

Variational Regularisation for Multi-Data Inverse Problems

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Abstract

This thesis covers analytical and numerical aspects of variational regularisation for multi-data inverse problems. Such problems emerge when splitting an inverse problem into subproblems possibly featuring different degrees of ill-posedness and different scales, noise levels and noise models. To address these different properties, a Tikhonov approach for such problems featuring joint regularisation and a weighted sum of discrepancies is proposed and lies in the focus of our considerations. The specific structure of the multi-data problem allows for partial solutions (solving some but not all subproblems) and emphasis lies on their properties. We show that with a suitable parameter choice rule, subsequential convergence to a partial solution can be obtained, and under additional source conditions, convergence rates for discrepancies and the Bregman distance are presented. Moreover, one sees that said limit partial solution solves a Tikhonov problem for the unsolved problems, featuring the solved subproblems as prior. The capabilities of norms and the Kullback-Leibler divergence as discrepancies are discussed, showing that they are indeed suitable discrepancies. As joint regularisation functional, a version of Total Generalised Variation (TGV) for vector-valued functions is considered. Its capability of promoting smooth solutions and penalising disjoint edge sets and features makes it suitable as joint regularisation in imaging. We apply a Tikhonov approach employing Kullback-Leibler divergence as discrepancies and joint TGV as regularisation functional to reconstruct multi-spectral Scanning Transmission Electron Microscopy (STEM) Computed Tomography. A primal-dual algorithm based scheme is proposed to solve such problems, and this reconstruction algorithm creates adequate, smooth yet sharp reconstructions superior in image quality to other standard methods.

Zusammenfassung

Diese Arbeit behandelt analytische und numerische Aspekte einer variationellen Regularisierung für multi-data inverse Probleme. Solche Probleme entstehen wenn ein inverses Problem in Subprobleme aufgespalten wird, welche unterschiedliche Grade von nicht Wohlgestelltheit, unterschiedliche Rauschniveaus und Rauschmodelle besitzen. Um diese Unterschiede miteinzubeziehen, wird ein Tikhonov Ansatz für solche Probleme mit einem gemeinsamen Regularisierungsfunktional und einer gewichteten Summe von Diskrepanz-Termen betrachtet und steht im Zentrum dieser Arbeit. Die spezifische Struktur des multi-data Problems ermöglicht die Betrachtung von Teillösungen und besonderes Augenmerk liegt auf deren Eigenschaften. Wir zeigen, dass mit geeigneter Parameterwahl Konvergenz zu einer Teillösung erzielt werden kann und mit zusätzlichen Voraussetzungen auch deren Konvergenzraten bestimmt werden können. Darüber hinaus sieht man, dass besagte Teillösung die Lösung eines Tikhonov Ansatzes für die ungelösten Probleme mit den gelösten Problemen als Prior ist. Es wird gezeigt, dass Normen und die Kullback-Leibler Divergenz geeignete Diskrepanzen sind. Zur Regularisierung wird eine Version von Total Generalised Variation (TGV) für vektorwertige Funktionen betrachtet, deren Eigenschaft glatte Lösungen zu erzeugen und disjunkte Kantenmengen zu bestrafen es zu einem geeigneten Regularisierungsfunktional für Imaging machen. Wir betrachten solch einen Tikhonov Ansatz mit Kullback-Leibler Divergenzen und TGV Regularisierung um multi-spektrale Scanning Transmission Electron Microscopy (STEM) Computed Tomography zu rekonstruieren. Basierend auf einem primalen-dualen Algorithmus wird eine Methode zur Lösung solcher Probleme abgeleitet. Dieser Algorithmus erzeugt glatte und scharfe Rekonstruktionen, und numerische Ergebnisse zeigen, dass dieser Algorithmus adäquate Rekonstruktionen erzeugt, die standard Rekonstruktionsmethoden in Qualität überlegen sind.

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Introduction

Many mathematical problems occurring in industrial and scientific applications cannot be solved by direct computation, but rather require the inversion of a process. This means considering a process T , which takes an input u , transforming it into an output f , but trying to find a suitable input leading to given output f . Hence, one considers problems of the form

$$Tu = f$$

typically featuring infinite-dimensional spaces, where the output f and the process $T: X \rightarrow Y$ are given, and one aims to solve this equation for the necessary input u . Such problems often occur when one obtains data f through a well-understood process modeled by T , but aims to reconstruct the cause u which would have led to f .

A simple example of such problems, which nicely illustrates the difference in thought between direct and inverse problems, is deconvolution, where one tries to solve

$$k * u = f, \quad \text{where} \quad k * u(\cdot) = \int_{\mathbb{R}^n} u(\cdot - y)k(y) dy,$$

with given f and k for u , meaning one tries to invert the convolution operation. This theoretical setting can for example be found in the backward heat equation for practical purposes. Imagine a rod of iron whose heat distribution over time is observed. Obtaining the heat distribution at some point in time from given starting distribution is a basic PDE problem one can solve via convolution $h * u_0 = u_1$, where u_0 denotes the initial distribution and h the heat-kernel. This would represent the direct problem, while obtaining a starting distribution which would have led to a given distribution later in time represents the inverse problem. Therefore, for given heat-distribution u_1 at time $t = 1$ one solves $h * u_0 = u_1$ for u_0 .

A problem we focus on more heavily in later sections is the inversion of the Radon transform used in CT [3]. The Computed Tomography (CT) method is used in medical practice to obtain 3-dimensional density distributions of patients. In order to do so, a sequence of X-ray images of the patient from different angles is taken. Through mathematical modelling it is easy to understand how to obtain the sinograms (X-ray data) from given density distribution, while the converse is not so obvious. Hence, in

order to obtain suitable CT reconstructions for the physician to analyse, one solves

$$Tu = f \tag{1}$$

where T models the forward operator, i.e. the procedure of obtaining the sinograms data from the density distribution, and f the sinogram data obtained from the examination of a patient. Such measurements f however typically suffer from noise, in particular Poisson distributed noise since the measurement is made via detection counts of the transmitted photons which typically is modelled to be Poisson distributed, see e.g. [50].

Unfortunately, solving an inverse problem is often not stable (in particular the ones mentioned above), i.e. small aberration in data f might result in massive changes in the corresponding solution u . Thus, regularisation methods are required in order to overcome this stability issue. Specifically, the Tikhonov regularisation [47, 48] is a commonly used method, and since this thesis will focus on Tikhonov regularisation, we quickly motivate its use:

Although an inverse problem is not always solvable, in practical applications one might still be interested in finding an approximate solution as this might appear sufficient. Therefore, it is reasonable to look for u^\dagger , such that Tu^\dagger is as close to f as possible, and consequently one could try to solve

$$u^\dagger \in \underset{u \in X}{\operatorname{argmin}} D(Tu, f) \tag{2}$$

instead, where $D(Tu, f)$ is a suitable measurement of the distance between f and Tu , commonly referred to as the discrepancy function. In case of working on a normed vector space, a natural choice would be the norm, i.e. $D(a, b) = \|a - b\|$, but more complex choices are possible and might be necessary.

However, Problem (2) might still not be solvable as $u \mapsto D(Tu, f)$ does not attain a minimum. Also, in practical applications, a procedure to measure data inherently contains measurement inaccuracies and noise, since theoretical assumptions are not being perfectly matched by reality. Thus, often only f^δ is available, which is a version of f with noise, and this poses a particular problem when solving (2) is not stable either.

Therefore, one introduces a regularisation parameter α and a regularisation function R and considers

$$u^\dagger \in \underset{u \in X}{\operatorname{argmin}} D(Tu, f) + \alpha R(u). \tag{3}$$

It is reasonable to choose R , such that (3) is solvable, and enforces desired properties of solutions, i.e. R should penalise undesired properties in u occurring due to noise in the data. Tikhonov regularisation methods are well studied, in particular the stability and convergence results for vanishing noise [25] play an integral role in this theory.

In order to get insight into the chemical make-up of a specimen, one uses Scanning Transmission Electron Microscopy (STEM), see [4, 36, 6, 35] and references therein. This enables one to obtain sinogram data corresponding to the density distribution of specific chemical components, thus allowing a CT reconstruction of the specific density distributions. Unfortunately, these data sets leave things to be desired in terms of quality due to the high time-consumption required to record several such data sets. Thankfully, one would expect the reconstructions of the individual spectra to contain complementing information, as one would expect a weighted sum of the densities to result in the mass-density distribution, or common edges to occur when the density of one element plumps and the others rise conversely. Therefore, one would like to reconstruct these multi-spectral data sets jointly, exploiting information contained in other spectra's data.

Following this idea, joint regularisation becomes more common, not solving problems individually, but several inverse problems jointly. This applies in particular to problems expected to have complementing information where a joint solution can take advantage of the information in the other inverse problems. Hence, one considers the problems

$$T_1u = f_1, \quad T_2u = f_2, \quad \dots \quad T_Mu = f_M. \quad (4)$$

Note that this setting does not solely allow for individual independent reconstructions being coupled for the sake of complementing information, but also incorporates inverse problems being coupled in nature, i.e. subproblems together posing a single inverse problem. It might be reasonable to split an inverse problem into such subproblems, as they might feature different degrees of ill-posedness, scales, noise levels and noise models which require individual consideration.

Relevant examples of the use of joint regularisation are CT reconstruction of Scanning Transmission Electron Microscopy (STEM) data or PET-MRI reconstructions in applied medicine, for example the Joint TGV reconstruction proposed in [29]. In the latter, the quality of PET is typically low and it is expected that complementing information from the MR images improve the quality of PET reconstructions.

In order to apply Tikhonov regularisation to such multi-data problems, one considers

$$u^\dagger \in \operatorname{argmin}_{u \in X} \left(\sum_{i=1}^M \lambda_i D_i(T_i u, f_i) \right) + R_\alpha(u) \quad (5)$$

with individual discrepancy terms and weights, but one joint regularisation function depending on a parameter α .

Although the general theory could be extended to the multi-data situation by considering it as a problem on the product space, it would not take into account the before mentioned properties of the individual subproblems. The structure of (4) and (5) raises the question of how the convergence result for vanishing noise in the single-data regularisation transfer into the multi-data setting if there are partial solutions, i.e. solutions to some, but not all problems simultaneously. This thesis will introduce a theory which considers such convergence results.

In order to bridge the gap between theoretical ideas and practical applications, we investigate how the theory works for specific discrepancies such as powers of norms and the Kullback-Leibler divergence [9]. The latter is particularly suitable for measuring the discrepancy of Poisson distributed noise which is present in many noise models and is thus regularly considered as a discrepancy function [40, 44, 16].

As application of this theory, we consider regularisation with the Total Generalised Variation (TGV) functional [14, 13], a regularisation commonly used in imaging, which generalises the Total Variation (TV) of functions [2]. TV regularisation has the specific advantage to other regularisation methods of promoting piece-wise constants solutions allowing hard transitions as would be expected to occur in many applications. However, piece-wise constant solutions are often not suitable, which is overcome by the TGV functional promoting piece-wise polynomial solutions. In particular this functional can also be used in a multi-dimensional setting [11, 29] and is shown to enforce common features such as complementing edges.

Finally, when using such approaches and being faced with a concrete problem, also a numerical framework is required in order to solve Tikhonov problems with concrete data and parameter. We show such a framework used onto the STEM CT reconstruction using TGV and the Kullback-Leibler divergence approaches which relies on a primal-dual optimisation method [17]. While a TV approach with norm discrepancies for individual reconstruction was used in [37] with promising results, one hopes that Kullback-Leibler divergence, which is more suitable for the occurring noise, and TGV, which allows for more realistic solutions, further improves the resulting reconstruction.

After a quick recapitulation of well-known mathematical foundations, this thesis is separated into four Parts. Part I discusses a general theory for Tikhonov regularisation. Therein the classical single-data Tikhonov regularisation is discussed as a basis for the subsequent multi-data Tikhonov approach, with particular focus on convergence results for partial solutions. In Part II, norms and the Kullback-Leibler divergence are investigated with respect to their properties required to be suitable choices as discrepancies with respect to the theory of Part I. In Part III, Total Deformation and Total Generalised Variation are introduced and their properties as regularisation functional are discussed. In particular, their applicability to linear inverse problems are investigated. Finally in Part IV, the application of the previously discussed to the multi-spectral STEM CT reconstruction is considered. Therein, the properties of the Radon transform, as well as a numerical framework and a discussion of results is presented.

1. Mathematical Foundation

In this chapter we establish some well-known theoretical aspects for the sake of completeness, to set notation and for later reference. Therefore, this chapter is more of a brief summary containing results required for the later theory than a chapter discussing these topics in detail. For more precise information and further details please look at the mentioned literature.

1.1. Topologies

For our observations, the notion of convergence will play an important role, and it is described in a general way by topological spaces. Also continuity and compactness properties which will play a part in inverse problems are related to topological aspects. For a more complete introduction and discussion of topologies, we refer to [38] and the references therein.

Definition 1.1. *Let X be a set and let $Pot(X)$ denote the power set of X . A set $\mathcal{T} \subset Pot(X)$ is called a topology, iff for any index set I , mapping $f: I \rightarrow \mathcal{T}$ and finite index set $J \subset I$ the properties*

$$X \in \mathcal{T}, \quad \emptyset \in \mathcal{T}, \quad \bigcup_{i \in I} f(i) \in \mathcal{T}, \quad \bigcap_{i \in J} f(i) \in \mathcal{T},$$

hold. In this case $A \in \mathcal{T}$ is called open, and the conditions state that X and \emptyset are open, arbitrary unions of open sets are again open, and finite intersections of open sets are open. A subset $B = A^c$ for A open is called closed. Moreover, the pair (X, \mathcal{T}) is called a topological space.

From this definition, one can derive a notion of convergence which is directly impacted by the open sets in \mathcal{T} .

Definition 1.2. *In a topological space (X, \mathcal{T}) we call a set $U \subset X$ a neighbourhood of $x \in X$, if $U \in \mathcal{T}$ and $x \in U$. We then say a sequence $(x^n)_n \subset X$ converges to x (also $x^n \xrightarrow{\mathcal{T}} x$ or $\lim_n x^n = x$) if and only if for every neighbourhood U of x there is a number $N(U) \in \mathbb{N}$ such that $x^n \in U$ for all $n \geq N(U)$. A topological space (X, \mathcal{T}) is called Hausdorff, if for all $x, y \in X$ with $x \neq y$ there exist disjoint neighbourhoods of x and y .*

Lemma 1.3. *In a Hausdorff space, a sequence has at most one limit.*

Based on the concept of convergence one can develop a notion of continuity and assign certain properties to subsets of X .

Definition 1.4. For two topological spaces (X, \mathcal{T}_X) and (Y, \mathcal{T}_Y) , we say a function $f: X \rightarrow Y$ is continuous with respect to the \mathcal{T}_X and \mathcal{T}_Y topologies (strictly speaking sequentially continuous) if for a sequence $(x^n)_n \subset X$, $x^n \xrightarrow{\mathcal{T}_X} x$ implies $f(x^n) \xrightarrow{\mathcal{T}_Y} f(x)$.

Definition 1.5. Let (X, \mathcal{T}_X) be a topological space.

- A set $K \subset X$ is called (sequentially) precompact, if every sequence $(x^n)_n \subset K$ admits a \mathcal{T}_x -convergent subsequence in X .
- A set $D \subset X$ is called dense, if for every $x \in X$ there is a sequence $(x^n)_n \subset D$ such that $x^n \xrightarrow{\mathcal{T}_X} x$.

Remark 1.6. We will in the following say continuity when meaning sequential continuity and precompact when meaning sequentially precompact, as we will mainly work with sequences and thus only use sequential continuity and precompactness.

However, sometimes continuity is a too strong requirement but a weaker notion would be sufficient. Closedness is such a weaker concept of regularity of functions.

Definition 1.7. A function $T: \text{dom}(T) \subset X \rightarrow Y$ between topological spaces X, Y is closed with respect to \mathcal{T}_X and \mathcal{T}_Y , if for any sequence $(x^n)_n \subset X$:

$$(x^n \rightarrow x, Tx^n \rightarrow y) \quad \Rightarrow \quad (x \in \text{dom}(T), Tx = y).$$

1.2. Normed Vector Spaces

In order to equip topological spaces with an algebraic structure, we introduce vector spaces which are commonly used in various fields. Their topology is typically adapted to the algebraic structure, thus making it possible to simplify topological problems. For a more detailed description, we refer to [42, 15] and the references therein.

Definition 1.8 (Vector space). Let V be a set such that there are operations

$$+: V \times V \rightarrow V \quad \text{and} \quad \cdot: \mathbb{R} \times V \rightarrow V, \quad (6)$$

such that the structure $(V, +)$ induces an Abelian group, i.e. let the addition be commutative, associative, contain a neutral element 0 and inverse elements to every $v \in V$

exist, typically denoted by $-v$. Furthermore, for $\alpha, \beta \in \mathbb{R}$ and $v, w \in V$, let

$$(\alpha + \beta)v = \alpha v + \beta v, \quad \alpha(v + w) = \alpha v + \alpha w, \quad \alpha(\beta v) = (\alpha\beta)v, \quad 1v = v.$$

Then V is called a vector space over \mathbb{R} .

Furthermore, a function $\|\cdot\|: V \rightarrow \mathbb{R}$ is called a norm if it is positive definite, absolutely homogeneous and satisfies a triangle inequality, i.e. for $v, w \in V$ and $\alpha \in \mathbb{R}$,

$$\|v\| \geq 0, \quad \|v\| = 0 \Leftrightarrow v = 0, \quad \|\alpha v\| = |\alpha|\|v\|, \quad \text{and} \quad \|v + w\| \leq \|v\| + \|w\|.$$

We call a vector space normed and write $(V, \|\cdot\|)$, if V is a vector space which admits a norm $\|\cdot\|$. Furthermore, $U \subset V$ such that U is a vector space with the same operations as V (restricted to U) is called a subspace.

A vector space is a solely algebraic structure, but normed spaces can be equipped with a topology adapted to these structures.

Proposition 1.9. *On a normed space $(V, \|\cdot\|_V)$, there is a topology such that for any sequence $(v^n)_n \subset V$, and any $v \in V$,*

$$\lim_{n \rightarrow \infty} v^n = v \quad \Leftrightarrow \quad \lim_{n \rightarrow \infty} \|v^n - v\| = 0.$$

This topology is called the norm topology (also topology induced by the norm). In particular, the topological space induced by a norm is a Hausdorff space. We will say convergence with respect to the norm or $\|\cdot\|$ when actually meaning convergence with respect to the norm topology.

Definition 1.10. *We call a sequence $(f^n)_n$ such that for every $\epsilon > 0$ there is $N(\epsilon) \in \mathbb{N}$ with $\|f^n - f^m\| \leq \epsilon$ for $n, m \geq N(\epsilon)$ a Cauchy sequence. A normed space V is called complete, if every Cauchy sequence possesses a limit in V . Such a normed complete space is also referred to as Banach space. In particular a closed subspace of a Banach space is itself complete.*

An important tool in both understanding and combining normed vector spaces are linear continuous functions between normed spaces.

