for the case of spatial measurements and [20] for the case of boundary measurements). So on each subinterval $(t_{i-1}, t_i)$, we can choose $f^*$ in a way that the initial state $V_i$ is mapped to the target state $V_{i-1}$ with starting point $V_T = 0$, such that

$$\|\varphi(\cdot, t_i, f^*) - V_i(\cdot)\|_{L_2(\Omega_0)} \leq L\frac{\varepsilon}{2^i K_i}, \qquad i = 0, ..., n-1. \tag{7.9}$$

Now we estimate

$$\begin{aligned}
|I| &\geq \left|\sum_{i=0}^{n-1} \int_\Omega \Delta t \Delta g(x, t_i)\varphi(x, t_i, f^*)\ dx\right| - C(\Delta t)^2 \\
&= \left|\sum_{i=0}^{n-1} \int_\Omega \Delta t \Delta g(x, t_i)(\varphi(x, t_i, f^*) - r(x, t_i) + r(x, t_i))\ dx\right| - C(\Delta t)^2 \\
&\geq \Bigg|\Big|\sum_{\{i\in\mathbb{N}_0, t_i\in[T_1,T_2]\}} \int_{\Omega_0} \Delta t \Delta g(x, t_i) r(x, t_i)\ dx\Big| \\
&\quad - \Big|\sum_{i=0}^{n-1} \int_\Omega \Delta t \Delta g(x, t_i)(\varphi(x, t_i, f^*) - r(x, t_i))\ dx\Big|\Bigg| - C(\Delta t^2).
\end{aligned} \tag{7.10}$$

Now, if we choose $K_i := \|\Delta g\|_{L_\infty}$, we have from (7.9)

$$\begin{aligned}
&\left|\sum_{i=0}^{n-1} \int_\Omega \Delta t \Delta g(x, t_i)(\varphi(x, t_i, f^*) - r(x, t_i))\ dx\right| \\
&\leq C_E \sum_{i=0}^{n-1} \|\Delta g\|_{L_\infty} \|\varphi(x, t_i, f^*) - r(x, t_i)\|_{L_2(\Omega_0)} \Delta t \\
&\leq \frac{\varepsilon L C_E T}{2}.
\end{aligned} \tag{7.11}$$

If we denote $\tilde{T} := \sum_{\{i\in\mathbb{N}_0, t_i\in[T_1,T_2]\}} \Delta t$, the calculations from (7.10) and (7.11) imply

$$|I| \geq L\Big(\tilde{T} - \varepsilon C_E T/2\Big) - C(\Delta t)^2 > 0 \qquad \text{if } \varepsilon \text{ and } \Delta t \text{ sufficiently small.} \tag{7.12}$$

So, since $f^* \neq 0$, this is a contradiction to $F(p_1) = F(p_2)$. □

For snapshot-measurements (iii), the situation is slightly more complicated. In this case, we have to ensure, that enough measurements are taken.

**Theorem 7.1.6.** *Let $m \in \mathbb{N}$ measurements of type* (iii) *be given and $\Delta g := g(p_1(x,t), u_2(x,t)) - g(p_2(x,t), u_2(x,t))$ be sufficiently smooth in time and assume that on a subset $\Omega_0 \times [T_1, T_2] \subset \Omega_T$ of positive measure $\Delta g$ is continuous in time and it holds $\Delta g \geq g^* > 0$. Further assume the number of measurements $K$ to be sufficiently big. Then, it holds $F(p_1) \neq F(p_2)$.*

*Proof.* We start out as in the proof of Theorem 7.1.5. So let $F(p_1) = F(P_2)$, then it follows from (7.8) that

$$I := \int_0^T \int_\Omega \Delta g(x,t) \varphi_k(x,t,f_k^*) \; dx \; dt = 0 \qquad \forall f_k^* \in L_2(\Omega).$$

Now, we choose a partition of the time interval, where each $t_i$ resembles the time measurement $i$ was taken and get

$$I = \sum_{i=0}^{K} \int_\Omega \Delta t \Delta g(x,t_i) \varphi_k(x,t_i,f_k^*) \; dx + C(\Delta t)^2.$$

Let now $r(x,t_i), L$ and $V_i$ be as in the proof of Theorem 7.1.5. From a density result [27, Theorem 1.1] follows, that on each subinterval $(t_{k-1}, t_k)$, we can choose $f_k^*$ in a way that the initial state $f_k^*$ is mapped to the target state $V_{i-1}$, such that

$$\|\varphi(\cdot, t_i, f_k^*) - V_i(\cdot)\|_{L_2(\Omega_0)} \leq L \frac{\varepsilon}{2^i K_i}, \qquad i = 0, ..., n-1.$$

Now we can proceed as in Theorem 7.1.5 and we arrive at an equation

$$|I| \geq L\Big(\tilde{T} - \frac{\varepsilon T}{2}\Big) - C(\Delta t)^2$$

This identity is greater than zero, if $\varepsilon$ and $\Delta t$ are small enough, which can only be guaranteed, if enough measurements are taken. So, if $K$ is sufficiently large, this is a contradiction to $F(p_1) = F(p_2)$. □

**Remark 7.1.7.** The result of Theorem 7.1.6 is not surprising, since without sufficient data uniqueness cannot be guaranteed in most cases. Theorem 7.1.6 gives no exact number of measurements needed, but in practice this number can be assumed to be reasonably low depending on the length of the experiment and the total variation of the solution and the parameters.

**Corollary 7.1.8.** *Let all the assumptions from Theorem 7.1.5 or Theorem 7.1.6 hold, depending on the type of measurements. Further let assumption 7.1.2 hold. Then $p_1 \neq p_2$ implies $u_1 \neq u_2$ on $\Omega_{T_1}$ and hence the solution to the inverse problem is unique in $\Omega_{T_1}$.*

*Proof.* The claim follows immediately from Theorem 7.1.5, Theorem 7.1.6 and Assumption 7.1.2. □

**Remark 7.1.9.** One could extend the results of Theorem 7.1.5 even further, by just using a subset of the parameter space and the solution space to show local uniqueness. For this, one would have to introduce a local approximate controllability condition, so that every $u \in F(P_0) \subset W$, where $P_0 \subset P$ is approximately controllable by the right hand side of the adjoint equation. However, in this case it has to be ensured that $V_j(x, t_j) \in F(P_0)$ for every $(x, t_j)$. In this case the same argument as in Theorem 7.1.5 can be applied to show the uniqueness of parameters in $P_0$.

**Remark 7.1.10.** State of the art until recent years was the derivation of uniqueness results with the help of $L_2$ weighted inequalities, the so called Carleman estimates, that often can give very general results that come with other benefits like Lipschitz continuity of the forward operator [43, 69]. However, so far the theory of Carleman estimates seems to be restricted to space dependent parameters only and thus does not fit well into our analysis.

**Remark 7.1.11.** An adjoint equation like (7.4) can also be derived in the system case. This has been done in [21] for the example equation from Section 2.3. At this point, we do not compute the explicit adjoint equation for (1.3). In a general case it provides little information. Also, if one can get uniqueness by an adjoint approach in the system case (if one makes the right restriction onto the parameters) is questionable. The adjoint equation itself is a coupled system. For example in that case, approximate controllability results are less general than in the scalar case [4]. However, in a concrete application an adjoint approach could help to derive conditions under which uniqueness holds. This might be an interesting starting point for future research.

## 7.2 Dealing with non-uniqueness in parabolic systems

In the previous sections we discussed an approach to showing that the solution of a specific inverse problem is unique. However, in many cases, especially in biological pattern formation, uniqueness does not hold. If one still performs Tikhonov regularization, one wants to find a way to improve the solution based on a priori knowledge available. In this section we propose an approach that is incorporating a priori information to improve the quality of solutions.

Assume that the solution of the system (1.3) in not unique, that means there exist $p_1, p_2$ with $u(p_1) = u(p_2)$. Let us make the assumption

$$g(p_1, u) = g(p_2, u) \qquad \text{a.e. in } \Omega_T,$$

which surely is fulfilled, if measurements on the full dataset are taken. Now assume additional a priori information. One may then want to consider the optimization problem

$$\min_{p\in\mathcal{D}(F)} \|F(p)-u^\delta\|^2 \qquad \text{s.t. a priori information.}$$

However, depending on the type of a priori information, this might not be the smartest approach, since the optimal solution is often not accessible in a reasonable amount of time. On the other hand, if one performs some kind of Tikhonov-regularization, the solution is probably not the one that one was looking for. But assume that we found a minimizer $p_\alpha^\delta$ of a Tikhonov functional for given data $u^\delta$, then it should approximately hold

$$g(p_1,u)=g(p_2,u)\approx g(p_\alpha^\delta,u(p_\alpha^\delta)).$$

Now we can define an operator

$$\begin{aligned}\tilde{F}:\mathcal{P}&\to L_2(\Omega_T)\\ p&\mapsto g(p,u)\end{aligned}$$

and then, it is only natural to consider the following optimization problem

$$\min_{p\in\mathcal{D}(F)} \|\tilde{F}(p)-g(p_\alpha^\delta,u(p_\alpha^\delta))\|^2 \qquad \text{s.t. a priori information.}$$

Note that this problem (depending on $\tilde{F}$) may still be hard to solve, but here, at least the forward operator is explicitly known and often of a much easier type. Also note that this problem can still be ill-posed, so it needs again to be regularized. Whether such an approach will work in practice proposes an interesting question.

# CHAPTER 8

# Numerics

There are lots of different methods to solve a PDE like (1.3). In our case we will use a finite element method combined with an implicit-explicit Euler method for the forward solver, i.e. the numerical solver of the PDE. In this chapter we will introduce the and discuss its advantages for our kind of problem. Then, we will show the applicability of the above theory with the help of the embryogenesis example from Section 2.4. This also highlights our findings of non-uniqueness of parameters as highlighted in Section 4.1.1.

## 8.1 Numerical solution of the forward problem

In this section, we shortly introduce the method that we used to solve the forward problem in our numerical experiments. The following overview is taken from the textbook [66]. Let us start with a weak solution of the problem (1.3), defined in (5.10), i.e.

$$\sum_{i=1}^{N} \langle u_i'(t), \varphi_i \rangle_{(\tilde{Y}^*,\tilde{Y})} + \sum_{i=1}^{N} \int_{\Omega} \nabla u_i(t) \cdot \nabla \varphi_i \, dx = \sum_{i=1}^{N} \int_{\Omega} g_i(u_i(t))\varphi_i \, dx \qquad \forall \varphi \in \tilde{Y}$$

To discretize this equation, two steps are performed. First we discretize the equation in space via finite elements and then in time via finite differences. For the discretization in space, we utilize a partition of $\Omega$ into disjoint triangles such that no vertice of any triangle lies on the interior of a side of another triangle and such that the union of triangles determine a polygonal domain $\Omega_h \subset \Omega$ with boundary vertices on $\partial\Omega$. Further we assume that there is a parameter $h$ that is related to the maximal length of the edges of the triangles. This set of triangles is called a *triangulation* $S_h$ of $\Omega$. We can now define a finite dimensional function space

$X_h$ on a triangulation $S_h$, a so called *finite element space*, such that $X_h \subset H^1(\Omega)$. This function space is uniquely determined by its basis functions, which in the simplest case can be chosen as so called hat or pyramid functions. These are piecewise linear functions that are uniquely determined by

$$\varphi_j = \delta_j P_j,$$

where the set $\{P_j\}$ denotes the set of vertices of the triangles. So each function in $X_h$ can be expressed via

$$\chi = \sum_{j=1}^{n_h} \alpha_j \varphi_j.$$

Now we can perform a space discretization of the weak formulation and get a differential equation on the finite dimensional space $X_h$

$$\sum_{i=1}^{N} \langle (u_i^{(h)})_t(t), \chi\rangle + \langle D^{(h)}(t)\nabla u_i^{(h)}(t), \nabla\chi\rangle$$
$$+ \langle g_i(p^{(h)}(t), u^{(h)}(t)), \chi\rangle = \sum_{i=1}^{N} \langle f_i^{(h)}(t), \chi\rangle \qquad \forall \chi \in X_h, t > 0,$$

with finite dimensional approximations $D_i^{(h)}$, $f_i^{(h)}$ and $p^{(h)}$ of $D_i$, $f_i$ and $p$, $i = 1, ..., N$ (note that this demands some regularity on $D$ and $p$). By expanding $u_h$ into the basis we get an expression

$$u_i^{(h)}(t) = \sum_{j=1}^{n_h} \alpha_{ij}(t)\varphi_j,$$

so the goal is to find coefficients $\alpha_{ij}$ with

$$\sum_{i=1}^{N}\sum_{j=1}^{n_h} \alpha'_{ij}(t)\langle\varphi_j, \varphi_k\rangle + \alpha_{ij}(t) D_i^{(h)}(t)\langle\nabla\varphi_j, \nabla\varphi_k\rangle$$
$$= \sum_{i=1}^{N} \langle f_i^{(h)}(t) - g_i(p^{(h)}(t), u^{(h)}(t)), \varphi_k\rangle, \qquad \forall k = 1, ..., n_h, t > 0,$$

where it is utilized that it is enough to test the equation with every basis function of $X_h$ instead of testing with every function $\chi \in X_h$. This identity can be rewritten in dependence of $\alpha$ as

$$M\alpha'(t) + S\alpha(t) = F(\alpha(t)),$$

where

$$M = \begin{pmatrix} M_1 & 0 & \dots & 0 \\ 0 & M_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & M_N \end{pmatrix}, \quad S = \begin{pmatrix} S_1 & 0 & \dots & 0 \\ 0 & S_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & S_N \end{pmatrix},$$

with $M_i = (\langle \varphi_j, \varphi_k \rangle)_{j=1,..,n_h,k=1,...,n_h}$ and $S_i = (\langle \nabla\varphi_j, \nabla\varphi_k \rangle)_{j=1,..,n_h,k=1,...,n_h}$. By our choice of the basis functions, the matrices $M$ and $D$ (under a positivity constraint onto the diffusion coefficient) are invertible and thus we get an equation for $\alpha$ via

$$\alpha'(t) = M^{-1}F(\alpha(t)) - M^{-1}S\alpha(t).$$

So our discrete scheme is just a system of ordinary differential equations. This system can now be solved by the well known Euler method, where one discretizes the time axis via finite differences and then integrates over time. In our case, we just assume equidistant time steps, i.e. for $[t_0 = 0, ..., t_K = 1]$ it holds $t_l = Kl$. Further we set $u^{(h)}(t_0) = Iu_0$, where $I$ is the function that interpolates the initial value $u_0$ to our triangulation $S_h$. To solve problem (1.3), we approximate the derivative

$$(u_i^{(h)})_t(t) = \frac{u_i^{(h)}(t_{l+1}) - u_i^{(h)}(t_l)}{K}$$

and insert this into the weak formulation in the following way

$$\begin{aligned} &\sum_{i=1}^{N} \langle u_i^{(h)}(t_{l+1}), \chi \rangle + K \langle D^{(h)}(t_l) \nabla u_i^{(h)}(t_{l+1}), \nabla\chi \rangle \\ =&\sum_{i=1}^{N} \langle u_i^{(h)}(t_l) + K(f_i^{(h)}(t_l) - g_i(p^{(h)}(t_l), u^{(h)}(t_l)), \chi \rangle \qquad \forall \chi \in X_h, \end{aligned}$$

which can be seen as an implicit-explicit Euler method. The implicit part (the evaluation of $\nabla u_i^{(h)}$ at the point $t_{l+1}$ is recommended due to possible stiffness of the equation). Again expanding this into the basis coefficients gives us

$$\begin{aligned} &\sum_{i=1}^{N} \sum_{j=1}^{n_h} \alpha_{ij}(t_{l+1}) \langle \varphi_j, \varphi_k \rangle + \alpha_{ij}(t_l) K D_i^{(h)}(t_{l+1}) \langle \nabla\varphi_j, \nabla\varphi_k \rangle \\ =&\sum_{i=1}^{N} \langle u_i^{(h)}(t_l) + K(f_i^{(h)}(t_l) - g_i(p^{(h)}(t_l), u^{(h)}(t_l)), \varphi_k \rangle, \qquad k = 1, ..., n_h, \end{aligned} \tag{8.1}$$