Definition 1.11. *Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be two normed spaces. We call a function $T: X \rightarrow Y$ linear, if for $v, w \in X$ and $\alpha \in \mathbb{R}$,*

$$T(\alpha v + w) = \alpha T(v) + T(w).$$

Moreover the function T is called continuous with respect to the norm topologies if

$$\|T\| = \sup_{\substack{v \in X \\ \|v\|_X \leq 1}} \|Tv\|_Y < \infty, \quad (7)$$

which is compatible with the notion of continuity defined in Definition 1.2. We call $\text{Ker}(T) = \{x \in X \mid Tx = 0\}$ the kernel and $\text{Rg}(T) = \{Tx \mid x \in X\}$ the range of T .

We define the dual space of X , denoted with X^* as

$$X^* = \{\xi: X \rightarrow \mathbb{R} \mid \xi \text{ is linear and continuous w.r.t. } \|\cdot\|_X \text{ and } |\cdot|\},$$

i.e. the space of all linear and continuous functionals from X onto \mathbb{R} . The dual space X^* equipped with the norm defined in (7) is a Banach space even if X is not complete.

For a linear continuous operator $T: X \rightarrow Y$ we define the adjoint operator as the unique operator such that

$$T^*: Y^* \rightarrow X^* \text{ with } \langle \eta, Tx \rangle_{Y^* \times Y} = \langle T^* \eta, x \rangle_{X^* \times X} \text{ for all } \eta \in Y^*, x \in X.$$

Proposition 1.12. *There is a topology $\mathcal{T}_{X,W}$ (called the weak topology) on a normed space $(X, \|\cdot\|_X)$ with the following properties: A sequence $(v^n)_n$ converges to v in $\mathcal{T}_{X,W}$ (also converges weakly or $v^n \rightharpoonup v$) if for every $\xi \in X^*$, $\lim_n \xi(v^n) = \xi(v)$. Alternatively, one can say that the weak topology is the weakest (coarsest) topology for which $\xi(\cdot)$ is continuous for every $\xi \in X^*$.*

Further, there exists a topology \mathcal{T}_{X^*,W^*} on X^* , which is the finest topology on X^* such that for all $x \in X$ the mapping $\xi \mapsto \xi(x)$ is continuous. Hence, for a sequence $(\xi^n)_n \subset X^*$ we say $\xi^n \rightharpoonup^* \xi$ (also $\xi^n \xrightarrow{\mathcal{T}_{X^*,W^*}} \xi$) if for all $x \in X$: $\xi^n(x) \rightarrow \xi(x)$ as $n \rightarrow \infty$.

Lemma 1.13. *The weak topology is indeed a topology, in fact $(V, \mathcal{T}_{V,W})$ is a Hausdorff space which is adapted to the vector space structure, i.e. addition and multiplication remain continuous under the weak topology. Convergence with respect to the norm implies weak convergence. Moreover, if $T: (X, \|\cdot\|_X) \rightarrow (Y, \|\cdot\|_Y)$ is continuous with respect to the norm topologies, it is also continuous with respect to the weak topologies, i.e. $T: X \rightarrow Y$ is continuous with respect to $\mathcal{T}_{X,W}$ and $\mathcal{T}_{Y,W}$.*

One can also consider the dual of the dual space to get further insight into the properties of a normed space and its weak topology.

Definition 1.14. *We call the space $X^{**} = (X^*)^*$ the bi-dual space of X , and define the*

canonical embedding

$$\tilde{t}: X \rightarrow X^{**}, \quad \tilde{t}(x)(\xi) = \xi(x) \quad \text{for all } \xi \in X^*, x \in X \quad (8)$$

which is isometric with respect to $\|\cdot\|_X$ and $\|\cdot\|_{X^{**}}$, but not necessarily surjective. If \tilde{t} is additionally surjective, the space X is called reflexive.

Theorem 1.15 (Alaoglu's Theorem for Reflexive Spaces). *Let $(X, \|\cdot\|_X)$ be a normed reflexive space. Then the set*

$$B(0, 1) = \{x \in X \mid \|x\|_X < 1\}$$

is sequentially precompact with respect to the weak topology.

Lemma 1.16. *Let X be a normed space, and $U \subset X$ a subspace. Then U is dense, if and only if for $\xi \in X^*$, $\xi(U) = \{0\}$ implies $\xi = 0$.*

So the properties of linear continuous functions on vector spaces are important, however, sometimes one only has the weaker property of closedness. Obviously being continuous is a stronger property than being closed, but in the linear setting and with suitable assumptions both are equivalent.

Theorem 1.17. *Let X and Y be Banach spaces and $T: X \rightarrow Y$ linear. Then T is continuous with respect to the norm topologies, if and only if T is closed with respect to the norm topologies. This in particular also holds if $\text{dom}(T)$ is a closed subspace of X .*

1.3. Measure Theory

Many applications in classical analysis rely on integration. However, the setting in which Riemann integration is applicable is limited. In order to generalise integrals to more universal situations and find a suitable theory concerning it, one introduces concepts of measurability and measures. A detailed description can be found in [19, 22].

Definition 1.18. *A system \mathcal{A} of subsets of a set $\Omega \neq \emptyset$ is called a σ -algebra if for $A \in \mathcal{A}$ and for a sequence $(A_n)_n \subset \mathcal{A}$*

$$\emptyset \in \mathcal{A}, \quad \Omega \in \mathcal{A}, \quad A^c \in \mathcal{A}, \quad \text{and} \quad \bigcup_{i=1}^{\infty} A_n \in \mathcal{A}. \quad (9)$$

The elements $A \in \mathcal{A}$ are called measurable and the tuple (Ω, \mathcal{A}) is called a measurable space. A function $f: \Omega_1 \rightarrow \Omega_2$ with measurable spaces $(\Omega_1, \mathcal{A}_1)$ and $(\Omega_2, \mathcal{A}_2)$ is called measurable (more precisely \mathcal{A}_1 - \mathcal{A}_2 measurable) if for $A \in \mathcal{A}_2$ the preimage $f^{-1}(A) \in \mathcal{A}_1$.

If (Ω, \mathcal{T}) is Hausdorff space, one can equip Ω with the Borel-algebra \mathcal{B} , the smallest σ -algebra containing all open sets in \mathcal{T} .

Such measurable functions play an integral role for measure theory, and thus verifying measurability of functions is necessary. Fortunately, many common operations on measurable functions maintain measurability.

Lemma 1.19. *Let $(\Omega_i, \mathcal{A}_i)$ be measurable spaces for $i = 1, 2, 3$ and let $f: \Omega_1 \rightarrow \Omega_2$ and $g: \Omega_2 \rightarrow \Omega_3$ be measurable functions in their respective senses. Then the composition $g \circ f: \Omega_1 \rightarrow \Omega_3$ is \mathcal{A}_1 - \mathcal{A}_3 measurable.*

If Ω_1 and Ω_2 are Hausdorff spaces equipped with the corresponding Borel-algebras \mathcal{B}_1 and \mathcal{B}_2 , and $f: \Omega_1 \rightarrow \Omega_2$ is continuous, then f is measurable with respect to \mathcal{B}_1 and \mathcal{B}_2 .

Next, one wants to introduce a measure, a function on \mathcal{A} which assigns each measurable set a value, and is adapted to disjoint set-union.

Definition 1.20. *For a measurable space (Ω, \mathcal{A}) a mapping $\mu: \mathcal{A} \rightarrow [0, \infty]$ such that for any sequence of disjoint sets $(A_n)_n \subset \mathcal{A}$*

$$\mu(\emptyset) = 0, \quad \text{and} \quad \mu\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{i=1}^{\infty} \mu(A_n) \quad (10)$$

holds, is called a measure, and the triple $(\Omega, \mathcal{A}, \mu)$ is called a measure space. Moreover, if $\mu(\Omega) < \infty$, μ is called a finite measure and if in addition $\mu(\Omega) = 1$, μ is referred to as probability measure and the measure space is called a probability space. Furthermore, a measure μ is called σ -finite if there is a sequence of measurable sets $(A_n)_n$ such that $\bigcup_n A_n = \Omega$ and $\mu(A_n) < \infty$.

Lemma 1.21. *There is a unique measure λ on $\Omega = \mathbb{R}^d$ equipped with the Borel-algebra induced by the standard l^2 topology in \mathbb{R}^d such that for $a = (a_1, \dots, a_d) \in \mathbb{R}^d$ and $b = (b_1, \dots, b_d) \in \mathbb{R}^d$ with $a_i < b_i$*

$$\lambda([a_1, b_1] \times \dots \times [a_d, b_d]) = \prod_{i=1}^d (b_i - a_i). \quad (11)$$

This measure is called the Lebesgue measure and can be interpreted as the measure whose

value of any cuboid is the product of its side-lengths, and is thus a natural measure to equip \mathbb{R}^d with.

In the upcoming integral theory, sets $A \in \mathcal{A}$ with measure $\mu(A) = 0$ do not have any impact, hence we use the following notation to denote such sets.

Definition 1.22. In a measure space $(\Omega, \mathcal{A}, \mu)$ a set $A \in \mathcal{A}$ such that $\mu(A) = 0$ is called a null-set. Moreover we say a Condition C is satisfied μ almost everywhere (a.e.) (almost surely in case of probability measures) if the set on which C is not fulfilled is subset of a null-set. Also, for a topological space X and a sequence of functions $(f_n)_n$ with $f_n: \Omega \rightarrow X$ measurable, we say f_n converges toward f almost everywhere if $\{x \in \Omega \mid f_n(x) \not\rightarrow f(x)\}$ is a null-set.

Now we have a good understanding of measures and measurability, however the aim is to define and derive a suitable notion of integrals with respect to measures.

Definition 1.23. Let $(\Omega, \mathcal{A}, \mu)$ be a measure space. We call a function $g: \Omega \rightarrow [0, \infty]$ simple if g is measurable with respect to the Borel-algebra on $[0, \infty]$ and attains only finitely many values on Ω . Then, for a measurable function $f: \Omega \rightarrow [0, \infty]$, we define the (Lebesgue-)integral

$$\int_{\Omega} f \, d\mu = \sup \left\{ \sum_z z \mu(\{h = z\}) \mid h \text{ is simple and } h \leq f \right\}, \quad (12)$$

where the value $+\infty$ is allowed.

Moreover, for measurable functions $f: \Omega \rightarrow [-\infty, \infty]$ we denote with $f^+ = \max(f, 0)$ and $f^- = -\min(f, 0)$, and define

$$\int_{\Omega} f \, d\mu = \int_{\Omega} f^+ \, d\mu - \int_{\Omega} f^- \, d\mu, \quad (13)$$

in case the value ∞ is attained by at most one of the integrals, but not both. Note that the integrals on the right-hand side are already defined, and we call a function integrable if the integral is well-defined and attains a finite value.

This notion of integrals carries some properties such as linearity and monotonicity which one knows and expects from classical integration theory.

Lemma 1.24. Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and let $f, g: \Omega \rightarrow \mathbb{R}$ be measurable and $\alpha \in \mathbb{R}$. Then

$$\left| \int_{\Omega} f \, d\mu \right| \leq \int_{\Omega} |f| \, d\mu, \quad \text{and} \quad \int_{\Omega} \alpha f + g \, d\mu = \alpha \int_{\Omega} f \, d\mu + \int_{\Omega} g \, d\mu, \quad (14)$$

and in particular f is integrable, if and only if $|f|$ is integrable. Moreover, if $f \geq g$ a.e., then $\int_{\Omega} f \, d\mu \geq \int_{\Omega} g \, d\mu$, and if $\int_{\Omega} |f| \, d\mu < \infty$, then also $|f| < \infty$ a.e..

These notions of measurable and integrable functions can be transferred into a space of integrable functions. However, as functions differing only on a null-set do have the same integrational properties, one needs to consider classes of equivalent functions.

Definition 1.25. Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, and we call two measurable functions f and g equivalent if $f = g$ a.e., which induces an equivalence relation on the measurable functions, and we denote with $[f]$ the equivalence class containing f . Then, for $p \in [1, \infty)$ we define for $f \in [f]$

$$\|f\|_{L_{\mu}^p} = \left(\int_{\Omega} |f|^p \, d\mu \right)^{\frac{1}{p}}, \quad \|f\|_{L_{\mu}^{\infty}} = \operatorname{ess-sup}_{\Omega}(|f|) = \inf\{C \in [0, \infty] \mid |f| \leq C \text{ a.e.}\} \quad (15)$$

which is independent of the representative. Further, for $p \in [1, \infty]$, we define the corresponding function spaces

$$L_{\mu}^p(\Omega) = \{[f] \mid f: \Omega \rightarrow \mathbb{R} \text{ measurable and } \|f\|_{L_{\mu}^p} < \infty\}. \quad (16)$$

Later, we will not explicitly talk about classes but functions, and implicitly refer to classes of the functions, which usually does not have any impact since the observations only require a.e. properties. We will also refer to $\|\cdot\|_{L_{\mu}^p}$ as $\|\cdot\|_p$ and call $\|\cdot\|_{\infty}$ the supremum norm.

Also, it is well-known that the corresponding dual spaces $(L_{\mu}^p(\Omega))^* = L_{\mu}^{p^*}(\Omega)$ with $\frac{1}{p} + \frac{1}{p^*} = 1$ for $p \in (1, \infty)$ and $p^* = \infty$ for $p = 1$ in case of a finite measure space. Particularly, for $p \in (1, \infty)$ the spaces $L_{\mu}^p(\Omega)$ are reflexive and for $p \in [1, \infty]$ the spaces $L_{\mu}^p(\Omega)$ are complete.

An important topic is also how convergence of a sequence of functions transfers to convergence of the corresponding integrals. One can show that point-wise convergence is not sufficient to ensure convergence of the integrals, thus in the following we present two well-known theorems partially solving the issue.

Theorem 1.26 (Fatou's Lemma). Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, let $f: \Omega \rightarrow [0, \infty]$ and let $(f_n)_n$ be a sequence of measurable functions such that $f_n: \Omega \rightarrow [0, \infty]$. Then,

$$f \leq \liminf_{n \rightarrow \infty} f_n \text{ a.e.} \quad \Rightarrow \quad \int_{\Omega} f \, d\mu \leq \liminf_{n \rightarrow \infty} \int_{\Omega} f_n \, d\mu. \quad (17)$$

Theorem 1.27 (Dominated Convergence, Lebesgue's Theorem). *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, let $f: \Omega \rightarrow [-\infty, \infty]$ and let $(f_n)_n$ be a sequence of measurable functions such $f_n: \Omega \rightarrow [-\infty, \infty]$ with $f_n(x) \rightarrow f(x)$ for almost all $x \in \Omega$. Further, let $g: \Omega \rightarrow [0, \infty]$ be integrable such that $|f_n| \leq g$ almost everywhere. Then,*

$$\lim_{n \rightarrow \infty} \int_{\Omega} f_n \, d\mu = \int_{\Omega} f \, d\mu. \quad (18)$$

For functions defined on product spaces of measurable spaces it is reasonable to consider product integrals featuring the individual measures. The theoretical basis for this is given by the following statements.

Definition 1.28. *Let $(\Omega_1, \mathcal{A}_1)$ and $(\Omega_2, \mathcal{A}_2)$ be measurable spaces. Then the product algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$ is the smallest σ -algebra on $\Omega_1 \times \Omega_2$ generated by sets $\{A_1 \times A_2 \in \Omega_1 \times \Omega_2 \mid A_1 \in \mathcal{A}_1, A_2 \in \mathcal{A}_2\}$.*

These product algebras raise the question of product measures and integration of functions on such algebras, which is summarised in the following theorem.

Theorem 1.29. *Let $(\Omega_1, \mathcal{A}_1, \mu)$ and $(\Omega_2, \mathcal{A}_2, \nu)$ be σ -finite measure spaces and let $f: \Omega_1 \times \Omega_2 \rightarrow [0, \infty]$ be measurable on the product algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$. Then, $y \mapsto f(x, y)$ is \mathcal{A}_2 measurable for all $x \in \Omega_1$ and $x \mapsto \int_{\Omega_2} f(x, y) \, d\nu(y)$ is well-defined and \mathcal{A}_1 measurable. Therefore, $\int_{\Omega_1} \int_{\Omega_2} f(x, y) \, d\nu(y) \, d\mu(x)$ is well-defined and independent of the integration order, i.e.*

$$\int_{\Omega_1} \int_{\Omega_2} f(x, y) \, d\nu(y) \, d\mu(x) = \int_{\Omega_2} \int_{\Omega_1} f(x, y) \, d\mu(x) \, d\nu(y). \quad (19)$$

This statement is called Fubini's Theorem, and remains true for functions $f: \Omega_1 \times \Omega_2 \rightarrow [-\infty, \infty]$ if a double integral of the modulus of f for an arbitrary integration order is finite.

On Hausdorff spaces with the corresponding Borel-algebras, the topological structure allows the question whether a measure is adapted to the topology.

Definition 1.30. *Let (X, \mathcal{B}, μ) a Borel-measure space on a Hausdorff space (X, \mathcal{T}) . Then a measure μ is called regular if for $B \in \mathcal{B}$*

$$\mu(B) = \inf \{ \mu(O) \mid O \supset B \text{ open} \} = \sup \{ \mu(C) \mid C \subset B \text{ compact} \}. \quad (20)$$

Also, one can drop the condition that a measure must be a non-negative scalar valued mapping and allow for real vector-valued measures.

Definition 1.31. On a measurable space (Ω, \mathcal{A}) a mapping $\mu: \mathcal{A} \rightarrow [-\infty, \infty]$ is called signed measure, if

$$\mu(\emptyset) = 0, \quad \text{and} \quad \mu\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{i=1}^{\infty} \mu(A_n), \quad (21)$$

where the sum is required to be well-defined and in particular independent of the summation order.

Definition 1.32. On a measurable space (Ω, \mathcal{A}) we call μ a vector-valued measure with dimension $d > 0$ if $\mu = (\mu_1, \dots, \mu_d)$ where μ_i are signed measures. In this setting, the integral of a function $f = (f_1, \dots, f_d): \Omega \rightarrow [-\infty, \infty]^d$ with f_1, \dots, f_d integrable is defined via

$$\int_{\Omega} f \, d\mu = \sum_{i=1}^d \int_{\Omega} f_i \, d\mu_i. \quad (22)$$

We denote with $\mathcal{M}(\Omega, \mathbb{R}^d)$ the space of regular, vector-valued, finite measures, and equip it with the norm

$$\|\mu\| = \sup \left\{ \int_{\Omega} \phi(x) \, d\mu(x) \mid \phi \in \mathcal{C}_0(\Omega) \text{ with } \phi(x) \leq 1 \text{ for a.e. } x \in \Omega \right\}. \quad (23)$$

Note that with this norm and the addition and scalar-multiplication of vector-valued measures, $\mathcal{M}(\Omega, \mathbb{R}^d)$ is a Banach space. Moreover, for $\mu \in \mathcal{M}(\Omega, \mathbb{R}^d)$ there is also a representation

$$\mu = \lambda |\mu|, \quad (24)$$

where $\lambda: \Omega \rightarrow \mathbb{R}^d$ is a $|\mu|$ measurable function also referred to as the density.