This is just a linear system in $\alpha$ of the form

$$(M + S)\alpha = F.$$

It can be shown, that the matrix $M + S$ is invertible. Further, the matrix $M + S$ is sparse and has a blockdiagonal structure, so (8.1) can efficiently be solved via numerical inversion methods, even if the discretization is fine. So we finally arrive at a solution on the fully discrete space $(X_h)^K \subset L_2([0,T], H^1(\Omega)^N)$. Under appropriate regularity assumptions on the parameters $D$ and $p$ (which are of course needed to make point evaluations of these functions on a finite grid possible), the above method can be shown to converge to a solution of (1.3) if $h \to 0$ and

$K \to \infty$, see [66, Chapter 13]. Note that the adjoint equation from (6.10), which is needed to compute the adjoint of the gradient of the Tikhonov functional, can be solved in an absolute similar way, that means a discrete solution $v(w)$ of (6.10) can be computed through $v(t_K) = 0$ and

$$\sum_{i=1}^{N}\sum_{j=1}^{n_h} \beta_{ij}(t_{l-1})\langle\varphi_j,\varphi_k\rangle + \beta_{ij}(t_{l-1})KD_i^{(h)}(t_l)\langle\nabla\varphi_j,\nabla\varphi_k\rangle$$
$$= \sum_{i=1}^{N}\langle v_i^{(h)}(t_l) + K(w_i^{(h)}(t_l) - (g_u)_i(p^{(h)}(t_l),u^{(h)}(t_l))v_i^{(h)}(t_l),\varphi_k\rangle \ \forall k = 1,...,n_h. \tag{8.2}$$

**Remark 8.1.1.** There are many different methods to solve problems like (1.3) numerically, for example one could consider a discretization in time before the space variable is discretized. For an overview over these methods, we refer to [66]. The method we proposed in this section just seems to fit our problem very well.

**Remark 8.1.2.** One could consider adaptive methods to compute solutions of a desired precision. In these, a triangulation is chosen based on an a posteriori error estimator. Then, for a given precision $\eta$, an optimal number of nodes is found such that $\|u(t_l) - u^{(h)}(t_l)\| \leq \eta$. In addition the time discretization can be chosen adaptively as well. Adaptive methods can greatly reduce the computational cost of the solution of the forward problem, especially, if a specific accuracy of the discretized solution is desired. In the case of inverse problems however, the situation is more complicated. It is known, that if $X_h \subset X$ is an increasing sequence of subspaces (i.e. $X_i \subset X_j$ for $i > j$) with $\cup X_h = X$, the sequence of minimizers

$$(x_\alpha^\delta)_h \in \operatorname*{argmin}_{x\in X_h} \|F_h(x) - y^\delta\|^2 + \alpha R(x),$$

where $F_h$ is a finite dimensional approximations of $F$, is still a regularization if $\alpha$ is chosen in dependence of $h$ and $\delta$ [53]. A similar result could so far only be shown for adaptive discretizations only under the additional assumption of the tangential cone condition [41]. Another problem is the minimization of the Tikhonov functional. If one uses an algorithm like Algorithm 4.2.23 to minimize the Tikhonov functional, an adaptive grid is likely to change in each iteration step, so convergence is not necessarily given. So far, only convergence of the iterative thresholding algorithm under the assumption of a linear operator has been shown [9]. If and under which assumptions these results can be generalized to nonlinear operators is an open problem.

## 8.2 Numerical Solution of the inverse problem

So let us assume that we have discretized the problem as described in the section before. To solve (and regularize) the inverse problem in the finite dimensional subspace $(X_h)^K$ defined in the section before, we will utilize the penalty

$$R_m(p) := R(p_m) := \sum_{l=0}^{K}\sum_{j=1}^{n_h} |\langle p_m(t_l), \varphi_j(t_l)\rangle|, \qquad m = 1, ..., M \tag{8.3}$$

i.e. we use a sparsity enforcing penalty term (or $\|\cdot\|_{\ell_1}$ penalty term). So the basis that we are using is the pixel basis for the time axis and the finite element basis in the space dimension. Note that the basis functions are not orthogonal, but since the mass matrix $(\langle\varphi_k, \varphi_j\rangle)_{k,j}$ is invertible, every function $p \in (X_h)^K$ has a unique representation in this basis, so that the results of Section 4.2.1 are applicable. As a second basis we also consider the pixel basis in space, where we penalize the parameter at all vertices of our triangulation, i.e.

$$R_m(p) := R(p_m) := \sum_{l=0}^{K}\sum_{j=1}^{n_h} |p_m(P_j, t_l)|, \qquad m = 1, ..., M. \tag{8.4}$$

The inverse problem itself will then be solved by Algorithm 4.2.24 (note that in our experiments we are assuming that data is given on the whole set $\Omega_T$). If we write this down for our problem, we arrive at

**Algorithm 8.2.1.**

1. Choose a triangulation of $\Omega$ and a step size $1/K$ for the time variable.

2. Interpolate the data $u^\delta$ and the initial value $u_0$ to the chosen grid.

3. Choose a starting value $p_0$ for the iteration, i.e. $p_0 = 0$. Choose an exit condition.

4. Solve the (discrete) forward problem

$$(u_n)_t - \nabla \cdot D\nabla u_n + g(p_n, u_n) = f, \qquad u_n(0) = u_0,$$

   where $u_n(p_n)(0) = u_n(p_n)(t_0) = u_0$ and $u_n(p_n)(t_{l+1})$ is computed via (8.1).

5. Solve the (discrete) adjoint problem

$$-(v_n)_t - \nabla \cdot D\nabla v_n + g_u(p_n, u_n)^* v_n = u_n - u^\delta, v_n(T) = 0,$$

   where $v_n(p_n)(T) = v(p_n)(t_K) = 0$ and $v_n(p_n)(t_{l-1})$ is computed via (8.2).

6. Generate the adjoint $h_n$ of $F$ at the point $p_n$ as

$$h_n = F'(p_n)(F(p_n) - u^\delta) = g(p_n, u_n)^* v_n$$

   .

7. If $n \geq 2$ compute a step size $s_n$ by

$$s_n = \frac{\langle p_n - p_{n-1}, h_n - h_{n-1} \rangle}{\langle h_n - h_{n-1}, h_n - h_{n-1} \rangle}.$$

8. Compute an update for $p_n$ as

$$\tilde{p}_{n+1} = p_n - s_n h_n.$$

9. Expand $\tilde{p}_{n+1}$ into the given basis, perform shrinkage and map the result back into the space $(X_h)^K$ to obtain an update $p_{n+1}$.

10. Check if $p_{n+1}$ is a valid update. If not set $s_n = 0.1 s_n$ and go to step 8.

11. Check if the exit condition is met. If not go to step 4.

**Remark 8.2.2.** We compute the adjoint of $F'(p_n)$ by discretizing the infinite dimensional adjoint. This operator however is not necessarily the adjoint of the finite dimensional solution operator, so if one applies Algorithm 8.2.1 one has to keep this in mind. From our experience this is not a problem in case of the identification of space and time dependent parameters, if the discretization is fine enough. However, if the parameters are only space or only time dependent, it can become a severe issue, since an additional numerical integration step is involved.

## 8.3 Experiments

For our numerical experiments, we consider the embryogenesis example from Section 2.4, where we only consider the cases $N = 1$, the case that one gene regulates itself and the case $N = 2$, where two genes interact with each other. We keep the parameters $D$, $\lambda$ and $R$ fixed, so that we only have to identify the parameter $W$ in the equation

$$u_t - \nabla \cdot D \nabla u + \lambda u = R\phi(Wu), \qquad u(0) = u_0.$$

The gradient of the Tikhonov functional then becomes

$$(F'(W)^*(F(W) - u^\delta))_i = v(F(W) - u^\delta)_i \phi'((Wu)_i) u_j, \qquad 1 \leq i, j \leq N,$$

where $v_i$ is the solution of the adjoint equation

$$-(v_i)_t - \nabla \cdot D_i \nabla v_i + \lambda_i v_i + \sum_{i=1}^{N} R_i \phi'(s_i) W_{ij} v_i = u(W)_i - u_i^\delta, \qquad i = 1, ..., N.$$

Note that the presence of $\phi'$ makes the gradient of the Tikhonov-functional very flat at places, where high concentrations are present, as it can be seen in Figure 8.3, which makes the minimization difficult.