Theorem 1.33 (Riesz' Representation). Let (X, \mathcal{T}) be a compact metric space and denote with $\mathcal{C}(X, \mathbb{R}^d)$ the space of continuous functions $X \rightarrow \mathbb{R}^d$ which is equipped with the supremum norm $\|f\|_{\infty} = \sup_{x \in X} |f|(x)$. Then, for every linear continuous functional $\xi: \mathcal{C}(X, \mathbb{R}^d) \rightarrow \mathbb{R}$ there exists a regular, vector-valued, finite measure μ such that

$$\xi(f) = \int_X f \, d\mu. \quad (25)$$

In particular the mapping $\xi \mapsto \mu$ is isometric and thus $\mathcal{C}(X, \mathbb{R})^* \hat{=} \mathcal{M}(X, \mathbb{R}^d)$.

1.4. Convex Analysis

When considering the Tikhonov regularisation of inverse problems often differentiable approaches are too restrictive and do not yield suitable results. Thus, one works with operations requiring nothing more than convexity, giving sufficient flexibility while still containing suitable structure for optimisation. More on the presented topics can be found in [18].

Definition 1.34. *Let X be a vector space and $A \subset X$. The function $\chi_A: X \rightarrow \{0, \infty\}$ such that*

$$\chi_A(x) = \begin{cases} 0 & \text{if } x \in A, \\ \infty & \text{otherwise,} \end{cases} \quad (26)$$

is called the characteristic function of A .

Definition 1.35. *Let X be a vector space and let $F: X \rightarrow (-\infty, \infty]$ be a function. We denote $(-\infty, \infty]$ by \mathbb{R}^∞ , call $\text{dom}(F) = \{x \in X \mid F(x) < \infty\}$ the domain, and say F is proper if $\text{dom}(F) \neq \emptyset$. The function F is called convex if for $\alpha \in [0, 1]$, $u, v \in X$,*

$$F(\alpha u + (1 - \alpha)v) \leq \alpha F(u) + (1 - \alpha)F(v). \quad (27)$$

A set $C \subset X$ is called convex if the characteristic function χ_C is convex. The function F is called strictly convex, if $\text{dom}(F)$ is convex, and for $\alpha \in (0, 1)$ and $u, v \in \text{dom}(F)$, $u \neq v$

$$F(\alpha u + (1 - \alpha)v) < \alpha F(u) + (1 - \alpha)F(v). \quad (28)$$

Note that if X is not a vector space, but a convex subset of a vector space Y , completely analogue definitions can be made.

Lemma 1.36. *Let X be a vector space, $F, G: X \rightarrow \mathbb{R}$ convex, $\alpha \geq 0$, $g: \mathbb{R}^\infty \rightarrow \mathbb{R}^\infty$ convex and monotone and $\{F^i\}_{i \in I}$ a set of convex functions. Then, also the following functions are convex:*

$$F + G, \quad \alpha F, \quad g \circ F, \quad \sup_{i \in I} F^i.$$

For convex functions, we generalise the notion of differentiability in a non-smooth context, allowing for a concept of differentiability containing relevant information for convex functions.

Definition 1.37. Let $(X, \|\cdot\|)$ be a normed space and $F: X \rightarrow (-\infty, \infty]$ a convex function. We call $\xi \in X^*$ a subgradient of F in a point x if for $y \in X$

$$F(y) - F(x) \leq \xi(y - x).$$

The set of all subgradients $[\partial F](x) = \{\xi \in X^* \mid \xi \text{ is subgradient of } F \text{ in } x\}$ is called the subdifferential.

Lemma 1.38. For $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ Banach spaces, F, G convex functions on X , $A: X \rightarrow Y$ linear and continuous and $\alpha > 0$, the following calculus rules hold:

$$\partial[\alpha F](x) = \alpha \partial[F](x), \quad \partial[F + G](x) \supset \partial[F](x) + \partial[G](x), \quad \partial[F \circ A](x) \supset A^* \partial[F](Ax)$$

where the inclusion of the addition holds with equality in case that there is an $u_0 \in \text{dom}(F) \cap \text{dom}(G)$ such that F is continuous in u_0 , and the inclusion for composition with linear continuous operations holds with equality in case F is continuous in some $u_0 \in \text{dom}(F) \cap \text{Rg}(A)$. Moreover, a convex function F attains a minimum in $x \in X$ if and only if $0 \in \partial[F](x)$.

Also, one requires certain regularity assumptions on the occurring functions in the Tikhonov regularisation, and while continuity would suffice, one can further relax to lower semi-continuity conditions.

Definition 1.39. Let (X, \mathcal{T}_X) be a topological space and $F: X \rightarrow \mathbb{R}^\infty$. We call F (sequentially) lower semi-continuous with respect to \mathcal{T}_X (\mathcal{T}_X -l.s.c.) if for any sequence $(x^n)_n$ in X such that $x^n \xrightarrow{\mathcal{T}_X} x$ for some $x \in X$,

$$F(x) \leq \liminf_{n \rightarrow \infty} F(x^n).$$

Lemma 1.40. For (X, \mathcal{T}_X) and (Y, \mathcal{T}_Y) topological spaces, F, G \mathcal{T}_X -lower semi-continuous and $\phi: \mathbb{R}^\infty \rightarrow \mathbb{R}^\infty$ l.s.c. and monotonely increasing, $\{F^n\}_{n \in I}$ a set of convex functions, $H: Y \rightarrow X$ linear and continuous, and $\alpha > 0$, the following functions are also lower semi-continuous:

$$F + G, \quad \alpha F, \quad \phi \circ F, \quad F \circ H, \quad \sup_{n \in I} F^n.$$

Lemma 1.41. Let $(X, \|\cdot\|_X)$ be a normed space, and U^* the dual of a normed space $(U, \|\cdot\|_U)$. Then, the mapping $x \mapsto \|x\|_X$ is weakly lower semi-continuous, and the mapping $\xi \mapsto \|\xi\|_{U^*}$ is weak* lower semi-continuous.

Lemma 1.42. *Let (X, \mathcal{T}_X) be a topological space, let $f, g: X \rightarrow \mathbb{R}^\infty$ be lower semi-continuous, and let $(x^n)_n$ be a sequence in X with $x_n \xrightarrow{\mathcal{T}_X} x$ such that $\lim_n f(x_n) + g(x_n) = f(x) + g(x) < \infty$. Then also $f(x_n) \rightarrow f(x)$ and $g(x_n) \rightarrow g(x)$.*

Proof. Due to lower semi-continuity

$$f(x) \leq \liminf_{n \rightarrow \infty} f(x_n), \quad \text{and} \quad g(x) \leq \liminf_{n \rightarrow \infty} g(x_n).$$

If we assume $f(x) = \liminf_n f(x_n) - c$ for some $c > 0$, then

$$f(x) + g(x) = \liminf_{n \rightarrow \infty} f(x_n) - c + g(x) \leq \limsup_{n \rightarrow \infty} f(x_n) + g(x_n) - c = f(x) + g(x) - c$$

yielding a contradiction, and consequently no such c can exist and $\liminf_n f(x_n) = \limsup_n f(x_n) = \lim_n f(x_n)$. \square

Lemma 1.43. *Let $(X, \|\cdot\|_X)$ be a normed space, and $F: X \rightarrow \mathbb{R}^\infty$ a convex and lower semi-continuous function. Then F is also weakly lower semi-continuous.*

The theory of convex analysis we derived so far is often used to solve minimisation problems $\min_{x \in X} F(x)$ with convex, lower semi-continuous $F: X \rightarrow \mathbb{R}^\infty$.

However, sometimes solving an optimisation problem directly is not possible, but there is a dual problem with a more suitable structure. Often, these dual problems offer more structure and thus can be solved, and their solutions give insight into the original problem and possibly even enable us to compute the solution to the original optimisation problem.

Definition 1.44. *For a Banach space $(X, \|\cdot\|_X)$ and $F: X \rightarrow \mathbb{R}^\infty$ a convex function, we define the convex conjugate function F^* as*

$$F^*: X^* \rightarrow \mathbb{R}^\infty, \quad F^*(\cdot) = \sup_{x \in X} \langle \cdot, x \rangle_{X^* \times X} - F(x).$$

Moreover, for $G: X^* \rightarrow \mathbb{R}^\infty$ we define

$$G^*: X \rightarrow \mathbb{R}^\infty, \quad G^*(\cdot) = \sup_{\xi \in X^*} \langle \xi, \cdot \rangle_{X^* \times X} - G(\xi). \quad (29)$$

Note that thus G^* is defined as a function on X and not on X^{**} .

This conjugation operation also fulfills the typical property that $T^{**} = T$ in a suitable setting.

Proposition 1.45. *Let $(X, \|\cdot\|_X)$ be a reflexive Banach space and denote by*

$$\begin{aligned}\Gamma_0(X) &= \left\{ F: X \rightarrow \mathbb{R}^\infty \mid F \text{ is proper, convex and lower semi-continuous} \right\}, \\ \Gamma_0(X^*) &= \left\{ G: X^* \rightarrow \mathbb{R}^\infty \mid G \text{ is proper, convex and lower semi-continuous} \right\}\end{aligned}$$

the spaces of proper convex and lower semi-continuous functions, on which in slight abuse of notation the conjugation operations $$: $\Gamma_0(X) \rightarrow \Gamma_0(X^*)$ and $*$: $\Gamma_0(X^*) \rightarrow \Gamma_0(X)$ are well-defined. Moreover, the former is invertible and the inverse operation is the latter, i.e.*

$$F = (F^*)^* \quad \text{on } \Gamma_0(X), \quad \text{and} \quad F(x) = \sup_{\xi \in X^*} \langle \xi, x \rangle - F^*(\xi) \quad \forall x \in X. \quad (30)$$

Theorem 1.46. *Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be Banach spaces, let $T: X \rightarrow Y$ be linear and continuous and $F: X \rightarrow \mathbb{R}^\infty$ and $G: Y \rightarrow \mathbb{R}^\infty$ both be proper, convex and lower semi-continuous. If we further assume*

$$Y = \bigcup_{\lambda > 0} \lambda(\text{dom}(G) - T \text{dom}(F)),$$

then we obtain the equivalent reformulation

$$\inf_{v \in X} F(v) + G(Tv) = \min_{\eta \in Y^*} F^*(-T^*\eta) + G^*(\eta). \quad (31)$$

Proof. See [5]. □

Part I.

General Tikhonov Regularisation

In this part we consider Tikhonov regularisation approaches to inverse problems with general discrepancies and regularisation functionals. This is a classical regularisation approach to ill-posed inverse problems, that features optimisation problems balancing the discrepancy in the data with costs generated by a function penalising undesired properties. First we consider the well-known single-data approach. Later, we present a multi-data approach applied to a set of subproblems collectively posing an inverse problem. Particular focus will be placed on suitable settings and assumptions for convergence results and concepts of partial solutions if not all problems can be solved simultaneously.

2. Single-Data Tikhonov Regularisation

In this chapter, we reiterate the well-established theory for Tikhonov regularisation of the single-data inverse problem

$$Tu = f^\dagger, \tag{32}$$

which will be a basis to build the theory for multi-data regularisation upon.

Problem 2.1 (Single-data Tikhonov problem). *Let X, Y be sets, $\alpha > 0$, let $D: Y \times Y \rightarrow [0, \infty]$ (called the discrepancy function), $R: X \rightarrow [0, \infty]$ (called the regularisation function) and $\alpha \in (0, \infty)$. Further, let $T: \text{dom}(T) \subset X \rightarrow Y$, and $f^\dagger \in Y$. The corresponding single-data Tikhonov Problem $\text{STIKH}_\alpha(f^\dagger)$ is defined as finding $u^\dagger \in X$ such that*

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_\alpha(u, f^\dagger) & \text{such that } F_\alpha(u^\dagger, f^\dagger) < \infty, \\ \text{with } F_\alpha(u, f^\dagger) = D(Tu, f^\dagger) + \alpha R(u). \end{cases} \quad \text{STIKH}_\alpha(f^\dagger)$$

Problem $\text{STIKH}_\alpha(f^\dagger)$ is expected to balance costs for not satisfying desired properties with costs for high discrepancy between Tu and f , thus ensuring adequate solutions. A suitable choice of α is in general not simple, however the rule of more noise requires greater α applies.

Note that the problem $\text{STIKH}_\alpha(f^\dagger)$ depends on two instances, α and f^\dagger , thus prominent questions are for which α, f^\dagger the problem $\text{STIKH}_\alpha(f^\dagger)$ is solvable and how it reacts

to changing α and f^\dagger .

2.1. Existence and Stability

First, we aim to find suitable conditions to ensure that $\text{STIKH}_\alpha(f^\dagger)$ is solvable and robust with respect to noise, i.e. disturbances in f^\dagger . The following properties are posed in a general setting in order to be widely applicable and fit many situations.

Definition 2.2. *Let (Y, \mathcal{T}_Y) be a Hausdorff space, and let $D: Y \times Y \rightarrow [0, \infty]$, and let \mathcal{T}_D be a Hausdorff topology on Y . Then D is called a basic discrepancy (with respect to \mathcal{T}_Y and \mathcal{T}_D), if the following hold:*

D1 The topology \mathcal{T}_D is stronger than convergence $D(f, f^n) \rightarrow 0$, i.e. \mathcal{T}_D is such that for a sequence $(f^n)_n \subset Y$ and $f \in Y$,

$$f^n \xrightarrow{\mathcal{T}_D} f \quad \Rightarrow \quad D(f, f^n) \rightarrow 0. \quad (33)$$

D2 For $v, f \in Y$, the value $D(v, f) = 0$ if and only if $v = f$.

D3 The function D is $\mathcal{T}_Y \times \mathcal{T}_D$ lower semi-continuous, i.e. for sequences $(v^n)_n \subset Y$, $(f^n)_n \subset Y$ and respective limits $f, v \in Y$,

$$\left(v^n \xrightarrow{\mathcal{T}_Y} v, f^n \xrightarrow{\mathcal{T}_D} f \right) \quad \Rightarrow \quad D(v, f) \leq \liminf_{n \rightarrow \infty} D(v^n, f^n). \quad (34)$$

A basic discrepancy is called v_0 -continuous in $f^\dagger \in Y$, if the mapping $f \mapsto D(v_0, f)$ is continuous in f^\dagger with respect to the \mathcal{T}_D topology.

Let $\psi: [0, \infty) \rightarrow [0, \infty)$ be a continuous and monotone function with $\psi(0) = 0$. We call a basic discrepancy strongly ψ -continuous on a set $V \subset Y$ in $f^\dagger \in Y$, if there is $\delta_0 > 0$ such that for all $v \in V$ and for $f \in Y$ with $D(f^\dagger, f) \leq \delta_0$, the discrepancy function satisfies the following modulus of continuity estimate:

$$|D(v, f^\dagger) - D(v, f)| \leq \psi(D(f^\dagger, f))(D(v, f^\dagger) + 1). \quad (35)$$

Note that these definitions are not standard, but will be used for the sake of readability. With this notation, we use the following assumptions.

Assumptions 2.3 (Single-Data Tikhonov Regularisation).

A1 Let (X, \mathcal{T}_X) be a Hausdorff space.

A2 Let (Y, \mathcal{T}_Y) be a Hausdorff space, and $T: \text{dom}(T) \subset X \rightarrow Y$ be a continuous operator with respect to \mathcal{T}_X and \mathcal{T}_Y , such that $\text{dom}(T)$ is closed with respect to \mathcal{T}_X .

A3 The function D is a basic discrepancy (see Definition 2.2).

A4 The function $R: X \rightarrow [0, \infty]$ is \mathcal{T}_X -lower semi-continuous.

A5 The Tikhonov functional F_1 (with parameter $\alpha = 1$) is uniformly coercive in the following sense: If $f^n \xrightarrow{\mathcal{T}_Y} f$, then for each $C > 0$ the set $\bigcup_{n=1}^{\infty} \{u \in X \mid F_1(u, f^n) < C\}$ is \mathcal{T}_X -precompact.

Some of these assumptions are standard, while some seem rather technical. It will become clear in the following theorems' proofs why they were required, and where weaker conditions would suffice.

While these assumptions will be applied throughout the entire chapter, in later stages additional continuity and source conditions will be required.

Hence, we can start answering whether $\text{STIKH}_\alpha(f^\dagger)$ is solvable, or more precisely for which data and parameter the minimisation problem attains a finite value.

Theorem 2.4 (Existence). *Let Assumptions 2.3 hold and let $f^\dagger \in Y$. Then, either for all $\alpha \in (0, \infty)$ $\text{STIKH}_\alpha(f^\dagger)$ possesses a solution, or $F_\alpha(\cdot, f^\dagger)$ is not proper for any $\alpha \in (0, \infty)$. Moreover, if $F_\alpha(\cdot, f^\dagger)$ is strictly convex, the solution is unique.*

Proof. Obviously, being proper is equivalent to the existence of an $u_0 \in \text{dom}(R) \cap \text{dom}(T)$ such that $D(Tu_0, f^\dagger) < \infty$, which does not depend on α . So either the problem is not proper for any α , or it is for all.

Hence, in the following we assume that $F_\alpha(\cdot, f^\dagger)$ is proper for $\alpha > 0$, and show that the minimum is attained by a standard approach, using the direct method. Obviously $F_\alpha(u, f^\dagger) = D(Tu, f^\dagger) + \alpha R(u) \geq 0$ and due to the properness assumptions $\inf_{u \in \text{dom}(T)} F_\alpha(u, f^\dagger) < \infty$. Thus, there exists an infimising sequence $(u^n)_n$ such that $\lim_{n \rightarrow \infty} F_\alpha(u^n, f^\dagger) = \inf_{u \in X} F_\alpha(u, f^\dagger)$. Basic computation shows that for some $C > 0$ $cF_1(u^n, f^\dagger) \leq F_\alpha(u^n, f^\dagger) \leq C$ for almost every n with $c = \alpha$ in case $\alpha \leq 1$, and $c = 1$ otherwise. Due to coercivity, there is a subsequence $(u^{n'})_{n'}$, such that $u^{n'} \xrightarrow{\mathcal{T}_X} u^\dagger \in X$. Using lower semi-continuity of $D(\cdot, f^\dagger)$ and R , and $Tu^{n'} \xrightarrow{\mathcal{T}_Y} Tu^\dagger$ by continuity, one obtains

$$F_\alpha(u^\dagger, f^\dagger) \leq \inf_{u \in X} F_\alpha(u, f^\dagger),$$

implying that u^\dagger is a solution to $\text{STIKH}_\alpha(f^\dagger)$. As strictly convex functions can attain at most one minimum, the uniqueness statement follows. \square

Remark 2.5. *Note that in this proof only weaker lower semi-continuity and coercivity properties than stated in Assumptions 2.3 were needed, since one only required lower semi-continuity with respect to the first component, and coercivity for fixed f^\dagger and for some $C > 0$ such that the level-set is not empty, not all C (although this C is usually not known a-priori).*

Next, we make sure that solving the Tikhonov problem is stable, i.e. slight changes in the data f will not affect the corresponding solutions significantly. To do so, we need an additional continuity property of the discrepancy, namely that D is a continuous discrepancy in a reasonable sense.

Theorem 2.6 (Stability). *Let Assumptions 2.3 hold, $f^\dagger \in Y$, $\alpha > 0$ and a sequence $(f^n)_n \subset Y$ such that $f^n \xrightarrow{\mathcal{T}_R} f^\dagger$. Further, let there be a solution to $STIKH_\alpha(f^\dagger)$ we denote by u_0 such that D is a Tu_0 -continuous discrepancy in f^\dagger .*

Then $STIKH_\alpha(f^n)$, the Tikhonov problem corresponding to data f^n , is solvable for sufficiently large n and we denote the corresponding solutions by u^n , i.e.

$$F_\alpha(u^n, f^n) = \min_{u \in \text{dom}(T)} F_\alpha(u, f^n) < \infty. \quad (36)$$

Moreover, the sequence $(u^n)_n$ admits a \mathcal{T}_X -convergent subsequence in X . Furthermore, every \mathcal{T}_X -limit u^\dagger of such a subsequence $(u^{n'})_{n'}$ is a solution to $STIKH_\alpha(f^\dagger)$, the Tikhonov problem with the true data f^\dagger , and these subsequences satisfy

$$R(u^\dagger) = \lim_{n' \rightarrow \infty} R(u^{n'}). \quad (37)$$

If the solution u_0 to the Tikhonov problem for f^\dagger and α is unique, then the entire sequence $(u^n)_n$ \mathcal{T}_X -converges towards the solution u_0 .

Proof. Note that this statement is a generalisation of [25, Thm 3.2, p 990] and the presented proof follows its general idea.

The continuity of $D(Tu_0, \cdot)$ in f^\dagger , which holds due to assumption, yields

$$F_\alpha(u_0, f^n) = D(Tu_0, f^n) + \alpha R(u_0) \xrightarrow{n \rightarrow \infty} D(Tu_0, f^\dagger) + \alpha R(u_0) < \infty$$

and consequently for n sufficiently large $\min_{u \in \text{dom}(T)} F_\alpha(u, f^n) < \infty$. Thus, Theorem 2.4 ensures the existence of u^n for n sufficiently large, and in the following we assume without loss of generality that the problems are solvable for all $n \geq 0$.

Due to the optimality of u^n for data f^n , we obtain for $u \in X$ that

$$F_\alpha(u^n, f^n) = D(Tu^n, f^n) + \alpha R(u^n) \stackrel{\text{opt.}}{\leq} D(Tu, f^n) + \alpha R(u) = F_\alpha(u, f^n). \quad (38)$$

Choosing $u = u_0$ yields

$$F_\alpha(u^n, f^n) \leq \underbrace{D(Tu_0, f^n)}_{n \xrightarrow{\infty} D(Tu_0, f^\dagger) < \infty} + R(u_0) \leq C < \infty.$$

Due to the uniform coercivity, the sequence $(u^n)_n$ admits a convergent subsequence $(u^{n'})_{n'}$ such that $u^{n'} \xrightarrow{\mathcal{T}_X} u^\dagger$. At this point, we may assume without loss of generality, that the entire sequence converges. Due to the lower semi-continuity of D and R ,

$$F_\alpha(u^\dagger, f^\dagger) \stackrel{\text{l.s.c.}}{\leq} \liminf_{n \rightarrow \infty} F_\alpha(u^n, f^n) \leq \limsup_{n \rightarrow \infty} F_\alpha(u^n, f^n) \stackrel{\text{opt.}}{\leq} \limsup_{n \rightarrow \infty} F_\alpha(u_0, f^n) \stackrel{\text{cont.}}{=} F_\alpha(u_0, f^\dagger), \quad (39)$$

where we applied the optimality of u^n for data f^n , as well as the fact, that for u_0 the discrepancy $D(Tu_0, \cdot)$ is continuous with respect to the topology \mathcal{T}_D in f^\dagger . Consequently, u^\dagger is a solution to the Tikhonov problem with data f^\dagger .

In case of a unique solution, the entire sequence converges as an immediate consequence of the previous result and a subsequence argument.

All that is left to show is that also the values of the regularisation function R converge. Therefore, let again $(u^{n'})_{n'}$ be a convergent subsequence $u^{n'} \xrightarrow{\mathcal{T}_X} u^\dagger$, and observe that since $F_\alpha(u^\dagger, f^\dagger) = F_\alpha(u_0, f^\dagger)$, (39) implies that

$$F_\alpha(u^\dagger, f^\dagger) = \liminf_{n' \rightarrow \infty} F_\alpha(u^{n'}, f^{n'}) = \limsup_{n' \rightarrow \infty} F_\alpha(u^{n'}, f^{n'}) \quad (40)$$

yielding convergence of the functional F_α . Since $F_\alpha(u, f) = D(Tu, f) + \alpha R(u)$ and both R and D are lower semi-continuous in a suitable sense, Lemma 1.42 implies convergence of both $D(Tu^{n'}, f^\dagger)$ and $R(u^{n'})$ respectively. \square

Remark 2.7. *The semi-continuity and continuity properties stated were both required in order to show the optimality of the limits u^\dagger . Also, here the uniform coercivity for a sequence $(f^n)_n$ was required to ensure the existence of convergent subsequences.*

2.2. Convergence

In the previous chapter the regularisation parameter α remained fixed and solely the data $(f^n)_n$ were changed, in order to show stability. However, for ever less disturbed data, it would be reasonable to reduce α towards 0, thus returning to the original unregularised problem $\min_{u \in \text{dom}(T)} D(Tu, f^\dagger)$. This raises the question how to choose α with respect to the noise level? Too fast reduction might lead to results strongly affected by the noise, while too slow reduction might yield results with high discrepancy. Furthermore, if the weight of R reduces towards zero, does this imply that solutions get ever-less regular, or can one expect the values of $R(u^n)$ to remain low?

To formalise the notion of vanishing noise, we use the following notation.

Definition 2.8. *Let $(\Delta_n)_{n \in \mathbb{N}} \subset (0, \infty)$ (the sequence of vanishing noise levels) be a sequence such that $(\Delta_n)_n$ is strictly monotone decreasing and the limit of $(\Delta_n)_n$ is 0. To simplify the notation, we associate n with δ such that $\Delta_n = \delta$, resulting in a sequence $(\delta)_{\delta \in \Delta}$. We will also index other sequences with δ , i.e. $(f^\delta)_\delta$ refers to a sequence $(f^n)_n$ with said relation between δ and n . Particularly, $\lim_{\delta \rightarrow 0} f^\delta$ refers to $\lim_{n \rightarrow \infty} f^n$, and analogously for other operations concerning sequences. Also, the phrase a property holds for δ sufficiently small refers to n sufficiently large, which indicates that after finitely many entries the property is satisfied by the elements of a sequence.*

In the following there will implicitly be a sequence $(\Delta_n)_n$ in the background without further mention, and we use the resulting sequence $(\delta)_{\delta \in \Delta}$ to index the other sequences.

In order to answer whether solutions to the Tikhonov problems remain regular when reducing noise and the regularisation parameter towards 0, one uses the concept of R -minimal solutions.

Definition 2.9 (R -Minimal Solutions). *For $f \in \text{Rg}(T)$ we call $\hat{u} \in X$ an R -minimal solution to $Tu = f$, if*

$$\hat{u} \in \underset{\substack{u \in \text{dom}(T) \\ Tu=f}}{\text{argmin}} R(u), \quad \text{such that} \quad R(\hat{u}) < \infty. \quad (41)$$

Obviously, for $f \in \text{Rg}(T)$ there exist solutions to $Tu = f$, however, R -minimal solutions are special in the way that they also minimise the regularisation functional.

Lemma 2.10. *Let the Assumptions 2.3 hold and let $f^\dagger \in \text{Rg}(T)$. Then either there exists an R -minimal solution to $Tu = f^\dagger$ or $R(u) \equiv \infty$ for all u with $Tu = f^\dagger$.*

Proof. We may assume there is an u_0 such that $Tu_0 = f^\dagger$ and $R(u_0) < \infty$, and thus, an R -infimising sequence $(v^n)_n$ exists, such that $Tv^n = f^\dagger$. Without loss of generality, $F_1(v^n, f^\dagger) = D(f^\dagger, f^\dagger) + R(v^n) \leq R(u_0) < \infty$, and by coercivity the sequence $(v^n)_n$ admits a convergent subsequence (reabeled v^n) with limit \hat{u} . Since the set $T^{-1}(f^\dagger)$ is \mathcal{T}_X -closed, and by lower semi-continuity of R , we see that

$$R(\hat{u}) \leq \liminf_{n \rightarrow \infty} R(v_n) = \inf_{u \in X: Tu=f^\dagger} R(u), \quad (42)$$

implying that $\hat{u} \in T^{-1}(f^\dagger)$ with minimal regularisation value. \square

Next, one is interested in whether for the sequence of data $(f^\delta)_\delta$ and parameter $(\alpha(\delta))_\delta$, the sequence of corresponding solutions $(u_\alpha^\delta)_\delta$ converges to an R -minimal solution, i.e. the regularity is the best it can be.

Theorem 2.11 (Convergence). *Let Assumptions 2.3 hold, let the sequence $(f^\delta)_\delta \subset Y$ and $f^\dagger \in T(\text{dom}(R))$ be such that the noise level $D(f^\dagger, f^\delta) = \delta$ and $f^\delta \xrightarrow{\mathcal{T}_R} f^\dagger$. Let there be an R -minimal solution u_0 to $Tu = f^\dagger$. Then the problems $STIKH_\alpha(f^\delta)$ are solvable for any α and δ sufficiently small.*

Moreover, if we choose $\alpha = \alpha(\delta)$ dependent on the noise level as $\alpha: (0, \infty] \rightarrow (0, \infty]$ such that

$$\lim_{\delta \rightarrow 0} \alpha(\delta) = 0, \quad \text{and} \quad \lim_{\delta \rightarrow 0} \frac{\delta}{\alpha(\delta)} = 0 \quad (43)$$

and denote the corresponding solutions to $STIKH_{\alpha(\delta)}(f^\delta)$ by u_α^δ , then the sequence of solutions $(u_\alpha^\delta)_\delta$ contains a \mathcal{T}_X -convergent subsequence. Every limit of such a subsequence is an R -minimal solution to $Tu = f^\dagger$. Moreover, if the R -minimal solution is unique, the entire sequence will converge.

Proof. This theorem is a generalisation of [25, Thm 3.5, p 991] and the following proof will use it as a blueprint.

First, we note that for any $\alpha > 0$,

$$F_\alpha(u_0, f^\delta) = D(Tu_0, f^\delta) + \alpha R(u_0) = \delta + \alpha R(u_0) < \infty,$$

and thus Theorem 2.4 implies solvability. We once again take advantage of the optimality of u_α^δ , obtaining

$$D(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)R(u_\alpha^\delta) = F_{\alpha(\delta)}(u_\alpha^\delta, f^\delta) \stackrel{\text{opt.}}{\leq} F_{\alpha(\delta)}(u, f^\delta) = D(Tu, f^\delta) + \alpha(\delta)R(u), \quad (44)$$

for arbitrary $u \in X$. Inserting $u = u_0$ in this equation and observing $Tu_0 = f^\dagger$ yields

$$D(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)R(u_\alpha^\delta) \leq \underbrace{D(Tu_0, f^\delta)}_{=\delta \rightarrow 0} + \underbrace{\alpha(\delta)R(u_0)}_{\rightarrow 0} \rightarrow 0. \quad (45)$$

Omitting either $D(Tu_\alpha^\delta, f^\delta) \geq 0$ or $\alpha(\delta)R(u_\alpha^\delta) \geq 0$ in this inequality, which holds due to the non-negativity of the occurring functions, one obtains

$$R(u_\alpha^\delta) \leq \underbrace{\frac{\delta}{\alpha(\delta)}}_{\rightarrow 0} + R(u_0) < \infty, \quad \text{and} \quad D(Tu_\alpha^\delta, f^\delta) \rightarrow 0. \quad (46)$$

Thus, through the uniform coercivity property of $F_1(\cdot, \cdot)$ the sequence $(u_\alpha^\delta)_\delta$ contains a convergent subsequence with limit u^\dagger . Due to the lower semi-continuity of D with respect to both arguments,

$$D(Tu^\dagger, f^\dagger) \leq \liminf_{\delta \rightarrow 0} D(u_\alpha^\delta, f^\delta) = 0, \quad (47)$$

which due to the positive definiteness property of D implies $Tu^\dagger = f^\dagger$. Furthermore, (46) together with lower semi-continuity of R implies that u^\dagger is an R -minimal solution.

The statement concerning convergence of the entire sequence in case of unique R -minimal solutions is again obtained via a subsequence argument and the already established statements. \square

Theorem 2.11 shows what suitable choices of α might be, in particular that one cannot reduce α too drastically. However, we are still unaware of how fast the solutions will converge, which in practical application might pose a problem. Note that until now no vector space structure was required, however in the following we will need convexity and Banach spaces to find suitable notions of distance to measure convergence rates. Also, to measure convergence rates, we use the following notation.

Definition 2.12. *Let δ be a sequence in the sense of Definition 2.8 with the corresponding $(\Delta_n)_n$, and let $(f^\delta)_\delta$ and $(g^\delta)_\delta$ be non negative real valued sequences. Then we use*

$$f = O(g) \quad \Leftrightarrow \quad \limsup_{\delta \rightarrow 0} \frac{f}{g} < \infty, \quad \text{and} \quad f = o(g) \quad \Leftrightarrow \quad \lim_{\delta \rightarrow 0} \frac{f}{g} = 0. \quad (48)$$

Also, we introduce the Bregman distance [32], a weak notion of distance, which is suitable to measure the rates of convergence for such problems.

Definition 2.13. Let X be a Banach space and $F: X \rightarrow \mathbb{R}^\infty$ a convex function. For $x_2 \in X$ and $\xi \in \partial[F](x_2)$, we define the Bregman distance

$$D_F^\xi(x_1, x_2) = F(x_1) - F(x_2) - \xi(x_1 - x_2). \quad (49)$$

Remark 2.14. We note that D_F^ξ is always non-negative, however in general it does not satisfy a positive definiteness property, i.e. $D_F^\xi(x_1, x_2) = 0$ does not imply $x_1 = x_2$. A simple instance where no positivity holds is the function $F(x) = |x|$ with $x \in \mathbb{R}$, $x_1 = 1$, $x_2 = 2$ and $\xi = 1 \in \partial[F](x_2)$.

Nonetheless, this gives a suitable notion of distance to measure convergence rates, however we will require some further technical assumptions to obtain rates.

Theorem 2.15 (Convergence Rates). *Let Assumptions 2.3 be satisfied, let X be a Banach space (but \mathcal{T}_X does not need to be the corresponding norm topology) and let R be convex. Let $f^\dagger \in Y$, $p \geq 1$, $\xi \in X^*$ be such that the following assumptions hold:*

1. *There exists an R -minimal solution u^\dagger to $Tu = f^\dagger$ with $\xi \in \partial[R](u^\dagger)$.*
2. *There are constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that for all $u \in X$ with $D(Tu, f^\dagger) \leq \epsilon_0$ and $R(u) \leq R(u^\dagger) + \epsilon_0$,*

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_R^\xi(u, u^\dagger) + \gamma_2 D(Tu, Tu^\dagger)^{1/p}. \quad (\text{SC1})$$

3. *D satisfies a quasi triangle inequality, in the sense that there is a constant $c > 0$ such that for $v, w \in Y$,*

$$D(v, f^\dagger)^{1/p} \leq c(D(v, w)^{1/p} + D(f^\dagger, w)^{1/p}). \quad (50)$$

Then the following convergence results in terms of Bregman distance hold for $(f^\delta)_\delta$ such that $f^\delta \xrightarrow{\mathcal{T}_D} f^\dagger$ and $D(f^\dagger, f^\delta) = \delta$.

- *For $p > 1$ and α chosen such that there are constants $c, C > 0$ and $c\delta^{\frac{p-1}{p}} \leq \alpha(\delta) \leq C\delta^{\frac{p-1}{p}}$, one obtains*

$$D_R^\xi(u_\alpha^\delta, u^\dagger) = O(\delta^{\frac{1}{p}}) \quad \text{and} \quad R(u_\alpha^\delta) \leq R(u^\dagger) + \frac{\delta^{\frac{1}{p}}}{c}. \quad (51)$$

- In the case of $p = 1$, for $1 > \epsilon > 0$ and the choice α such that $c\delta^\epsilon \leq \alpha(\delta) \leq C\delta^\epsilon$ for some constants $c, C > 0$, one obtains

$$D_R^\xi(u_\alpha^\delta, u^\dagger) = O(\delta^{1-\epsilon}) \quad \text{and} \quad R(u_\alpha^\delta) \leq R(u^\dagger) + \frac{\delta^{1-\epsilon}}{c}. \quad (52)$$

In both cases, one obtains

$$D(Tu_\alpha^\delta, f^\delta) = O(\delta). \quad (53)$$

Proof. Again, this theorem is a generalisation of [25, Thm. 4.4, p 995] and the following proof uses its ideas.