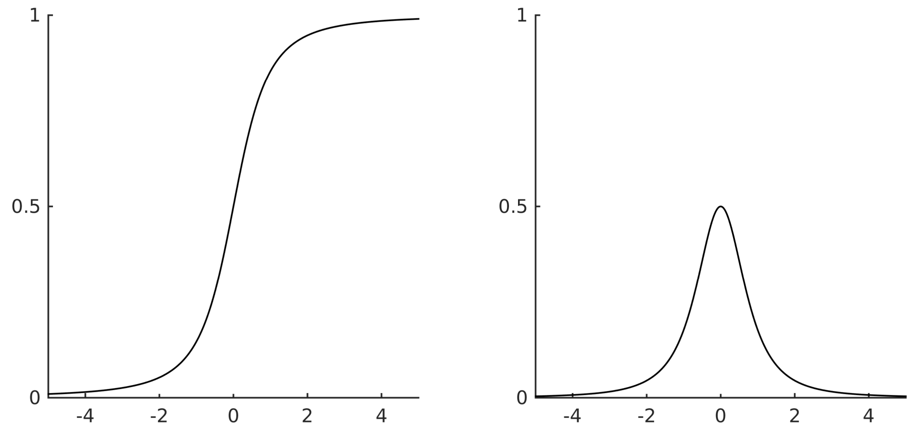


Figure 8.1: The function $\phi$ (left) and its derivative $\phi'$ (right).

In both cases we performed a considerable number of experiments, and the results for some characteristic examples are shown in this chapter. The bottom line of all our experiments is basically that the reconstruction of parameters in the case $N = 1$ works very well for space time dependent parameters (as long as the respective coefficients are chosen appropriately, see remark 8.3.1 below), but it does not in the case of a system. The main reason for this is local non-uniqueness of the parameter $W$ as stated in Theorem 4.1.2. In this case, it can be seen the parameter $W$ inherits certain structure from the solution $u$.

All our experiments are performed within the PDE-toolbox `FreeFem++`, see [33], where we implemented Algorithm 8.2.1. The visualizations are then done in `MATLAB` [50]. Note that all experiments are based on simulated data. To avoid a so called inverse crime, our simulated data is generated on a finer / different finite dimensional space $(\tilde{X}_h)^{\tilde{K}}$ by choosing an initial value $u_0$ and then applying the method from Section 8.1 to solve the forward problem with parameter $W^\dagger$ to generate the data. Then the data is interpolated to the grid $(X_h)^K$ that we use for the inversion. Note that the interpolation from one grid to another automatically generates a considerable amount of noise.

**Remark 8.3.1.** The coefficients for the forward problem have to be chosen, such that an influence of the parameter onto the solution can be measured in our finite dimensional subspace, i.e. a change of the pattern is recognizable. If this is not the case, the problem is too ill posed when noisy data is given. This is for example the case, if the diffusion or decay coefficients are too large so that every change in the pattern $u$ immediately diffuses or decays.

### 8.3.1 Space and time dependent parameter in a scalar equation

In this section we consider the identification of a space time dependent parameter in a scalar equation. For the domain $\Omega$ we choose the unit circle, i.e.

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 1\}.$$

The initial value we use is given as

$$u_0(x, y) = 1 + 6 \cdot \Big(1 - \Big(3\big(\sqrt{x^2 + y^2}\big)^2 - 2\big(\sqrt{x^2 + y^2}\big)^3\Big)\Big). \tag{8.5}$$

We fix the following parameters

$$D = 0.05, \lambda = 4.0, R = 40.0$$

and the parameter we want to identify is set to

$$W^\dagger(x, y, t) = \begin{cases} -1.4 & (x, y, t) \in [0.2, 0.5]^2 \times [0.2, 0.6] \\ -0.6 & (x, y, t) \in [-0.6, -0.2] \times [0.2, 0.6] \times [0.2, 0.8] \\ 0 & \text{elsewhere} \end{cases},$$

i.e. it is piecewise constant. The data generation is performed on a (uniform) triangulation with 7921 nodes, where 1000 timesteps are given. In addition 1% gaussian noise is added to the data. Then the data is interpolated to a mesh with 2023 nodes and 100 timesteps, where inversion is performed.

The solution of the forward problem with this initial value is displayed in Figure 8.2. It can be seen that the pattern quickly evolves over time before it completely diffuses. At places, where $W^\dagger$ has a negative entry, the inhibiting influence of $W^\dagger$ on the synthesis of $u$ is clearly visible.

This data is now used for the reconstruction of the parameter. In all our experiments we set a tolerance $\varepsilon = 10^{-10}$ and a maximum number of iterations $IT = 10000$ and terminated Algorithm 8.2.1, when either $\|p_n - p_{n-1}\| < \varepsilon$ or the maximum number of iterations was reached. For $\alpha \leq 10^{-6}$ the full number of 10000 iterations was needed.

Reconstructions over time are displayed in Figure 8.4 for the finite element basis and in Figure 8.5 for the pixel basis. In both cases the smaller peak is reconstructed very well at all points in time. While the larger peak in the center is detected immediately, the reconstruction of its height is slightly off and only good in the middle of the time interval. This, on the one hand is related to the strong diffusion that is present, but also might have to do with the nonlinear function $\phi$, which is almost linear for input arguments around zero and almost constant for large input arguments, see Figure 8.3. If we compare the best achievable reconstructions done in the pixel basis with the ones done in the finite element basis the $L_2$-error in the finite element basis is considerably smaller. On the other hand, the best achievable reconstruction from a visual point of view seems to be better in the pixel basis. Note that both reconstructions (with respect to the norm) already inherit some noise artifacts in both cases. If $\alpha$ is chosen smaller, these become much stronger, but the reconstruction of the peaks becomes better, see Figure 8.3. Note that for $\alpha = 10^{-9}$, the original peaks could hardly be distinguished from noise artifacts anymore.

If we used the squared $L_2$ norm as penalty, the best achievable reconstructions were not even close to those in the sparsity case, see Figure 8.6. The reconstruction of the peaks is much worse than in the original. Also the noise artifacts are larger.

Further, we performed experiments, where instead of the original gradient $\tilde{F}'$ of the discrepancy term $\tilde{F} := \|F(x) - u^\delta\|^2$, a smoothed version $\tilde{F}'_\kappa$ of $\tilde{F}'$ is used. We compute $D_\kappa$ as

$$\begin{aligned} \kappa\Delta\tilde{F}'_\kappa(t) + \tilde{F}'_\kappa(t) &= \tilde{F}'(t), \qquad \text{in } \Omega, \\ \tilde{F}'_\kappa(t) &= 0, \qquad \text{on } \partial\Omega, \end{aligned}$$

which is also called *Sobolev smoothing* of $\tilde{F}'$ [30]. This approach lead to great improvements in an elliptic parameter identification problem [30]. While for our problem, noise artifacts are smoothed out very well, the reconstruction of the peaks is not as good as it was before, see Figure 8.6. However, we did only a very limited number of experiments and might have chosen $\kappa$ to large. With a more optimized parameter choice for $\kappa$, the results concerning this can probably be improved.

Also, note that in all reconstructions, there were big noise artifacts in the first few time points, peaking at the initial value. This indicates that the degree of ill posedness of the problem has somewhat of a time dependence.

Finally, for future experiments, one could for example consider a total variation penalty term, which based on the structure of our solution should yield good results.