From the optimality of u_α^δ , the fact that $R(u^\dagger) < \infty$ and $Tu^\dagger = f^\dagger$ since u^\dagger is an R -minimal solution, we see that

$$D(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)R(u_\alpha^\delta) \stackrel{\text{opt.}}{\leq} \underbrace{D(Tu^\dagger, f^\delta)}_{=\delta \rightarrow 0} + \alpha(\delta)R(u^\dagger) = \delta + \alpha(\delta)R(u^\dagger) \quad (54)$$

which can be equivalently reformulated to

$$D(Tu_\alpha^\delta, f^\delta) + \alpha(\delta) \underbrace{(R(u_\alpha^\delta) - R(u^\dagger) - \langle \xi, u_\alpha^\delta - u^\dagger \rangle_{X^* \times X})}_{D_R^\xi(u_\alpha^\delta, u^\dagger)} \leq \alpha(\delta) \langle \xi, u^\dagger - u_\alpha^\delta \rangle_{X^* \times X} + \delta. \quad (55)$$

Furthermore, for δ sufficiently small u_α^δ satisfies the requirements for (SC1) as $R(u_\alpha^\delta) \leq R(u^\dagger) + \frac{\delta}{\alpha(\delta)} \rightarrow R(u^\dagger)$ due to (54) when omitting $D(Tu_\alpha^\delta, f^\delta)$ and with the triangle inequality (50) one obtains

$$D(Tu_\alpha^\delta, f^\dagger)^{\frac{1}{p}} \leq c\delta^{\frac{1}{p}} + cD(Tu_\alpha^\delta, f^\delta)^{\frac{1}{p}} \stackrel{(54)}{\leq} c\delta^{\frac{1}{p}} + c(\delta + \alpha(\delta)R(u^\dagger))^{\frac{1}{p}} \rightarrow 0. \quad (56)$$

Consequently, using the Source Condition (SC1), $Tu^\dagger = f^\dagger$ and the triangle inequality, one obtains

$$\begin{aligned} \langle \xi, u^\dagger - u_\alpha^\delta \rangle_{X^*, X} &\stackrel{(\text{SC1})}{\leq} \gamma_1 D_R^\xi(u_\alpha^\delta, u^\dagger) + \gamma_2 D(Tu_\alpha^\delta, \underbrace{Tu^\dagger}_{=f^\dagger})^{1/p} \\ &\leq \gamma_1 D_R^\xi(u_\alpha^\delta, u^\dagger) + c\gamma_2 (D(Tu_\alpha^\delta, f^\delta)^{1/p} + \delta^{\frac{1}{p}}). \end{aligned} \quad (57)$$

Case $p = 1$: Combining (55) and (57) yields

$$(1 - c\alpha(\delta)\gamma_2)D(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)(1 - \gamma_1)D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta + c\alpha(\delta)\gamma_2\delta. \quad (58)$$

Due to $\gamma_1 < 1$ and $c\alpha(\delta)\gamma_2 < 1$ for δ sufficiently small, one can rearrange in order to obtain

$$\begin{aligned} D(Tu_\alpha^\delta, f^\delta) &\leq \delta \frac{1 + c\alpha(\delta)\gamma_2}{(1 - c\alpha(\delta)\gamma_2)} = O(\delta), \\ D_R^\xi(u_\alpha^\delta, u^\dagger) &\leq \frac{\delta(1 + c\alpha(\delta)\gamma_2)}{\alpha(\delta)(1 - \gamma_1)} = O(\delta^{1-\epsilon}). \end{aligned}$$

Case $p > 1$: Similar to the case $p = 1$ we combine the results (55) and (57) in order to obtain

$$D(Tu_\alpha^\delta, f^\delta) - c\alpha(\delta)\gamma_2 D(Tu_\alpha^\delta, f^\delta)^{\frac{1}{p}} + \alpha(\delta)(1 - \gamma_1)D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta + c\alpha(\delta)\delta^{\frac{1}{p}}\gamma_2. \quad (59)$$

Application of Young's inequality

$$ab \leq \frac{a^p}{p} + \frac{b^{p^*}}{p^*} \quad \text{for } a, b \geq 0, \quad \frac{1}{p} + \frac{1}{p^*} = 1,$$

with $a = D(Tu_\alpha^\delta, f^\delta)^{1/p}$ and $b = c\alpha(\delta)\gamma_2$ results in

$$c\alpha(\delta)\gamma_2 D(Tu_\alpha^\delta, f^\delta)^{\frac{1}{p}} \leq \frac{1}{p} D(Tu_\alpha^\delta, f^\delta) + \frac{(c\gamma_2\alpha(\delta))^{p^*}}{p^*}.$$

Thus, for δ sufficiently small,

$$\begin{aligned} D(Tu_\alpha^\delta, f^\delta) &\leq \frac{p}{p-1} \left(\delta + c\alpha(\delta)\delta^{\frac{1}{p}}\gamma_2 + \frac{(c\alpha(\delta)\gamma_2)^{p^*}}{p^*} \right) = O(\delta), \\ D_R^\xi(u_\alpha^\delta, u^\dagger) &\leq \frac{\delta + c\alpha(\delta)\delta^{\frac{1}{p}}\gamma_2 + \frac{1}{p^*}(c\alpha(\delta)\gamma_2)^{p^*}}{\alpha(\delta)(1 - \gamma_1)} = O(\delta^{\frac{1}{p}}). \end{aligned}$$

□

Remark 2.16. *Note that the Condition (SC1) is a variational inequality source condition as described in [26], using the Bregman distance D_R^ξ as the error functional. These variational inequality source conditions yield a wider theory of conditions allowing for convergence results obtained similarly to the computations done above.*

Since the Source Condition (SC1) is still quite abstract, the following shows a sufficient condition in a common setting.

Theorem 2.17. *Let (X, \mathcal{T}_X) and (Y, \mathcal{T}_Y) be Hausdorff spaces, and let R be \mathcal{T}_X -lower semi-continuous. Let $(X, \|\cdot\|_X), (Z, \|\cdot\|_Z), (Y, \|\cdot\|_Y)$ be Banach spaces such that $T: X \rightarrow Y$ is linear and continuous with respect to \mathcal{T}_X and \mathcal{T}_Y . Let $Z \subset Y$ such that $\|\cdot\|_Z$ is lower semi-continuous with respect to \mathcal{T}_Y in Y when understanding $\|y\|_Z = \infty$ if $y \notin Z$. Further, we denote by $\tilde{T}: \text{dom}(\tilde{T}) = \{u \in X \mid Tu \in Z\} \subset X \rightarrow Z$ the restriction of T to suitable spaces and we assume without loss of generality that \tilde{T} is densely defined. We consider the Tikhonov functional $F_\alpha(\cdot, f) = \|T \cdot - f\|_Z^p + \alpha R(\cdot)$, i.e. with a norm discrepancy $D(v, f) = \|v - f\|_Z^p$ for some $p \geq 1$. We further assume, that $F_\alpha(\cdot, f)$ is coercive for any $f \in Y$ and that the topology \mathcal{T}_Y is shift invariant, i.e. such that $f^n \xrightarrow{\mathcal{T}_Y} f$ iff $f^n - g \xrightarrow{\mathcal{T}_Y} f - g$ for any $g \in Y$. Let $f^\dagger \in Z$ and $(f^\delta)_\delta \subset Z$ be a sequence such that $\|f^\dagger - f^\delta\|_Z^p = \delta$ and $\delta \rightarrow 0$ (we use an extension of the norm topology in Z as the \mathcal{T}_D topology on Y). Further, let u^\dagger be an R -minimal solution to $Tu = f^\dagger$ such that*

$$\text{there is } \omega \in \text{dom}(\tilde{T}^*) \text{ such that } \tilde{T}^*\omega \in \partial R(u^\dagger), \quad (\widetilde{SC1})$$

where \tilde{T}^* is the adjoint of \tilde{T} . For $\xi = \tilde{T}^*\omega$ we gain:

- For $p > 1$, the choice of α such that $c\delta^{\frac{p-1}{p}} \leq \alpha(\delta) \leq C\delta^{\frac{p-1}{p}}$ results in

$$D_R^\xi(u_\alpha^\delta, u^\dagger) = O(\delta^{\frac{1}{p}}), \quad \text{and} \quad \|Tu_\alpha^\delta - f^\delta\|_Z^p = O(\delta). \quad (60)$$

- For $p = 1$ and α such that there are constants $c, C > 0$ with $c\delta^\epsilon \leq \alpha(\delta) \leq C\delta^\epsilon$ for some $\epsilon > 0$ results in

$$D_R^\xi(u_\alpha^\delta, u^\dagger) = O(\delta^{1-\epsilon}), \quad \text{and} \quad \|Tu_\alpha^\delta - f^\delta\|_Z = O(\delta). \quad (61)$$

Proof. We just need to verify, that indeed the assumptions of Theorem 2.15 are fulfilled. Obviously, for $D(v, f) = \|v - f\|_Z^p$ we obtain $D \geq 0$ and $D(v, f) = 0$ if and only if $v = f$. In order to show lower semi-continuity, we compute

$$\|v - f\|_Z \leq \liminf_{n \rightarrow \infty} \underbrace{\|v^n - f\|_Z}_{\xrightarrow{\mathcal{T}_Y} v-f} - \underbrace{\lim_{n \rightarrow \infty} \|f - f^n\|_Z}_{=0} \leq \liminf_{n \rightarrow \infty} \|v^n - f^n\|_Z.$$

That the subgradient of R in u^\dagger is non-empty is apparent, since $\tilde{T}^*\omega \in \partial R(u^\dagger)$. Also, the quasi triangle inequality is simply the standard triangle inequality of norms for $\|\cdot\|_Z$, which only leaves to show the estimate on the dual pairing. Therefore, we note that both $u_\alpha^\delta, u^\dagger \in \text{dom}(\tilde{T})$, since F_α is proper by assumption, and u^\dagger and u_α^δ are optimal in

their respective senses. Also $\xi \in \text{dom}(\tilde{T}^*)$, resulting in

$$\begin{aligned} \langle \xi, u^\dagger - u_\alpha^\delta \rangle_{X^* \times X} &= \langle \omega, \tilde{T}(u^\dagger - u_\alpha^\delta) \rangle_{Z^* \times Z} \leq \|\omega\|_{Z^*} \|Tu_\alpha^\delta - Tu^\dagger\|_Z = \|\omega\|_{Z^*} D(Tu_\alpha^\delta, Tu^\dagger)^{1/p} \\ &= 0D_R^\xi(u, u^\dagger) + \|\omega\|_{Z^*} D(Tu_\alpha^\delta, Tu^\dagger)^{1/p}, \end{aligned}$$

i.e. (SC1) is satisfied with $\gamma_1 = 0$ and $\gamma_2 = \|\omega\|_{Z^*}$. \square

Remark 2.18. *A classical situation in which one uses this Theorem is, if $T: (X, \|\cdot\|_X) \rightarrow (Y, \|\cdot\|_Y)$ is linear and continuous, and the relevant topologies \mathcal{T}_X and \mathcal{T}_Y represent the respective weak topologies. Moreover, $\|\cdot\|_Z$ is a stronger norm than the one on Y , and is only defined on a subspace of Y (e.g. $Y = L^2$ but Z is the Sobolev space H^1).*

So to summarise, under reasonable assumptions the Tikhonov problem is solvable. Moreover, with additional continuity assumptions, solving the Tikhonov problem is stable. Finally, with a suitable parameter choice rule, one can obtain convergence to R -minimal solutions, and with an additional source condition, rates can be estimated.

3. Multi-Data Tikhonov Regularisation

Based on this classical approach to Tikhonov regularisation, one can extend the setting by breaking down an inverse problem into several inverse problems. Hence, in this section one tries to solve

$$T_1 u = f_1^\dagger, \dots, T_M u = f_M^\dagger \quad (62)$$

for $u \in X$, $f_i^\dagger \in Y_i$ and operators $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$. We will use product space notation $T = (T_1, \dots, T_M)$, $Y = Y_1 \times \dots \times Y_M$ and $f^\dagger = (f_1^\dagger, \dots, f_M^\dagger)$ and problem (62) can be understood as the inverse problem $Tu = f^\dagger$ being broken down into several subproblems. Considering these subproblems will give us more control to deal with the individual subproblems' properties.

As motivated in the introduction, we aim to consider a Tikhonov functional $F_{\lambda, \alpha}(u, f^\dagger) = \sum_{i=1}^M \lambda_i D_i(T_i u, f_i^\dagger) + R_\alpha(u)$ using multiple discrepancies with individual parameter. Splitting the problem into these subproblems and applying such Tikhonov approaches allows to consider adequate noise models and corresponding discrepancies to the individual problems. Also, the individual problems might have different scales and noise levels, and moreover the degree of ill-posedness might vary strongly between the individual problems, making individual regularisation parameters essential to obtaining a suitable approach. Furthermore, splitting the problem allows to consider a multitude of behaviour in the data. Important questions which arise from this setting are:

- How are the parameter supposed to be chosen in order to get suitable results?
- How do sequences of solutions obtained through such a Tikhonov approach to data disturbed by noise behave if the data of some (but not all) problems converge to a ground truth? In this case, does the problem converge to a limit problem with appropriate interpretation (like R -minimal)?
- Can one obtain convergence rates for the individual problems, and if so, how do they incorporate the noise levels of the other problems, what is their interplay?

3.1. Preliminaries

Before we come to the main focus of multi-data Tikhonov regularisation, we have to adapt the assumptions and confirm basic existence and stability results.

While the split problem (62) could be interpreted as a single inverse problem on the product space $Y = Y_1 \times \dots \times Y_M$ and regularised accordingly, we discuss a multi-data

Tikhonov approach as follows in order to address mentioned issues.

Problem 3.1 (Multi-Data Tikhonov Problem). *For $i \in \{1, \dots, M\}$ let X, Y_i, \mathcal{A} be sets and let $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$. Further, let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$, $\lambda \in (0, \infty)^M$ and a family of functions $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha: X \rightarrow [0, \infty]$ be given. We say u^\dagger is a solution to the multi-data Tikhonov regularisation regarding $T_i u = f_i^\dagger$ for $i \in \{1, \dots, M\}$ with discrepancies D_i , weights λ_i and regularisation R_α with regularisation parameter $\alpha \in \mathcal{A}$, if*

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda, \alpha}(u, f^\dagger) & \text{such that } F_{\lambda, \alpha}(u^\dagger, f^\dagger) < \infty, \\ \text{with } F_{\lambda, \alpha}(u, f^\dagger) = \left(\sum_{i=1}^M \lambda_i D_i(T_i u, f_i^\dagger) \right) + R_\alpha(u). \end{cases} \quad (\text{MTIKH}_{\lambda, \alpha}(f^\dagger))$$

Here, one uses a single regularisation functional R_α , while individual weighting parameters λ_i and individual discrepancies D_i suitable for the i -th inverse problem are applied, in order to exert more control over individual discrepancies.

Such approaches are already used in practice in order to solve independent inverse problems with complementing information, i.e. solving $T_i u_i = f_i^\dagger$ for u_i via Tikhonov approaches with joint regularisation which is expected to transfer information between the problems. While such problems satisfies the setting of multi-data regularisation, this multi-data approach is not limited to such situations.

In order to develop the theory, we generalise the assumptions from the single-data setting to the multi-data setting, and those will be used throughout the entire chapter. As we allow now for slightly more general regularisation functionals, we require the following definition.

Definition 3.2. *Let (X, \mathcal{T}_X) and $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ be Hausdorff spaces, and for any $\alpha \in \mathcal{A}$, let $R_\alpha: X \rightarrow [0, \infty]$. Then we call the family $(R_\alpha)_{\alpha \in \mathcal{A}}$ continuous, if the following hold:*

R1 The mapping $(u, \alpha) \mapsto R_\alpha(u)$ is $\mathcal{T}_X \times \mathcal{T}_\mathcal{A}$ -lower semi-continuous, i.e. for sequences $(u^n)_n \subset X$ and $(\alpha^n)_n \subset \mathcal{A}$,

$$\left(u^n \xrightarrow{\mathcal{T}_X} u \text{ and } \alpha^n \xrightarrow{\mathcal{T}_\mathcal{A}} \alpha \right) \Rightarrow R_\alpha(u) \leq \liminf_{n \rightarrow \infty} R_{\alpha^n}(u^n). \quad (63)$$

R2 For fixed $u \in X$, and a sequence $(\alpha^n)_n \subset \mathcal{A}$ such that $\alpha^n \xrightarrow{\mathcal{T}_\mathcal{A}} \alpha$, also $\lim_{n \rightarrow \infty} R_{\alpha^n}(u) = R_\alpha(u)$.

R3 For $\alpha, \beta \in \mathcal{A}$, there is a constant $c(\alpha, \beta)$ such that $R_\alpha(u) \leq c(\alpha, \beta)R_\beta(u)$ for all $u \in X$, i.e. the functions R_α are topologically equivalent for different parameter $\alpha \in \mathcal{A}$. Moreover, for a sequence $(\alpha^n)_n \subset \mathcal{A}$ with $\alpha^n \xrightarrow{\mathcal{T}_\mathcal{A}} \alpha$ the constants $c(\alpha, \alpha^n)$ stay bounded.

Furthermore, for continuous $\psi_{R_{\alpha^\dagger}}: [0, \infty) \rightarrow [0, \infty)$ with $\psi_{R_{\alpha^\dagger}}(0) = 0$, we say the family $(R_\alpha)_{\alpha \in \mathcal{A}}$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on a set $U \subset X$ in $\alpha^\dagger \in \mathcal{A}$, iff $(\mathcal{A}, d_\mathcal{A})$ is a metric space equivalent to $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ and there is $\epsilon_0 > 0$ such that for all $u \in U$ and for $\beta \in \mathcal{A}$ with $d_\mathcal{A}(\beta, \alpha^\dagger) < \epsilon_0$, the family of regularisation functions $(R_\alpha)_\alpha$ satisfies the following modulus of continuity estimate:

$$|R_\beta(u) - R_{\alpha^\dagger}(u)| \leq \psi_{R_{\alpha^\dagger}}(d_\mathcal{A}(\beta, \alpha^\dagger))(R_{\alpha^\dagger}(u) + 1). \quad (64)$$

Recall that for single-data Tikhonov problems we required Hausdorff spaces, a continuous operator, a basic discrepancy (a non-negative function with positivity properties which is lower semi-continuous), a topology stronger than the discrepancy, a non-negative and lower semi-continuous regularisation functional and a coercivity statement. The following assumptions are similar, however now feature several discrepancies and corresponding spaces and topologies.

Assumptions 3.3 (Multi-data Tikhonov Regularisation). *Let the following conditions hold:*

M1 *The spaces (X, \mathcal{T}_X) and $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ are Hausdorff spaces.*

M2 *For $i \in \{1, \dots, M\}$, the space (Y_i, \mathcal{T}_{Y_i}) is a Hausdorff space, and the operator $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$ is continuous with respect to \mathcal{T}_X and \mathcal{T}_{Y_i} and $\text{dom}(T_i)$ is closed with respect to \mathcal{T}_X .*

M3 *There are topologies \mathcal{T}_{D_i} on Y_i for $i \in \{1, \dots, M\}$ such that D_i is a basic discrepancy with respect to \mathcal{T}_{Y_i} and \mathcal{T}_{D_i} (see Definition 2.2).*

M4 *The family $(R_\alpha)_{\alpha \in \mathcal{A}}$ is continuous (see Definition 3.2).*

On the product space $Y = Y_1 \times \dots \times Y_M$, we denote by \mathcal{T}_Y and \mathcal{T}_D the product topologies induced by $\{\mathcal{T}_{Y_i}\}_{i=1}^M$, $\{\mathcal{T}_{D_i}\}_{i=1}^M$ respectively.

M5 *There is $\alpha_0 \in \mathcal{A}$ such that the Tikhonov functional $F_{\mathbf{1}, \alpha_0}$ with $\mathbf{1} = (1, \dots, 1)$ is uniformly coercive in the following sense: For a sequence $(f^n)_n \subset Y$ with $f^n \xrightarrow{\mathcal{T}_Y} f$ and for each $C > 0$, the set $\bigcup_{n=1}^\infty \{u \in X \mid F_{\mathbf{1}, \alpha_0}(u, f^n) < C\}$ is \mathcal{T}_X -precompact.*

Remark 3.4. *While most of these assumptions are simply generalisations of the single-data setting, allowing the regularisation to be dependent on a parameter $\alpha \in \mathcal{A}$ will allow for more general settings without any substantial problems arising from it. This parameter α can be understood as a fine-tuning of the regularisation, while the main weighting is done through λ .*

The existence and stability properties of $MTIKH_{\lambda,\alpha}(f^\dagger)$ are inherited from the corresponding results for single-data Tikhonov regularisation.

Theorem 3.5. *Let the Assumptions 3.3 hold and $f^\dagger \in Y$. Either for all $\lambda \in (0, \infty)^M$ and $\alpha \in \mathcal{A}$ the Problem $MTIKH_{\lambda,\alpha}(f^\dagger)$ is solvable, or $F_{\lambda,\alpha}(\cdot, f^\dagger) \equiv \infty$ for all $\lambda \in (0, \infty)^M$ and $\alpha \in \mathcal{A}$. Moreover, if there is a solution u_0 to $MTIKH_{\lambda,\alpha}(f^\dagger)$ and if D_i is $T_i u_0$ -continuous in f_i^\dagger for $i \in \{1, \dots, M\}$ (i.e. $D_i(T_i u_0, \cdot)$ is continuous in f^\dagger with respect to the \mathcal{T}_{D_i} topology), then solving $MTIKH_{\lambda,\alpha}(f^\dagger)$ is stable.*

Proof. For fixed $\alpha \in \mathcal{A}$ and $\lambda \in (0, \infty)^M$ we consider the discrepancy and regularisation functions $\tilde{D}(v, f) = \sum_{i=1}^M \lambda_i D_i(v_i, f_i)$, $\tilde{R}(u) = R_\alpha(u)$ and $\tilde{F}_1(u, f) = \tilde{D}(Tu, f) + \tilde{\alpha} \tilde{R}(u) = \tilde{F}_{\tilde{\alpha}}(u, f)$ with $\tilde{\alpha} = 1$, where $T = (T_1, \dots, T_M)$, $v, f \in Y$ and $u \in X$. Using the single-data Tikhonov functional $\tilde{F}_1(u, f)$ to the inverse problems $Tu = f$ yields an approach satisfying Assumptions 2.3. Hence, Theorem 2.4 states that $\tilde{F}_1(\cdot, f^\dagger)$ either attains a minimum or is constantly ∞ . Moreover, due to the topological equivalence of R_α and R_β for $\alpha, \beta \in \mathcal{A}$, the properness of the problems does not depend on the specific α , thus making the problem either be solvable for all $\alpha \in \mathcal{A}$ or non-proper. The same argument can be made for different parameter λ , showing that being proper does not depend on α or λ , and consequently the existence statement is valid.

To show stability, we apply Theorem 2.6 to the functional \tilde{F}_1 for fixed $\alpha \in \mathcal{A}$ and $\lambda \in (0, \infty)^M$, where Tu_0 -continuity of \tilde{D} is satisfied due to the continuity assumptions on D_i for $i \in \{1, \dots, M\}$. \square

3.2. Convergence to Partial Solutions

In this section, we aim to answer the questions stated in the beginning of Chapter 3. In particular, the question of how solutions behave if the data concerning some of the problems converge to a ground truth while the other data converge to data not representing the true data. This leads to the concept of partial solutions, i.e. $u \in X$ such that for an index set $I = \{i_1, \dots, i_{|I|}\} \subset \{1, \dots, M\}$ with $T_I = (T_{i_1}, \dots, T_{i_{|I|}})$ and $f_I = (f_{i_1}, \dots, f_{i_{|I|}})$, $T_I u = f_I$ holds. As we consider the data of some subproblems

converging to a ground truth, one might expect to obtain partial solutions solely solving said subproblems. We will see, that convergence to such partial solutions can be attained and the problems themselves converge towards a limit problem not unlike the problem $\min_{Tu=f^\dagger} R(u)$. As we will see, this limit problem can be understood as a Tikhonov approach to the unsolved subproblems, using the solved problems as a prior.

To answer the posed questions, we aim to generalise the theory of vanishing noise to incorporate convergence to partial solutions. Again a suitable parameter choice is required in order to guarantee convergence towards partial solutions. Note that we again use sequences indexed by δ , however, now $\delta = (\delta_1, \dots, \delta_M) \in (0, \infty)^M$ is a vector of positive reals.

Remark 3.6. *Note that in Chapter 2 continuity of D was required for the stability result in Theorem 2.6, but not for the convergence result in Theorem 2.11, since $\alpha(\delta) \rightarrow 0$ enforced the convergence one previously only attained due to continuity assumptions. The following theory of convergence to partial solutions is a mixture of the two, and thus requires a mixture of the assumptions and techniques used in the respective proofs.*

In particular, we need to adapt the notion of R -minimal solutions in case of partial solutions to also incorporate discrepancies of the unsolved problems.

Definition 3.7. *Let D_i and R_α as in the Tikhonov functional in Problem 3.1. For an index set $I \subset \{1, \dots, M\}$, $f \in Y$, weights $\lambda \in (0, \infty]^M$ and $\alpha \in \mathcal{A}$, we define the extended regularisation functional*

$$R_{\alpha, \lambda, I}(u, f) = R_\alpha(u) + \sum_{i \in I^c} \lambda_i D_i(T_i u, f_i). \quad (65)$$

Note that in this setting, we allow $\lambda_i = \infty$ in which case we set $\lambda_i D_i(T_i u, f_i) = \chi_{\{f_i\}}(T_i u)$, where χ denotes the characteristic function in Definition 1.34.

For $f^\dagger \in Y$, we call $u^\dagger \in X$ an $R_{\alpha, \lambda, I}$ -minimal I -partial solution to $Tu = f^\dagger$ if

$$u^\dagger \in \underset{\substack{u \in \text{dom}(T) \\ Tu = f_I^\dagger}}{\text{argmin}} R_{\alpha, \lambda, I}(u, f^\dagger), \quad \text{and} \quad R_{\alpha, \lambda, I}(u^\dagger, f^\dagger) < \infty, \quad (66)$$

where for $I = \{i_1, \dots, i_{|I|}\}$ with $i_1 < i_2 < \dots < i_{|I|}$, $T_I = (T_{i_1}, \dots, T_{i_{|I|}})$ and $f_I^\dagger = (f_{i_1}^\dagger, \dots, f_{i_{|I|}}^\dagger)$. When setting $\lambda_i = \infty$ for $i \in I$ one can understand this minimisation problem equivalently as $\underset{u \in \text{dom}(T)}{\text{argmin}} R_{\alpha, \lambda, \{1, \dots, M\}}(u, f^\dagger)$ since for $i \in I$ the convention $\lambda_i D_i(T_i u, f_i) = \chi_{\{f_i\}}(T_i u)$ enforces $T_I u = f_I^\dagger$.

Remark 3.8. Note that $R_{\alpha,\lambda,I}$ is again a multi-data Tikhonov functional to the problem $T_{I^c}u = f_{I^c}^\dagger$, and thus $R_{\alpha,\lambda,I}$ -minimal solutions are solutions to a Tikhonov problem regarding $T_{I^c}u = f_{I^c}^\dagger$ using $T_Iu = f_I^\dagger$ as prior.

Theorem 3.9 (Convergence to Partial Solutions). *Let Assumptions 3.3 hold, let the sequence $(f^\delta)_\delta$ in Y with $f^\delta \xrightarrow{\mathcal{T}_D} f^\dagger$ be given and denote with $D_i(f_i^\dagger, f_i^\delta) = \delta_i$ the noise level of the individual subproblems and set $\delta = (\delta_1, \dots, \delta_M)$. Further, let $I \subset \{1, \dots, M\}$ and $\lambda^\dagger \in (0, \infty]^M$ be such that $\lambda_i^\dagger = \infty$ for $i \in I$ and finite otherwise, let $\alpha^\dagger \in \mathcal{A}$ and $f^\dagger \in Y$ such that $f_I^\dagger \in \text{Rg}(T_I)$. Assume there is an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u_0 to $Tu = f^\dagger$ such that for all $i \in I^c$, the discrepancy D_i is T_iu_0 -continuous in f_i^\dagger (i.e. $D_i(T_iu_0, \cdot)$ is continuous in f_i^\dagger with respect to \mathcal{T}_{D_i}).*

Then, for every $\lambda \in (0, \infty)^M$, $\alpha \in \mathcal{A}$ and f^δ with δ sufficiently small $MTIKH_{\lambda,\alpha}(f^\delta)$ possesses a solution. Furthermore, if sequences $(\alpha^\delta)_\delta$ and $(\lambda^\delta)_\delta$ with $\alpha^\delta \xrightarrow{\mathcal{T}_A} \alpha^\dagger$ and $\lambda^\delta \rightarrow \lambda^\dagger$ are chosen such that

$$\begin{cases} \lambda_i^\delta \rightarrow \lambda_i^\dagger \in (0, \infty) & \text{for } i \in I^c, \\ \lambda_i^\delta \delta_i \rightarrow 0, \lambda_i^\delta \rightarrow \infty = \lambda_i^\dagger & \text{for } i \in I, \end{cases} \quad (67)$$

then the corresponding sequence of solutions to $MTIKH_{\lambda^\delta, \alpha^\delta}(f^\delta)$ denoted by $(u^\delta)_\delta$ contains a \mathcal{T}_X -convergent subsequence. Moreover, any limit u^\dagger of such a subsequence is an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution to $Tu = f^\dagger$ and

$$\begin{aligned} R_{\alpha^\dagger}(u^\dagger) &= \lim_{\delta \rightarrow 0} R_{\alpha^\delta}(u^\delta), & D_i(T_iu^\dagger, f_i^\dagger) &= \lim_{\delta \rightarrow 0} D_i(T_iu^\delta, f_i^\delta) & \text{for } i \in I^c, & (68) \\ D_i(T_iu^\delta, f_i^\delta) &= o((\lambda_i^\delta)^{-1}) & & & \text{for } i \in I. & \end{aligned}$$

Remark 3.10. *We note that this theorem is a combination of stability and convergence results, where the $i \in I$ represent the vanishing noise portion, while the $i \in I^c$ represent the stability portion. Thus, only I^c requires the continuity assumption as was required for the stability but not for the convergence results.*

Also, the convergence to an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution can be understood as approximating a Tikhonov problem for $T_{I^c}u = f_{I^c}^\dagger$ with prior $T_Iu = f_I^\dagger$. Thus solving the multi-data Tikhonov problem for vanishing noise can be used as an approximation scheme for solving a Tikhonov problem with prior (as direct solution might not be possible).

Proof Theorem 3.9. We note that due to the continuity assumption on D_i for $i \in I^c$, we

can compute

$$F_{\mathbf{1}, \alpha^\dagger}(u_0, f^\delta) = R_{\alpha^\dagger}(u_0) + \left(\sum_{i \in I} \underbrace{D_i(T_i u_0, f_i^\delta)}_{=\delta_i \rightarrow 0} \right) + \left(\sum_{i \in I^c} \underbrace{D_i(T_i u_0, f_i^\delta)}_{\xrightarrow{\text{cont.}} D_i(T_i u_0, f_i^\dagger) < \infty} \right) < \infty \quad (69)$$

for δ sufficiently small since u_0 is an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal solution. Thus, Theorem 3.5 ensures existence of solutions for any f^δ with δ sufficiently small and all $\lambda \in (0, \infty)^M$, $\alpha \in \mathcal{A}$. We use the optimality of u^δ , the continuity condition on D_i for $i \in I^c$ and the continuity of the family $(R_\alpha)_\alpha$ to estimate

$$\begin{aligned} F_{\lambda^\delta, \alpha^\delta}(u^\delta, f^\delta) &\stackrel{\text{opt.}}{\leq} F_{\lambda^\delta, \alpha^\delta}(u_0, f^\delta) \stackrel{\text{def.}}{=} \left(\sum_{i \in I} \lambda_i^\delta D_i(\overbrace{T_i u_0, f_i^\delta}^{=f_i^\dagger}) \right) + \left(\sum_{i \in I^c} \lambda_i^\delta D_i(T_i u_0, f_i^\delta) \right) + R_{\alpha^\delta}(u_0) \\ &= \left(\sum_{i \in I} \underbrace{\delta_i \lambda_i^\delta}_{\xrightarrow{(67)} 0} \right) + \left(\sum_{i \in I^c} \underbrace{\lambda_i^\delta}_{\xrightarrow{\text{def.}} \lambda_i^\dagger < \infty} \underbrace{D_i(T_i u_0, f_i^\delta)}_{\xrightarrow{\text{cont.}} D_i(T_i u_0, f_i^\dagger)} \right) + \underbrace{R_{\alpha^\delta}(u_0)}_{\xrightarrow{\text{cont.}} R_{\alpha^\dagger}(u_0)} \\ &\leq c + R_{\alpha^\dagger, \lambda^\dagger, I}(u_0, f^\dagger) < \infty \end{aligned} \quad (70)$$

for δ sufficiently small. Also, for α_0 as in M5 of Assumption 3.3 such that $F_{\mathbf{1}, \alpha_0}$ is coercive, the uniform boundedness of $c(\alpha^\dagger, \alpha^\delta)$ for the continuous family $(R_\alpha)_\alpha$ and the fact that $\underline{\lambda}^\delta = \min_{i=1, \dots, M} \lambda_i^\delta$ is uniformly bounded away from zero imply

$$\begin{aligned} \sum_{i=1}^M D_i(T_i u, f_i^\delta) &\leq \frac{1}{\underline{\lambda}^\delta} \sum_{i=1}^M \lambda_i^\delta D_i(T_i u, f_i^\delta), \quad \text{and} \\ R_{\alpha_0}(u^\delta) &\leq c(\alpha_0, \alpha^\dagger) R_{\alpha^\dagger}(u^\delta) \leq c(\alpha_0, \alpha^\dagger) c(\alpha^\dagger, \alpha^\delta) R_{\alpha^\delta}(u^\delta). \end{aligned} \quad (71)$$

Together with (70), this yields the boundedness of $F_{\mathbf{1}, \alpha_0}(u^\delta, f^\delta)$, and the precompactness of the corresponding level sets implies that $(u^\delta)_\delta$ admits a \mathcal{T}_X -convergent subsequence (relabelled u^δ) with limit u^\dagger . Due to lower semi-continuity and $f^\delta \xrightarrow{\mathcal{T}_R} f^\dagger$, one obtains that $D_i(T_i u^\dagger, f_i^\dagger) \leq \liminf_\delta D_i(T_i u^\dagger, f_i^\delta) = \liminf_\delta \delta_i = 0$ for $i \in I$ and with convergence

of $\lambda_i^\delta \rightarrow \lambda_i^\dagger$ for $i \in I^c$ and $\alpha^\delta \xrightarrow{\mathcal{T}_A} \alpha^\dagger$, one computes

$$\begin{aligned}
R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) &\stackrel{\text{l.s.c.}}{\leq} \liminf_{\delta \rightarrow 0} R_{\alpha^\delta, \lambda^\delta, I}(u^\delta, f^\delta) \leq \limsup_{\delta \rightarrow 0} R_{\alpha^\delta, \lambda^\delta, I}(u^\delta, f^\delta) \\
&\leq \limsup_{\delta \rightarrow 0} R_{\alpha^\delta, \lambda^\delta, I}(u^\delta, f^\delta) + \sum_{i \in I} \lambda_i^\delta D_i(T_i u^\delta, f_i^\delta) \\
&\stackrel{\text{opt.}}{\leq} \limsup_{\delta \rightarrow 0} R_{\alpha^\delta, \lambda^\delta, I}(u_0, f^\delta) + \sum_{i \in I} \lambda_i^\delta \underbrace{D_i(T_i u_0, f_i^\delta)}_{=\delta_i \rightarrow 0} \stackrel{\text{cont.}}{=} R_{\alpha^\dagger, \lambda^\dagger, I}(u_0, f^\dagger)
\end{aligned} \tag{72}$$

where the last inequality is due to optimality and the final equality holds since $(\alpha, \lambda, f) \mapsto R_{\alpha, \lambda, I}(u_0, f)$ is continuous in $(\alpha^\dagger, \lambda^\dagger, f^\dagger)$ due to the continuity condition on D_i for $i \in I^c$ and the continuity of the family $(R_\alpha)_\alpha$. In particular, these results imply that u^\dagger is an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution to $Tu = f^\dagger$.

Note that since both u^\dagger and u_0 are $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solutions, $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) = R_{\alpha^\dagger, \lambda^\dagger, I}(u_0, f^\dagger)$ holds. So all inequalities in (72) hold with equality, yielding the convergence $R_{\alpha^\delta, \lambda^\delta, I}(u^\delta, f^\delta) \xrightarrow{\delta \rightarrow 0} R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$ and $\sum_{i \in I} \lambda_i^\delta D_i(T_i u^\delta, f_i^\delta) \rightarrow 0$ resulting in $D_i(T_i u^\delta, f_i^\delta) = o((\lambda_i^\delta)^{-1})$ for $i \in I$. Application of Lemma 1.42 to the extended regularisation functional $R_{\alpha^\delta, \lambda^\delta, I}(u_\alpha^\delta, f^\delta) = (\sum_{i \in I^c} \lambda_i^\delta D_i(T_i u_\alpha^\delta, f_i^\delta)) + R_{\alpha^\delta}(u^\delta)$ yields convergence of $R_{\alpha^\delta}(u^\delta)$ and $D_i(T_i u^\delta, f_i^\delta)$ for $i \in I^c$. \square

Remark 3.11. *This proof follows the idea of the proof for Theorem 2.11 by considering $R_{\alpha, \lambda, I}$ as regularisation functional. The additional continuity is required to ensure the existence of a convergent subsequence, and the $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimality of u^\dagger as an I -partial solution. Also, the stability result stated in Theorem 3.5 can be understood to be a special case of Theorem 3.9 when setting $I = \emptyset$, $\lambda^\delta = \lambda^\dagger$, $\alpha^\delta = \alpha^\dagger$ and solely changing f^δ , in fact one even gets a slightly stronger stability result since we obtain stability for λ, α not fixed, but converging $\lambda \rightarrow \lambda^\dagger \in (0, \infty)^M$, $\alpha \rightarrow \alpha^\dagger \in \mathcal{A}$.*

Also, for $I = \{1, \dots, M\}$ one attains subsequential \mathcal{T}_X -convergence of $(u^\delta)_\delta$ to solutions of the multi-data inverse problem $Tu = f^\dagger$, analog to the vanishing noise result presented in Theorem 2.11. Further, we point out that the continuity conditions are solely required to ensure $D_i(T_i u_0, f_i^\delta) \xrightarrow{\delta \rightarrow 0} D_i(T_i u_0, f_i^\dagger)$ for $i \in I^c$, and consequently is only needed for those $i \in I^c$ which have $f_i^\delta \neq f_i^\dagger$ for infinitely many δ .