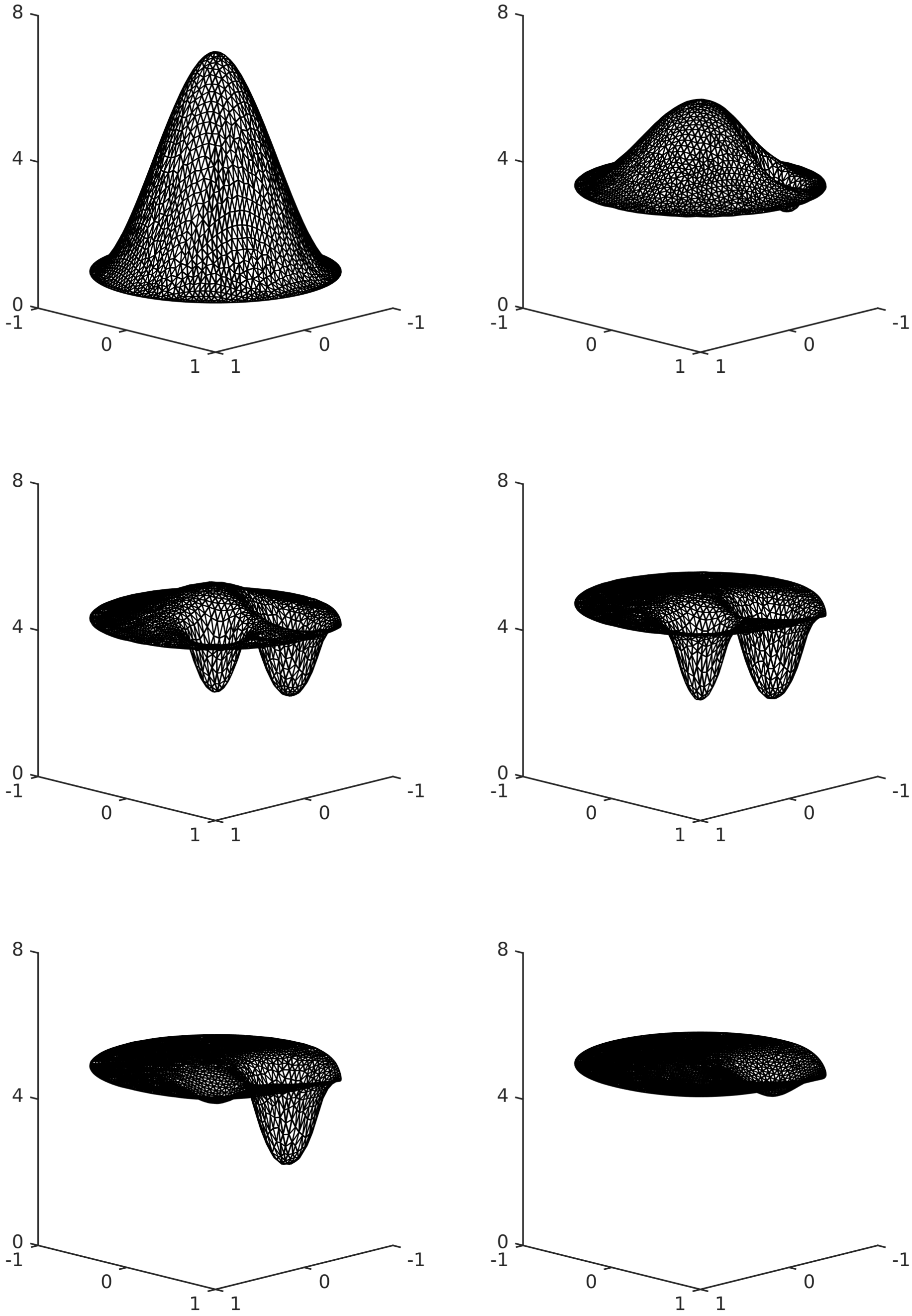


Figure 8.2: Evolution of the solution $u$ over time, starting with $u_0$ from (8.5) on the top left at $t = 0$. The other snapshots are taken at $t = 0.2$, $t = 0.4$, $t = 0.6$, $t = 0.8$ and $t = 1$.

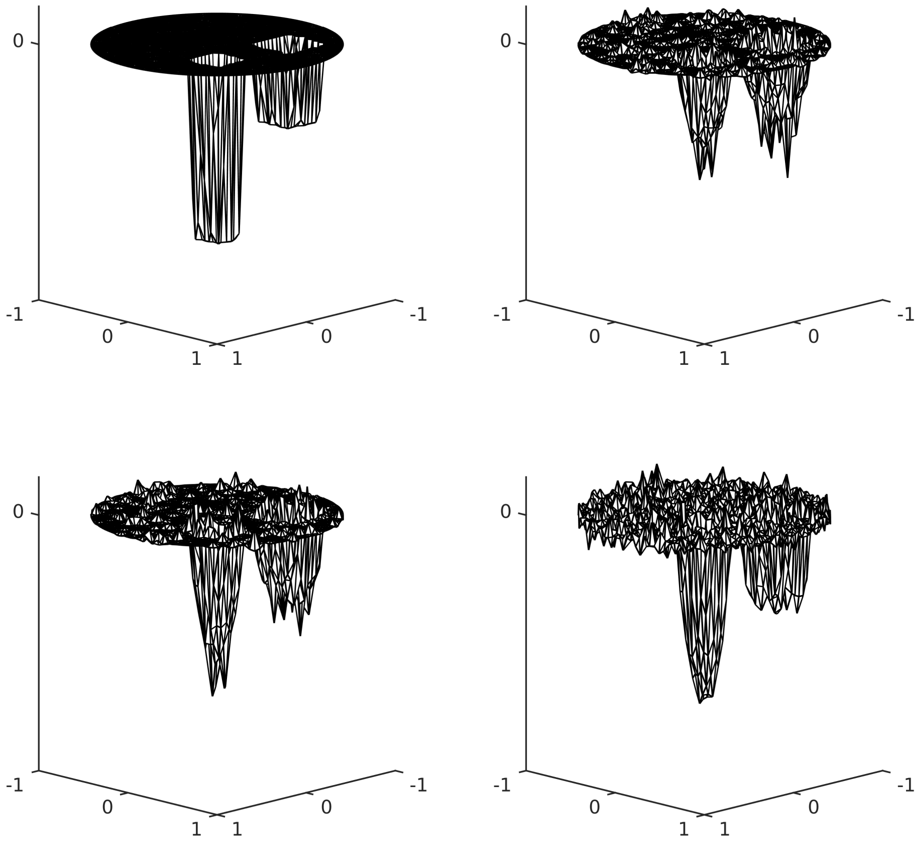


Figure 8.3: The parameter $W^{\dagger}$ (top left) and its reconstructions using the penalty term (8.3) for $\alpha = 10^{-4}$, $\alpha = 10^{-5}$ and $\alpha = 10^{-6}$ at time $t = 0.5$.