Next, we aim to obtain convergence rates for the Bregman distance and the occurring discrepancies. The main difference to the result in Theorem 2.15 is that when one considers $R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)$ as the regularisation functional, there is an explicit dependence on $f^\dagger, \lambda^\dagger$ and α^\dagger , whose information is not contained in the $MTIKH_{\lambda^\delta, \alpha^\delta}(f^\delta)$ problems

for fixed δ . In order to overcome this issue, one requires further continuity assumptions on D_i and R_α , and convergence rates on $\lambda_i^\delta \rightarrow \lambda_i^\dagger$ and $\alpha^\delta \xrightarrow{\mathcal{T}_\mathcal{A}} \alpha^\dagger$. Therefore, we require sets $U \subset X$ and $V_i \subset Y_i$ and functions $\psi_i, \psi_{R_{\alpha^\dagger}} : [0, \infty) \rightarrow [0, \infty)$ such that for $i \in \{1, \dots, M\}$, the discrepancy D_i is strongly ψ_i -continuous on V_i in f_i^\dagger , and that $(R_\alpha)_\alpha$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on U in α^\dagger (see Definitions 2.2 and 3.2). Recall that this means there are functions ψ_i for $i \in \{1, \dots, M\}$ and a function $\psi_{R_{\alpha^\dagger}}$ such that the functions D_i and the regularisation family $(R_\alpha)_\alpha$ satisfy the modulus of continuity estimates for $v_i \in V_i$, $u \in U$:

$$|D_i(v_i, f_i^\dagger) - D_i(v_i, f_i)| \leq \psi_i(D_i(f_i^\dagger, f_i))(D_i(v_i, f_i^\dagger) + 1), \quad (73)$$

$$|R_\alpha(u) - R_{\alpha^\dagger}(u)| \leq \psi_{R_{\alpha^\dagger}}(d_\mathcal{A}(\alpha, \alpha^\dagger))(R_{\alpha^\dagger}(u) + 1), \quad (74)$$

for $D_i(f_i^\dagger, f_i)$ and $d_\mathcal{A}(\alpha, \alpha^\dagger)$ sufficiently small, where $d_\mathcal{A}$ is a metric on \mathcal{A} that metricises the topology $\mathcal{T}_\mathcal{A}$.

Remark 3.12. *We note that the right side of the modulus of continuity estimates may depend multiplicatively on one of the function values. This allows for more general moduli of continuity without affecting the resulting convergence rates. In particular, this ensures applicability to a larger range of discrepancy functions.*

Note that for $v_i \in V_i$ this estimate implies continuity of $D_i(v_i, \cdot)$ in f_i^\dagger . Furthermore, if for $i \in \{1, \dots, M\}$ the true data f_i^\dagger satisfies $f_i^\dagger \in V_i$, then $\psi_i(t) \geq ct$ with some constant $c \geq 1$.

Theorem 3.13 (Error Estimates to Partial Solutions). *Let Assumptions 3.3 hold and let $(\mathcal{A}, d_\mathcal{A})$ be a metric space. Let $\alpha^\dagger \in \mathcal{A}$, let $I \in \{1, \dots, M\}$ and $\lambda^\dagger \in (0, \infty]^M$ be such that $\lambda_i^\dagger = \infty$ for $i \in I$ and finite otherwise, and f^\dagger be the true parameters and true data, and let parameter $\lambda \in (0, \infty)^M$ and $\alpha \in \mathcal{A}$ and data $f \in Y$ be such that $D_i(f_i^\dagger, f_i) = \delta_i$ sufficiently small that (73) and (74) holds, and such that*

$$\begin{cases} \lambda_i \delta_i < 1 \text{ for } i \in I, & |\lambda_i - \lambda_i^\dagger| < 1 \text{ for } i \in I^c, \\ \lambda_i \psi_i(\delta_i) \leq 1 \text{ for } i \in I^c, & \psi_i(\delta_i) \leq \frac{1}{2} \text{ for all } i, \quad \psi_{R_{\alpha^\dagger}}(d_\mathcal{A}(\alpha^\dagger, \alpha)) < 1. \end{cases} \quad (75)$$

Let \hat{u} denote a solution to $MTIKH_{\lambda, \alpha}(f)$, and let there be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u^\dagger to $Tu = f^\dagger$. Further, let there be sets $V_i \subset Y_i$ and $U \subset X$ and functions $\psi_i, \psi_{R_{\alpha^\dagger}} : [0, \infty) \rightarrow [0, \infty)$ such that the discrepancies D_i are strongly ψ_i -continuous on V_i in f_i^\dagger for $i \in \{1, \dots, M\}$ and the family of functions $(R_\alpha)_\alpha$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on U in α^\dagger and such that $\hat{u}, u^\dagger \in U$ and $T_i \hat{u}, T_i u^\dagger \in V_i$ for all i . Then there is a constant

$c > 0$ such that

$$R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + c \left(\left(\sum_{i \in I} \lambda_i \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) \right). \quad (76)$$

In particular, this constant c does not depend on $\hat{u}, f, \lambda, \alpha$ but solely on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$ and $\alpha^\dagger, \lambda^\dagger, f^\dagger$.

Additionally, let X be a Banach space and let R_{α^\dagger} and $D_i(T_i \cdot, f^\dagger)$ for $i \in I^c$ be convex, and let there be $\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ as well as constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\lambda_i - 2\gamma_2 \geq 1$ for $i \in I$, such that

$$-\langle \xi, \hat{u} - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) + \gamma_2 \sum_{i \in I} D_i(T_i \hat{u}, T_i u^\dagger). \quad (\text{SC2})$$

Then, there is a constant $c > 0$ such that the following estimates for $j \in I$ hold:

$$D_j(T_j \hat{u}, f_j) \leq c \left((\lambda_j)^{-1} \left(\left(\sum_{i \in I} \lambda_i \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) \right) \right), \quad (77)$$

$$D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) \leq c \left(\left(\sum_{i \in I} \lambda_i \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) \right). \quad (78)$$

Note that the constant c does not depend on $\hat{u}, f, \lambda, \alpha$, but the estimate is uniform for all such tuples satisfying the stated assumptions and only depends on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$, $\alpha^\dagger, \lambda^\dagger, f^\dagger$ and the constants γ_1, γ_2 .

Remark 3.14. Note that the Source Condition (SC1) allowed for exponent $\frac{1}{p}$ on the discrepancy, while (SC2) does not. This is solely for the sake of simplicity, Theorem 3.21 will present a more general source condition for multi-data regularisation.

We provide the proof after remarking important consequences concerning the applicability of this theorem to sequences of solutions.

Remark 3.15. While in the previous theorem the estimate is made for one tuple $\hat{u}, f, \lambda, \alpha$, classical application of such results would be to use these estimates on sequences u^δ, f^δ ,

$\alpha^\delta, \lambda^\delta$ with $\delta \rightarrow 0$ to obtain convergence rates. To do so, one would require the estimate (75) and the Condition (SC2) to hold for all instances of the sequences.

For parameter choice rules $\delta \mapsto (\lambda^\delta, \alpha^\delta)$ as in Theorem 3.9 and data f^δ there is $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ such that $\delta_i \leq \bar{\delta}_i$ guarantees that (75) is fulfilled. Hence, these estimates hold for $\delta < \bar{\delta}$ independent of all other factors, and in particular independent of the sequence f^δ itself as long as the parameter choice rules are fixed.

The Source Condition (SC2) needs to hold for the instances of the sequence $(u^\delta)_\delta$, the sequence of corresponding solutions. Typically, one assumes that this estimate holds for u with sufficiently small Tikhonov function values, more precisely (SC2) holds for u such that $R_{\lambda^\dagger, \alpha^\dagger, I}(u, f^\dagger) \leq R_{\lambda^\dagger, \alpha^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f^\dagger) \leq \epsilon_0$ for some constant $\epsilon_0 > 0$. Again, these assumption are fulfilled for the sequence after finitely many δ , as can be seen from Theorem 3.9. Thus the estimates of Theorem 3.13 transfers to a convergence rates for sequences of data with vanishing noise.

Theorem 3.16 (Convergence Rates to Partial Solutions). *Let Assumptions 3.3 hold and let $(\mathcal{A}, d_{\mathcal{A}})$ be a metric space. Let $\alpha^\dagger \in \mathcal{A}$, let $I \in \{1, \dots, M\}$ and $\lambda^\dagger \in (0, \infty]^M$ be such that $\lambda_i^\dagger = \infty$ for $i \in I$ and finite otherwise, and f^\dagger be the true parameters and true data, and $(f^\delta)_\delta \subset Y$ be a sequence such that $D(f_i^\dagger, f_i^\delta) = \delta_i$ and $f^\delta \xrightarrow{T_R} f^\dagger$. Let parameter choice rules λ^δ and α^δ be such that $\lambda^\delta \rightarrow \lambda^\dagger$ and $\alpha^\delta \rightarrow \alpha^\dagger$ with*

$$\begin{cases} \lambda_i^\delta \rightarrow \lambda_i^\dagger \in (0, \infty) & \text{for } i \in I^c, \\ \lambda_i^\delta \delta_i \rightarrow 0, \lambda_i^\delta \rightarrow \infty = \lambda_i^\dagger & \text{for } i \in I. \end{cases} \quad (79)$$

Denote with u^δ the solutions to $MTIKH_{\lambda^\delta, \alpha^\delta}(f^\delta)$, and let there be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u^\dagger to $Tu = f^\dagger$. Further, let there be sets $V_i \subset Y_i$ and $U \subset X$ such that the discrepancies D_i are strongly ψ_i -continuous on V_i in f_i^\dagger for $i \in \{1, \dots, M\}$ and the family of functions $(R_\alpha)_\alpha$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on U in α^\dagger and these sets are such that $u^\delta, u^\dagger \in U$ and $T_i u^\delta, T_i u^\dagger \in V_i$ for all δ and all i .

Then there is $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ and a constant $c > 0$ such that for $\delta < \bar{\delta}$,

$$\begin{aligned} R_{\alpha^\dagger, \lambda^\dagger, I}(u^\delta, f^\dagger) &\leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + c \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \\ &\quad \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \end{aligned} \quad (80)$$

Additionally, let X be a Banach space and let R_{α^\dagger} and $D_i(T_i \cdot, f^\dagger)$ be convex for $i \in I^c$, and let there be constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that the follow-

ing source condition holds: There is $\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ such that for u satisfying $R_{\alpha^\dagger, \lambda^\dagger, I}(u, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f_i^\dagger) \leq \epsilon_0$,

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} D_i(T_i u, T_i u^\dagger). \quad (\text{SC2})$$

Then, there are constants $c > 0$ and $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ such that for $\delta < \bar{\delta}$ the following estimates for $j \in I$ hold:

$$D_j(T_j u^\delta, f_j^\delta) \leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} \lambda_i^\delta \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right), \quad (81)$$

$$D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) \leq c \left(\left(\sum_{i \in I} \lambda_i^\delta \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right). \quad (82)$$

In particular, this constant c solely depends on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$, γ_1 , γ_2 , λ^\dagger , α^\dagger , f^\dagger and $\bar{\delta}$, but not on the specific sequences $(u^\delta)_\delta$, $(f^\delta)_\delta$ or even $(\delta)_{\delta \in \Delta}$.

To avoid technical difficulties in the proof of Theorem 3.13, we first prove the following lemma. The need for this lemma arises as the extended regularisation functional $R_{\alpha, \lambda, I}(u, f)$ does not solely depend on u , but also on f , α , λ , and one needs to be able to estimate the difference between said functional when using some f , α , λ (or f^δ , α^δ , λ^δ) and f^\dagger , α^\dagger , λ^\dagger .

Lemma 3.17. *Let the assumptions in Theorem 3.13 leading up to equation (76) be satisfied, and let the corresponding notations for \hat{u} , u^\dagger , f , f^\dagger , δ etc. be used. Then there is a constant $c_1 > 0$ such that for $\delta_i = D_i(f_i^\dagger, f_i)$,*

$$|R_{\alpha, \lambda, I}(u^\dagger, f) - R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)| \leq c_1 \left(\psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) + \sum_{i \in I^c} \lambda_i \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right), \quad (83)$$

$$|R_{\alpha, \lambda, I}(\hat{u}, f) - R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger)| \leq c_1 \left(\psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) + \sum_{i \in I^c} \lambda_i \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right). \quad (84)$$

In particular, the constant c_1 does solely depend on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$ and λ^\dagger , but not on λ , α , f , \hat{u} .

Proof Lemma 3.17. In order to obtain a suitable estimate, we must first compute some subestimates. To this point, we use the moduli of continuity statements and the definition of the extended regularisation functional to compute for $u \in \{\hat{u}, u^\dagger\} \subset U$ the effect of changing the parameter for the extended regularisation function, first from f to f^\dagger , then λ to λ^\dagger and finally α to α^\dagger :

$$\begin{aligned}
|R_{\alpha,\lambda,I}(u, f) - R_{\alpha,\lambda,I}(u, f^\dagger)| &\stackrel{\text{per}}{\stackrel{\text{def.}}{=}} \left| \sum_{i \in I^c} \lambda_i (D_i(T_i u, f^\dagger) - D_i(T_i u, f)) \right| \\
&\stackrel{\text{mod.}}{\stackrel{\text{cont.}}{\leq}} \sum_{i \in I^c} \lambda_i \psi_i(\delta_i) (D_i(T_i u, f_i^\dagger) + 1), \\
|R_{\alpha,\lambda,I}(u, f^\dagger) - R_{\alpha,\lambda^\dagger,I}(u, f^\dagger)| &\stackrel{\text{per}}{\stackrel{\text{def.}}{=}} \left| \sum_{i \in I^c} (\lambda_i^\dagger - \lambda_i) D_i(T_i u, f_i^\dagger) \right| \leq \sum_{i \in I^c} |\lambda_i^\dagger - \lambda_i| D_i(T_i u, f_i^\dagger), \\
|R_{\alpha,\lambda^\dagger,I}(u, f^\dagger) - R_{\alpha^\dagger,\lambda^\dagger,I}(u, f^\dagger)| &\stackrel{\text{per}}{\stackrel{\text{def.}}{=}} |R_{\alpha^\dagger}(u) - R_\alpha(u)| \stackrel{\text{mod.}}{\stackrel{\text{cont.}}{\leq}} \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) (R_{\alpha^\dagger}(u) + 1).
\end{aligned}$$

Combining these results one obtains

$$\begin{aligned}
|R_{\alpha,\lambda,I}(u, f) - R_{\alpha^\dagger,\lambda^\dagger,I}(u, f^\dagger)| &\leq \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) (R_{\alpha^\dagger}(u) + 1) \\
&\quad + \sum_{i \in I^c} D_i(T_i u, f_i^\dagger) (|\lambda_i^\dagger - \lambda_i| + \lambda_i \psi_i(\delta_i)) + \lambda_i \psi_i(\delta_i).
\end{aligned} \tag{85}$$

For $u = u^\dagger$ the right-hand sides of (85) can be further estimated since $\sum_{i \in I^c} D_i(T_i u^\dagger, f^\dagger) < \infty$ and $R_{\alpha^\dagger}(u^\dagger) < \infty$, thus yielding (83).

In order to obtain the estimate (84), we consider (85) for $u = \hat{u}$, and show that $D_j(T_j \hat{u}, f_j^\dagger)$ for $j \in I^c$ and $R_{\alpha^\dagger}(\hat{u})$ are bounded independent of $\hat{u}, f, \lambda, \alpha$ (so we get the estimate independent of specific $\hat{u}, f, \alpha, \lambda$). Indeed, one obtains for $j \in I^c$, when reformulating the modulus of continuity condition and since $\psi_j(\delta_j) \leq \frac{1}{2}$ due to assumption (75), that

$$D_j(T_j \hat{u}, f_j^\dagger) \stackrel{\text{mod.}}{\stackrel{\text{cont.}}{\leq}} \frac{1}{1 - \psi_j(\delta_j)} (D_j(T_j \hat{u}, f_j) + \psi_j(\delta_j)) \leq 2(D_j(T_j \hat{u}, f_j) + \psi_j(\delta_j)), \tag{86}$$

and via the estimates (83) we already proved, it follows that

$$\begin{aligned}
R_\alpha(\hat{u}) + \lambda_j D_j(T_j \hat{u}, f_j) &\stackrel{\text{opt.}}{\leq} \left(\sum_{i=1}^M \lambda_i D_i(T_i u^\dagger, f_i) \right) + R_{\alpha, \lambda, I}(u^\dagger, f) = \left(\sum_{i \in I} \lambda_i \delta_i \right) + R_{\alpha, \lambda, I}(u^\dagger, f) \\
&\stackrel{(83)}{\leq} c_1 \left(\sum_{i \in I^c} \lambda_i \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) \\
&\quad + c_1 \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) + \left(\sum_{i \in I} \lambda_i \delta_i \right) + R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) \leq C < \infty
\end{aligned} \tag{87}$$

for $j \in I^c$, where C does not depend on $\hat{u}, f, \alpha, \lambda$. Note that this constant C is indeed uniform as the contributing terms are bounded due to Assumption (75). Hence, $D_j(T_j \hat{u}, f_j^\dagger)$ and $R_{\alpha^\dagger}(\hat{u}) \leq c(\alpha^\dagger, \alpha) R_\alpha(\hat{u})$ are bounded due to (86), and consequently one obtains through (85),

$$|R_{\alpha, \lambda, I}(\hat{u}, f) - R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger)| \leq c_1 \left(\psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\dagger, \alpha)) + \left(\sum_{i \in I^c} \lambda_i \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) \right), \tag{88}$$

where the constant c_1 depends solely on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$ and $\lambda^\dagger, f^\dagger, \alpha^\dagger$ but not on $\hat{u}, f, \alpha, \lambda$. \square

With this technical result, some issues originating from the extended regularisation functional can be tackled, and the proof for Theorem 3.13 unfold similarly to the one for Theorem 2.15.

Proof of Theorem 3.13. Optimality of \hat{u} , i.e.,

$$\begin{aligned}
F_{\lambda, \alpha}(\hat{u}, f) &= \left(\sum_{i \in I} \lambda_i D_i(T_i \hat{u}, f_i) \right) + R_{\alpha, \lambda, I}(\hat{u}, f) \\
&\leq \left(\sum_{i \in I} \lambda_i D_i(T_i u^\dagger, f_i) \right) + R_{\alpha, \lambda, I}(u^\dagger, f) = F_{\lambda, \alpha}(u^\dagger, f)
\end{aligned}$$

yields

$$\left(\sum_{i \in I} \lambda_i D_i(T_i \hat{u}, f_i) \right) + R_{\alpha, \lambda, I}(\hat{u}, f) \leq R_{\alpha, \lambda, I}(u^\dagger, f) + \sum_{i \in I} \lambda_i \delta_i. \tag{89}$$

However, to proceed we require an estimate similar to (89) with $R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)$ instead of $R_{\alpha, \lambda, I}(\cdot, f)$, and by the estimates given in Lemma 3.17 and the inequality (89) one

indeed obtains

$$\begin{aligned}
R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger) &\leq R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger) + \sum_{i \in I} \lambda_i D_i(T_i \hat{u}, f_i) \\
&\leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \left(\sum_{i \in I} \lambda_i \delta_i \right) + 2c_1 \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + 2c_1 \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)),
\end{aligned} \tag{90}$$

which confirms the error estimate on $R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger)$ stated in (76).