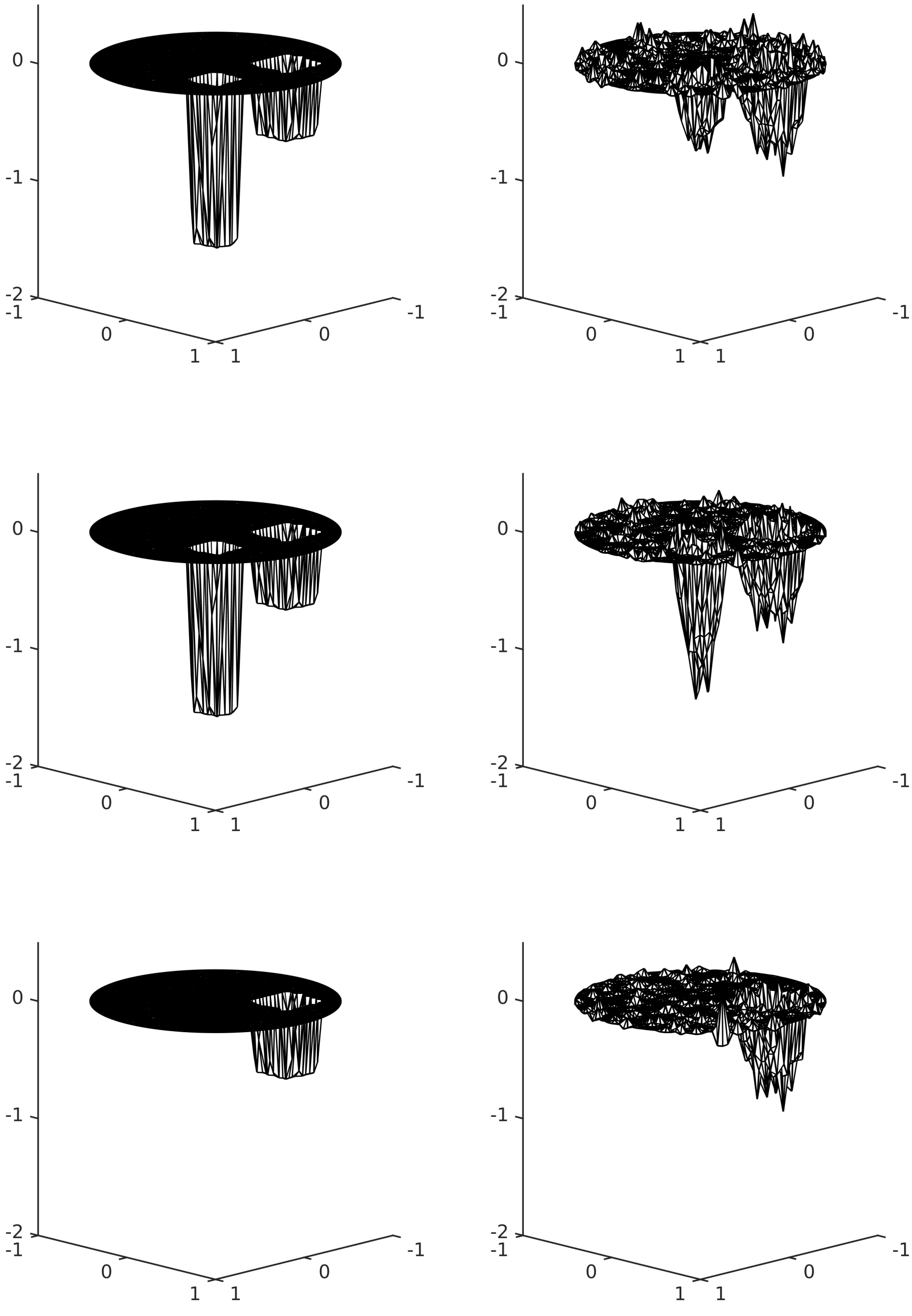


Figure 8.4: The parameter $W^\dagger$ (left column) and its reconstructions (right column) using the penalty term (8.3) at times $t = 0.25$, $t = 0.5$, $t = 0.75$. The reconstructions were done with regularization parameter $\alpha = 10^{-5}$.

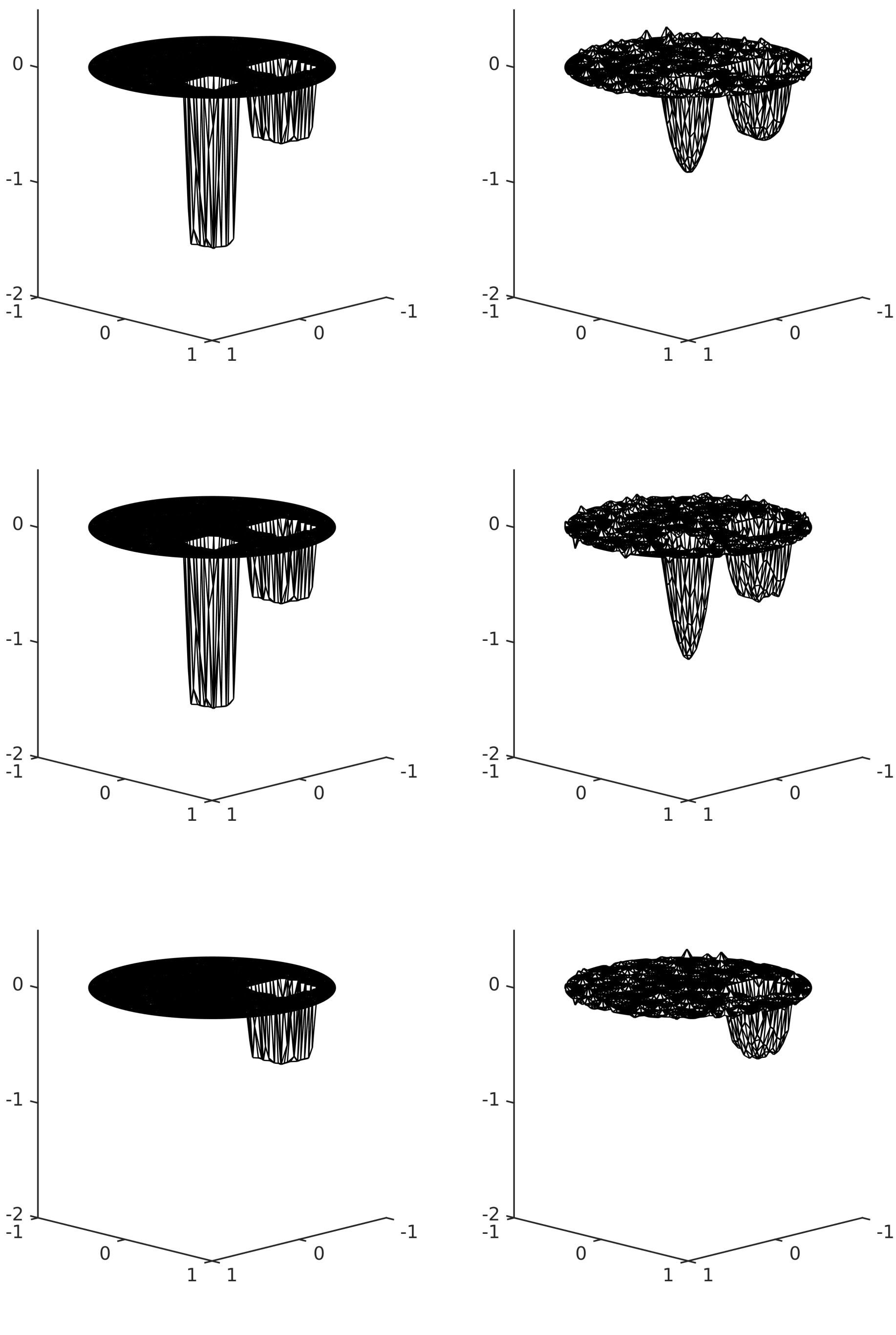


Figure 8.5: The parameter $W^\dagger$ (left column) and its reconstructions (right column) using the penalty term (8.4) at times $t = 0.25$, $t = 0.5$, $t = 0.75$. The reconstructions were done with regularization parameter $\alpha = 10^{-2}$.

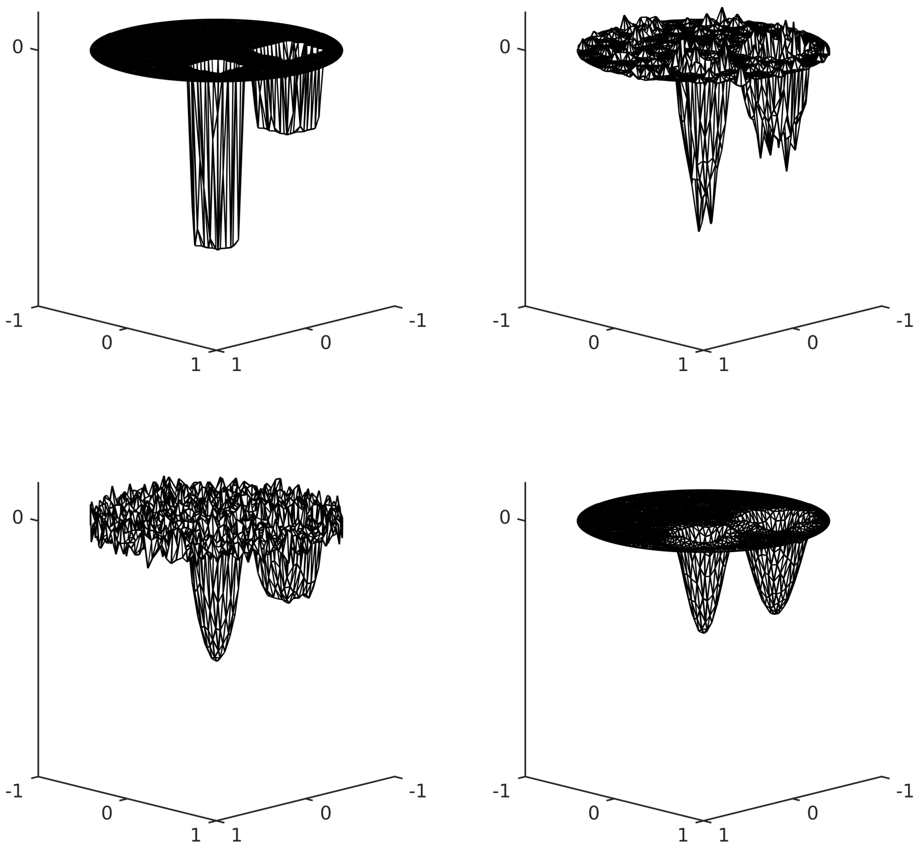


Figure 8.6: The parameter $W^{\dagger}$ (top left) and its reconstructions at time $t = 0.5$. In the top right, the finite element penalty term (8.3) with $\alpha = 10^{-5}$ is used for reconstruction. In the bottom left the $L_2$-norm with $\alpha = 10^{-1}$ is used. In the bottom right reconstructions with the Sobolev gradient $F'_{\kappa}$ combined with the finite element penalty term (8.3) are shown. The parameters used for this reconstruction were $\kappa = 0.8$ and $\alpha = 10^{-5}$.

### 8.3.2 Parameter identification in a system

In this section we discuss how parameter identification in a system works out, when we want to identify a matrix of parameters. The domain $\Omega$ is given as

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 4\}.$$

Again we fix the parameters

$$D_1 = D_2 = 0.002,\ \lambda_1 = \lambda_2 = 1.0,\ R_1 = 35.0,\ R_2 = 45.0.$$

As initial values we choose

$$u_{01} = \begin{cases} 30.0(1 - (3K_1^2 - 2K_1^3)) & K_1 \leq 1 \\ 0 & \text{otherwise} \end{cases}$$
$$u_{02} = \begin{cases} 30.0(1 - (3K_2^2 - 2K_2^3)) & K_2 \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

with

$$K_1 = \sqrt{(x - 0.25)^2 + (y + 0.25)^2},$$
$$K_2 = \sqrt{(x + 0.25)^2 + (y - 0.25)^2}.$$

The functions $u_{01}$ and $u_{02}$ are two (smooth) hills of the same structure, where one is located to the top left, while the other one is located to the bottom right of the center of $\Omega$.

The parameter $W^\dagger$ is the matrix

$$W^\dagger = \begin{pmatrix} -0.5 & 0.5 \\ -0.5 & -0.05 \end{pmatrix},$$

so presence of $u_1$ has an inhibiting influence on its own synthesis, while the presence of $u_2$ promotes the synthesis of $u_1$. On the other hand, strong presence of $u_1$ inhibits the synthesis of $u_2$, while $u_2$ inhibits its own synthesis.

Here, data generation is performed on a mesh with 926 nodes and 1000 time steps, while inversion is performed on a mesh with 243 nodes and 100 time steps. For the reconstruction, we still used a small regularization parameter ($\alpha = 10^{-8}$) due to possible interpolation noise. Also we only performed 10000 iterations in our iterative scheme, where we ended with a discrepancy $\|u(p) - u^\delta\|_{L_2(\Omega_T)} \approx 0.2$, which is an almost non visible difference.

One can see in Figure 8.7 that in $u_1$ the hill grows to the right side but its height gets smaller. In $u_2$ a valley begins to form, where concentrations of $u_1$ are high. These are exactly the results that we expected to see, when we have chosen the parameter $W^\dagger$.

We can see the reconstruction of the space time dependent parameters $W_{11}$, $W_{12}$, $W_{21}$ and $W_{22}$ from the simulated data in Figure 8.8. There are some spatial and temporal changes, but only where the functions $u_1 > 0$ and $u_2 > 0$. This is no surprise, since where $u$ is close to zero, the parameter $W$ does hardly influence the solution. On the set where the peaks are located, the reconstruction of $W$ is much better. At some points however parameter $W_{i1}$ has some artifacts of $W_{i2}$ and vice versa. This can be attributed to the non uniqueness shown in Theorem 4.1.2 for these kind of problems. At points, where $u_1$ and $u_2$ are peaking, the values of $W_{21}$ and $W_{22}$ are overestimated by quite a margin. The reason for this is the function $\phi$ combined with the large values of the functions $u_1$ and $u_2$ at their peak. For this to see, note that the argument of $\phi$, i.e. $W_{11}u_1 + W_{22}u_2$ is big at those points as well (especially much greater than 2 for almost all components of $W$). The function $\phi$ is very flat at those points, that means a sizable discrepancy between $W$ and $W^\dagger$ at those points has only minimal effect. On the other hand a very slight discrepancy between true solution and reconstructed solution can completely destroy a lot of information at those points. So alone the presence of the function $\phi$ amplifies the ill posedness of the problem a lot.

**Remark 8.3.2.** Note that we were not able to identify the constant parameters (using the real number gradient from Section 6.9 instead of the space time dependent gradient), as soon as data generation was done on a different grid than inversion. Algorithm 8.2.1 did still converge, but to a local minimum that had no visible relation to the parameters we originally used to generate the data. If the grid for data generation was the same as for inversion and no noise was present, we always found the true solution $W^\dagger$, when we used the starting value $W = 0$. Even with small noise, we could still achieve good results in this cases. Note that it cannot be ruled out that there might just be some numerical reasons (for example related to numerical integration, the interior interpolation process, or the grid being not fine enough) that caused the problems, when the data is generated on a different grid.

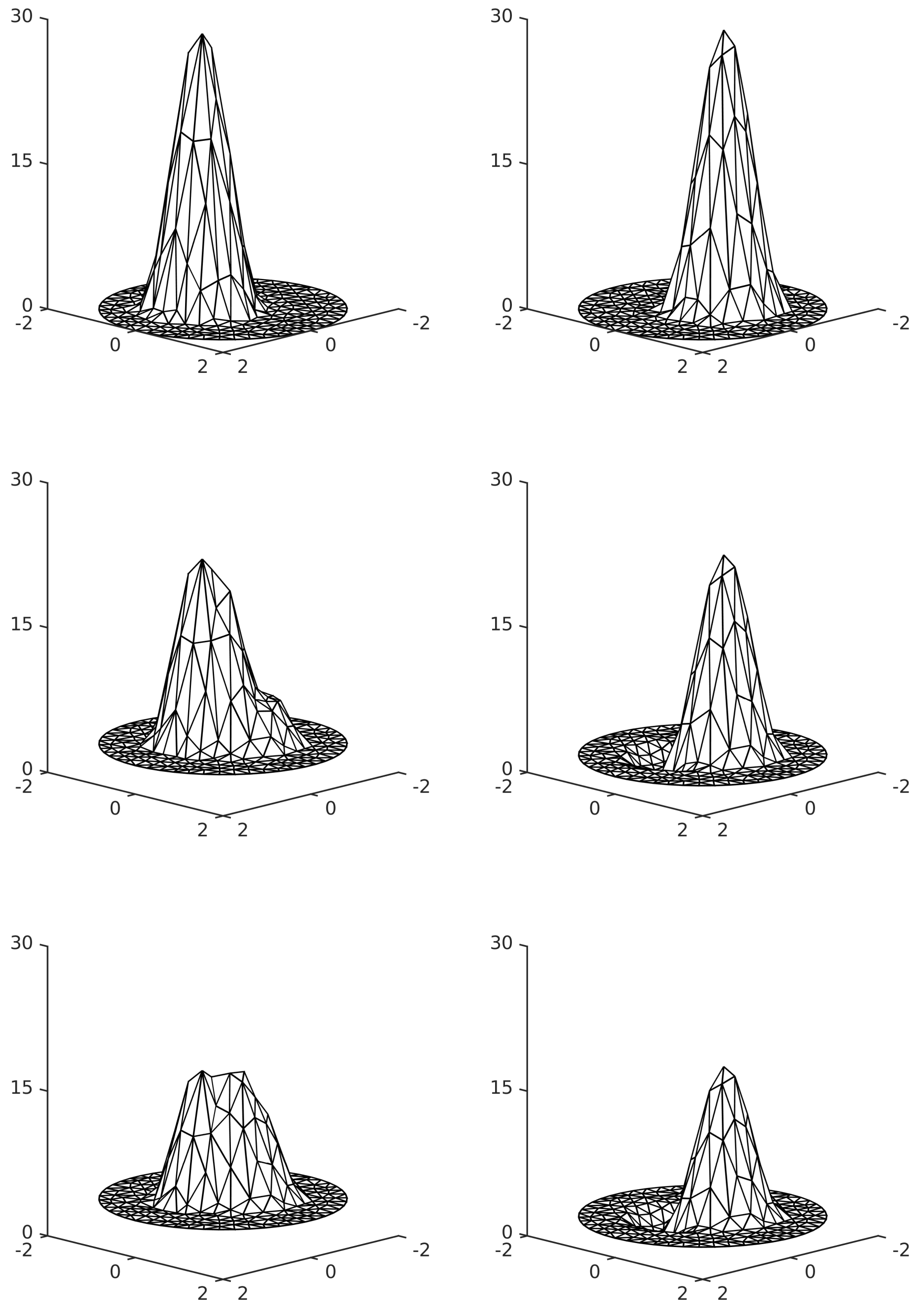


Figure 8.7: Evolution of $u_1$ on the left and $u_2$ on the right. Snapshots were taken at $t = 0$, $t = 0.25$ and $t = 0.5$.

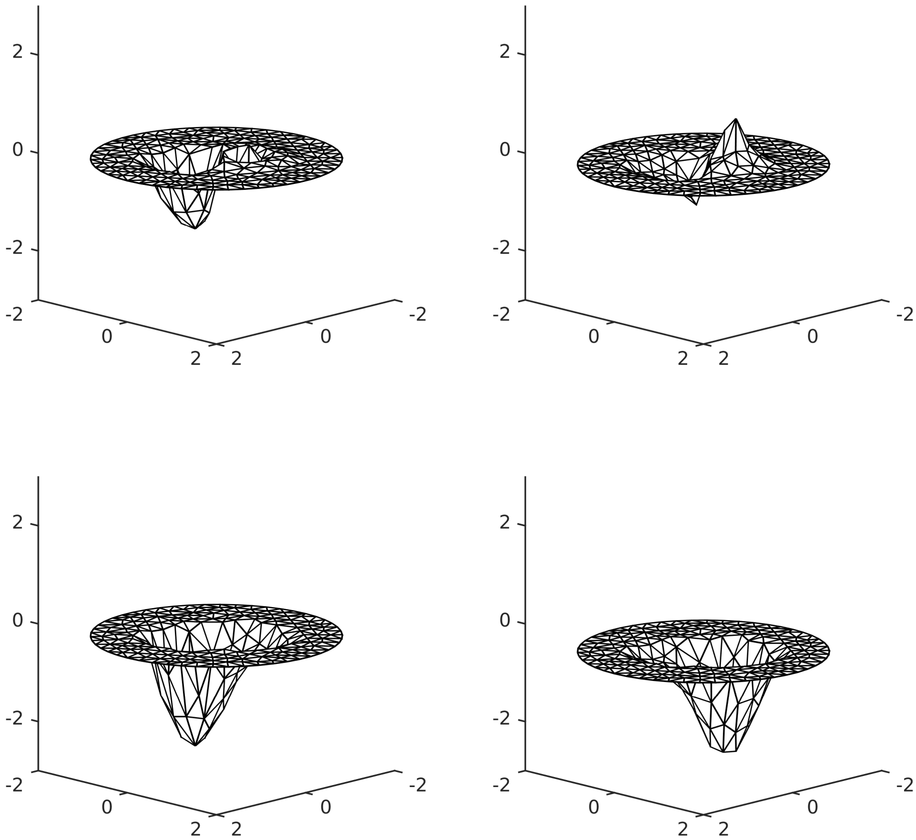


Figure 8.8: Space time dependent reconstruction of $W$ at time $t = 0.5$. From the top left to the bottom right the order is $W_{11}$, $W_{12}$, $W_{21}$, $W_{22}$.

# CHAPTER 9

## Conclusion

In this thesis we have investigated parameter identification in general systems of semilinear reaction-diffusion equations, where the parameters are space and time dependent. The first thing we noticed is that the solution of a parameter identification problem associated with those systems is not unique in general and in some cases not even locally. To deal with ill-posedness in the sense of non continuous dependence of the parameters on the data, we analyzed regularization properties of the parameter-to-state map associated with the underlying partial differential equation. We only proposed a variational regularization approach, i.e. Tikhonov regularization, but in principle the introduced concepts should carry over to other regularization methods.

Before we analyzed the problem itself, we stated the well known regularization theory of Tikhonov regularization for nonlinear inverse problems, which we slightly adapted for our needs. We therefore introduced a special concept of the weak sequential closedness property, which we called $\tau$-weak sequential closedness and can includes stronger compactness properties. Also the minimization of Tikhonov functionals under certain constraints onto the forward operator was discussed.

Then, we introduced the weak solution theory for nonlinear parabolic PDEs in general manner and a regularity theory from [32], which allows to obtain stronger embeddings for the solution space. This then can be used to show that the parameter-to-state is differentiable, as long as the superposition operator that is given through the nonlinearity $g$ is well behaved. The differentiability of the parameter-to-state map was derived as in [58, 57] with the help of the implicit function theorem. For this, results concerning superposition operators [5] dictated that the growth of the nonlinearity $g$ has to be examined. Depending on this, the parameter space for the problem may have to be chosen as an $L_p$ space with $p > 2$, if the function $g$ is nonlinear in one of the arguments.

To ensure that regularization happens, assumptions that help showing the $\tau$-

weak sequential closedness property of the forward operator are discussed. It turned out, that if $g$ is not linear in $p$, we had to restrict the domain of definition operator. We have shown, that if the domain is chosen as a subset of $L_\infty(\Omega_T) \cap BV(\Omega_T)$ the $\tau$-weak sequential closedness property can still be shown. Further, this restriction turned out to be not too strong for most parameter identification problems.

In order to minimize the Tikhonov functional numerically, we derived the adjoint of the derivative of the parameter-to-state map. This was done strict functional analytic sense for general semilinear systems, where we exploited the theory of densely defined unbounded operators to stay in the correct spaces for our setting. After that we also looked at restricted measurements which are given via a linear observation operator and ensured, that all previous results stay applicable in three common cases of measurements.

The adjoint of the derivative of the parameter-to-state map is also necessary if one wants discuss source conditions. It turned out that source conditions for equations of our type can indeed be interpreted as smoothness conditions. In particular, an element of the subdifferential of the penalty term can only fulfill a source condition if it is located in a subspace of the solution space and fulfills a final condition. In the case of a system of equations, there is also a coupling condition onto the parameters. Also, we found an interesting connection between approximate controllability and approximate source conditions.

While we were not able to survey restrictions that can lead to uniqueness of solutions of the parameter identification problem in systems, we at least showed that for three different types of measurement restrictions in scalar equations uniqueness can be shown. This was done with the help of an adjoint approach proposed in [21]. Especially the results concerning snapshot measurements are to the authors best knowledge new results.

Finally, we discussed the numerical implementation and performed numerical experiments in the scalar as well as in the system case, with special focus on the application of sparsity regularization. In the scalar case we were able to reconstruct parameters in a nonlinear example equation coming from the biochemical evolution of genes. While we were not able to obtain similar results in the system case due to non uniqueness, at least we have shown that the numerical identification of space time dependent parameters in a system in principle is possible.

Future research can for example be concerned with the derivation of properties of parameters, under which uniqueness of a solution of the parameter identification can be shown. Also an extension of the proposed theory to quasilinear parabolic partial differential including nonlinear boundary equations could be considered. At least the solution theory we utilized stays valid in this case [32]. For the numerical part one could try utilizing adaptive solvers to speed up the inversion process or more advanced algorithms in order to minimize the Tikhonov functional. Also an application of the theory to real world problems is desirable, especially for the embryogenesis example that we frequently used to explain our abstract concepts in concrete situations.

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