Now, analogous to the proof concerning convergence rates for a single discrepancy, the Source Condition (SC2) and a modulus of continuity estimate analogue to (86) for $i \in I$ imply

$$\begin{aligned}
-\langle \xi, \hat{u} - u^\dagger \rangle &\stackrel{\text{(SC2)}}{\leq} \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) + \gamma_2 \sum_{i \in I} D_i(T_i \hat{u}, f_i^\dagger) \\
&\stackrel{\text{mod.}}{\leq} \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) + 2\gamma_2 \sum_{i \in I} \left(D_i(T_i \hat{u}, f_i) + \psi_i(\delta_i) \right).
\end{aligned} \tag{91}$$

Combining the equations (90) and (91), and using the definition of the Bregman distance $R_{\alpha^\dagger, \lambda^\dagger, I}(\hat{u}, f^\dagger) - R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) - \langle \xi, \hat{u} - u^\dagger \rangle = D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger)$ results in

$$\begin{aligned}
&\left(\sum_{i \in I} (\lambda_i - 2\gamma_2) D_i(T_i \hat{u}, f) \right) + (1 - \gamma_1) D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) \\
&\leq \left(2 \sum_{i \in I} \lambda_i \delta_i + \gamma_2 \psi_i(\delta_i) \right) + 2c_1 \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + 2c_1 \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)).
\end{aligned} \tag{92}$$

From this one obtains for $j \in I$ and some constant $c > 0$, that

$$\begin{aligned}
D_j(T_j \hat{u}, f) &\leq c(\lambda_j)^{-1} \left(\left(\sum_{i \in I} \lambda_i \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) \right), \\
D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(\hat{u}, u^\dagger) &\leq c \left(\left(\sum_{i \in I} \lambda_i \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha, \alpha^\dagger)) \right).
\end{aligned}$$

We note that the constant c occurring here depends on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$, $\gamma_1, \gamma_2, f^\dagger, \lambda^\dagger, \alpha^\dagger$ and $\bar{\delta}$, but not on $\hat{u}, f, \alpha, \lambda$ as long as the stated assumptions are fulfilled. \square

Proof of Theorem 3.16. This proof is a direct consequence from Theorem 3.13 when substituting \hat{u} by u^δ since the estimates occurring in said theorem are independent of the specific δ . The Conditions (75) are fulfilled for δ sufficiently small independent of the specific f^δ or u^δ . Also, due to the parameter choice rule, the requirements to apply the Source

Condition (SC2) are satisfied by u^δ with $\delta < \bar{\delta}$ for some $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ due to the estimate in (68) and (76) (stating convergence of $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\delta, f^\dagger)$ and $D_j(T_j u^\delta, f_j^\delta)$) which is independent of the specific u^δ, f^δ . So application of Theorem 3.13 to $(u^\delta, f^\delta, \alpha^\delta, \lambda^\delta)$ for $(\hat{u}, f, \alpha, \lambda)$ yields the desired estimates. \square

Remark 3.18. *Theorem 3.16 grants us insight into suitable convergence requirements for $\lambda^\delta \rightarrow \lambda^\dagger$, $\alpha^\delta \rightarrow \alpha^\dagger$ and the behaviour of u^δ .*

- *Note that $(u^\delta)_\delta$ and u^\dagger are not known a-priori, and consequently confirming that $u^\delta, u^\dagger \in U$ and $T_i u^\delta, T_i u^\dagger \in V_i$ beforehand might not be possible.*
- *We note that the estimates on the j -th discrepancy is affected by the noise of all problems, not solely the δ_j , which is to be expected since the problems are solved jointly and the noise of the other problems also impacts the Tikhonov functional.*
- *We note that the estimate on $D_j(T_j u^\delta, f_j^\delta)$ is $o((\lambda_j^\delta)^{-1})$ since all the other occurring terms in (81) vanish in the estimate, thus at least confirming the rate in Theorem 3.9.*
- *One sees that for $i \in I^c$, the convergence rate of the parameter choice $\lambda_i^\delta \rightarrow \lambda_i^\dagger$ has an impact on the estimates, and should thus be chosen such that $|\lambda_i^\delta - \lambda_i^\dagger| = O(\psi_i(\delta_i))$. Also, the convergence rate $d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)$ should be chosen such that $\psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) = O(\max_i \psi_i(\delta_i))$ to not slow down the estimates.*
- *For $i \in I$, the rate at which λ_i^δ converges to infinity plays a role on the estimate. If $\lim_{\delta \rightarrow 0} \frac{\delta_i}{\psi_i(\delta_i)} = 0$, a reasonable choice is such that $c \frac{\psi_i(\delta_i)}{\delta_i} \leq \lambda_i^\delta \leq C \frac{\psi_i(\delta_i)}{\delta_i}$ for some constants $c, C > 0$, and in particular this choice would satisfy (79) making it a applicable choice without any further assumptions.*
- *As can be expected, quick convergence for $\lambda_j^\delta \rightarrow \infty$ can lead to faster convergence of the discrepancy of the j -th problem. However, this might in turn slow down convergence rates for the discrepancies corresponding to the other problems and for the Bregman distance.*

Hence there is a balance between speeding up the rates for one specific discrepancy, and slowing convergence rates on the other discrepancies.

The following corollaries show some possible technical relaxations of the assumptions, as well as results for specific parameter choices we did not show in the main theorem for the sake of readability and generality.

Corollary 3.19. *Let the assumptions of Theorem 3.13 hold, and let additionally λ^δ and α^δ be chosen such that for $\epsilon_i \in (0, 1)$ and constants $c, C > 0$*

$$c\delta_i^{1-\epsilon_i} \leq \lambda_i^\delta \leq C\delta_i^{1-\epsilon_i} \text{ for } i \in I, \quad |\lambda_i^\delta - \lambda_i^\dagger| = O(\psi_i(\delta_i)) \quad (93)$$

and $\psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) = O(\max_i \psi_i(\delta_i))$. Then, one obtains the rates

$$D_j(T_j u^\delta, f_j^\delta) = O\left(\delta_j^{1-\epsilon_j} \left(\sum_{i \in I} (\delta_i^{\epsilon_i} + \psi_i(\delta_i)) + \sum_{i \in I^c} (\psi_i(\delta_i)) \right)\right) \text{ for } j \in I, \quad (94)$$

$$D_{R_{\alpha^\dagger, \lambda^\dagger, I}^\xi}(\cdot, f^\dagger)(u^\delta, u^\dagger) = O\left(\sum_{i \in I} (\delta_i^{\epsilon_i} + \psi_i(\delta_i)) + \sum_{i \in I^c} (\psi_i(\delta_i))\right). \quad (95)$$

Furthermore, we note that when considering the multi-data inverse problem as a single vector-valued one, considering $\hat{D}(T \cdot, f) = \sum_{i=1}^M D_i(T_i \cdot, f_i)$ and corresponding $\hat{\delta} = \sum_{i=1}^M \delta_i \geq \delta_i$ for all $i > 0$ and $\psi_i(\delta) = \delta^{\frac{1}{p_i}}$, these results imply the results for the single-data regularisation stated in Theorem 2.15.

Remark 3.20. *Sometimes, the strong ψ_i -continuity of D_i required to obtain the rates might be a too strong requirement. When dealing with just one specific sequence of data $(f^\delta)_\delta$, we can relax the ψ_i -continuity of D_i on a set V_i in f_i^\dagger (i.e. the modulus of continuity estimate) to hold solely for these specific f^δ (compared to f sufficiently close to f^\dagger in the original), i.e. for $v_i \in V_i$*

$$|D_i(v_i, f_i^\dagger) - D_i(v_i, f_i^\delta)| \leq \psi_i(D_i(f_i^\dagger, f_i^\delta)) (D_i(v_i, f_i^\dagger) + 1). \quad (96)$$

This simply means instead of a general modulus of continuity, it is sufficient to reduce the estimate to a specific sequence of data. With this instead of strong continuity of D_i , convergence results for this one specific sequence can be derived in an analogous manner, however no uniform estimate can be observed for all sequences.

We note that in the setting of Theorem 3.13, for $i \in I$ the estimate in Source Condition (SC2) would contain D_i , while in the single-data setting in (SC1) stated in Theorem 2.15 $D^{\frac{1}{p}}$ would appear. Thus the following corollary relaxes the source condition (SC2) to (SC3), so that (SC3) is indeed a generalisation of (SC1).

Theorem 3.21. *Let all assumptions of Theorem 3.13 hold except the strong ψ_i -continuity of the discrepancies D_i and the Source Condition (SC2) which holds in the slightly weaker*

form

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u, T_i u^\dagger), \quad (\text{SC3})$$

under the same requirements for u and where $\psi_i: [0, \infty) \rightarrow [0, \infty)$ is a monotone continuous function with $\psi_i(0) = 0$. Here for $i \in I$, the function $\phi_i: Y_i \times Y_i \rightarrow [0, \infty]$ is such that for $v_i \in Y_i$ and f_i with $D_i(f_i^\dagger, f_i)$ sufficiently small,

$$\phi_i(v_i, f_i^\dagger) \leq \Phi_i(D_i(f_i^\dagger, f_i))D_i(v_i, f_i) + \psi_i(D_i(f_i^\dagger, f_i)),$$

where $\Phi_i: [0, \infty] \rightarrow [0, \infty]$ is such that $\Phi_i(\delta_i) \leq \frac{1}{4\gamma_2} \lambda_i^\delta$ for δ_i sufficiently small. Also, let D_i be strongly ψ_i -continuous on V_i in f_i^\dagger for $i \in I^c$ (and not for all i) for sets V_i and functions ψ_i as in Theorem 3.16 and let $T_i u^\dagger, T_i u^\delta \in V_i$ for $i \in I^c$. Then the convergence estimates of Theorem 3.16 remain valid.

Proof. First note that the Lemma 3.17 holds even if the strong continuity is only satisfied for $i \in I^c$, as the $i \in I$ do not play any role in the statement or proof. The proof for Theorem 3.16 remains exactly the same except the equations (91) and (92), however due to the assumptions on ϕ these equations hold in slightly different form as

$$\begin{aligned} -\langle \xi, u^\delta - u^\dagger \rangle &\stackrel{(\text{SC3})}{\leq} \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u^\delta, f_i^\dagger) \\ &\stackrel{\text{def.}}{\leq} D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) + 2\gamma_2 \sum_{i \in I} \left(\Phi_i(\delta) D_i(T_i u^\delta, f_i^\dagger) + \psi_i(\delta_i) \right), \end{aligned} \quad (97)$$

which for δ sufficiently small results in

$$\begin{aligned} &\left(\sum_{i \in I} \underbrace{(\lambda_i^\delta - 2\gamma_2 \Phi_i(\delta_i))}_{\geq \frac{1}{2} \lambda_i^\delta} D_i(T_i u^\delta, f_i^\dagger) \right) + (1 - \gamma_1) D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) \\ &\leq 2 \left(\sum_{i \in I} \lambda_i^\delta \delta_i + \psi_i(\delta_i) \right) + 2c_1 \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)). \end{aligned} \quad (98)$$

which leads to analogous estimates. \square

Remark 3.22. *This Source Condition (SC3) is indeed a generalisation of the Source Condition (SC1), and allows us to omit the strong continuity requirement for $i \in I$ by in turn requiring a potentially stronger source condition.*

Note that here ψ_i -continuity of D_i is required for $i \in I^c$ while for $i \in I$, ψ_i denotes a function resulting from estimates in (SC3).

So to summarise, one can generalise the theory for single-data to multi-data in a natural way. In particular, convergence and rates towards $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solutions to $Tu = f^\dagger$ can be obtained. These partial solutions can be interpreted as solutions to a Tikhonov approach for the unsolved problems $T_I^c u = f_{I^c}^\dagger$ using $T_I u = f_I^\dagger$ as prior.

Part II.

Specific Discrepancies

In this part, we aim to discuss how the theory of Part I applies to commonly used discrepancy functions. Furthermore, we try to reduce the assumptions made on the discrepancies concerning specific choices for D_i into conditions which are more practically verifiable, or show that some properties are automatically fulfilled.

First classical norms and afterwards lower semi-continuous subnorms are considered with regard to said properties required from the discrepancies. Then, the Kullback-Leibler divergence, a suitable discrepancy for data affected by Poisson noise is considered. While this discrepancy requires more technical effort to discuss, in the end it is applicable under reasonable assumptions.

4. Norm Discrepancies

4.1. Classical Norms

When dealing with a normed vector space Y , it is common to use norms or the power of norms as discrepancies in the single-data case, i.e. for $p \in [1, \infty)$ use

$$D(v, f) = \|v - f\|_Y^p.$$

This makes sense as this discrepancy is a reasonable measure of distance in Y , is a convex function and is compatible with the linear structure.

Therefore we study norm discrepancy functions and how they fits into the multi-data setting we previously derived. To do so, in this chapter we consider following the Tikhonov problem.

Problem 4.1. *Let (X, \mathcal{T}_X) , (Y_i, \mathcal{T}_{Y_i}) for $i \in \{1, \dots, M\}$ and $(\mathcal{A}, \mathcal{T}_{\mathcal{A}})$ be Hausdorff spaces and let $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$ be continuous operators with respect to \mathcal{T}_X and \mathcal{T}_{Y_i} and with closed domain. Moreover, let $J \subset \{1, \dots, M\}$ be such that for $j \in J$ the space $(Y_j, \|\cdot\|_{Y_j})$ is a normed vector space, let $p_j \in [1, \infty)$ and $D_j: Y_j \times Y_j \rightarrow [0, \infty)$ with $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$. Let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ for $i \in J^c$ be non-negative functions, let $\lambda \in (0, \infty)^M$ and let $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha: X \rightarrow [0, \infty]$ be a family of functions. We say u^\dagger is a solution to the Tikhonov regularisation ($N\text{-MTIKH}_{\lambda, \alpha}(f^\dagger)$) regarding $Tu = f^\dagger$*

with discrepancies D_i , weights λ_i and regularisation R_α with parameter $\alpha \in \mathcal{A}$, if

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda, \alpha}(u, f^\dagger) \text{ such that } F_{\lambda, \alpha}(u^\dagger, f^\dagger) < \infty \\ \text{with } F_{\lambda, \alpha}(u, f^\dagger) = \left(\sum_{j \in J} \|T_j u - f_j^\dagger\|_{Y_j}^{p_j} \right) + \left(\sum_{i \in J^c} D_i(T_i u, f_i^\dagger) \right) + R_\alpha(u). \end{cases} \quad (N\text{-MTIKH}_{\lambda, \alpha}(f^\dagger))$$

So this problem is a multi-data Tikhonov approach where for $j \in J$ the discrepancy $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$ is the norm of the difference to the p_j -th power.

We aim to discuss whether using norm discrepancies $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$ fits the general theory derived in Part I, and what assumptions are required to apply it.

Recall that for Part I we required basic discrepancies, i.e. we needed discrepancy functions to be non-negative, indeed positive unless its arguments are equal, there needed to be a topology \mathcal{T}_{D_i} stronger than D_i such that D_i is lower semi-continuous in $\mathcal{T}_{Y_i} \times \mathcal{T}_{D_i}$. The following assumptions for $j \in J$ will be the basis of this discussion.

Assumptions 4.2 (Norms).

Let $J \subset \{1, \dots, M\}$ be the set such that $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$ is the discrepancy function for $j \in J$. The following conditions are satisfied for each $j \in J$:

N1 There is a topology \mathcal{T}_{D_j} on Y_j , such that

$$f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j \quad \Rightarrow \quad \|f_j - f_j^n\|_{Y_j} \rightarrow 0 \quad (99)$$

N2 The norm $\|\cdot\|_{Y_j}$ is \mathcal{T}_{Y_j} -lower semi-continuous.

N3 The topology \mathcal{T}_{Y_j} is translation invariant in the sense that

$$v_j^n \xrightarrow{\mathcal{T}_{Y_j}} v_j \quad \Rightarrow \quad \left(v_j^n + f_j \xrightarrow{\mathcal{T}_{Y_j}} v_j + f_j \quad \text{or} \quad v_j^n + f_j \xrightarrow{\|\cdot\|_{Y_j}} v_j + f_j \right) \quad (100)$$

for every $f_j \in Y_j$.

We again use the product space notation $T = (T_1, \dots, T_M)$, $Y = Y_1 \times \dots \times Y_M$ with product topologies \mathcal{T}_Y and \mathcal{T}_D .

Proposition 4.3. *With Assumptions 4.2, for $j \in J$ the norm discrepancy $D_j: Y_j \times Y_j \rightarrow [0, \infty)$, $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$ is a basic discrepancy on Y_j with respect to the corresponding topologies \mathcal{T}_{Y_j} and \mathcal{T}_{D_j} (see Definition 2.2).*

Proof. Let $j \in J$ and $v_j, f_j \in Y_j$. That the topology \mathcal{T}_{D_j} is stronger than the topology induced by $\|v_j - f_j\|_{Y_j}$ is clear due to the assumptions, and since the function $g(t) = t^{p_j}$ is continuous and $g(0) = 0$, also $\|f_j - f_j^n\|_{Y_j} \rightarrow 0$ if and only if $\|f_j - f_j^n\|_{Y_j}^{p_j} \rightarrow 0$ confirming that \mathcal{T}_{D_j} is stronger than D_j .

The positivity of $D_j(v_j, f_j)$ for $v_j \neq f_j$ is obviously satisfied due to the positive definiteness property of norms, which is not obstructed by taking the p_j -th power.

Finally, concerning the lower semi-continuity with respect to $\mathcal{T}_{Y_1} \times \mathcal{T}_{D_1}$, let sequences $(v_j^n)_n$ and $(f_j^n)_n$ be in Y_j with $v_j^n \xrightarrow{\mathcal{T}_{Y_j}} v_j$ and $f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j$. Due to the inverse triangle inequality, and $\|f_j - f_j^n\|_{Y_j} \rightarrow 0$ as well as $v_j^n - f_j \rightarrow v_j - f_j$ either in \mathcal{T}_{Y_1} or in the norm topology, one computes

$$\liminf_{n \rightarrow \infty} \|v_j^n - f_j^n\|_{Y_j} \geq \liminf_{n \rightarrow \infty} \|v_j^n - f_j\|_{Y_j} - \|f_j - f_j^n\|_{Y_j} \stackrel{\text{l.s.c.}}{\geq} \|v_j - f_j\|_{Y_j} \quad (101)$$

where we used that both topologies either through $N1$ or directly imply the lower semi-continuity estimate on $\|v_j^n - f_j\|$. Since the function $g(t) = t^{p_j}$ is continuous and monotone, application of g leaves the lower semi-continuity of $\|\cdot_1 - \cdot_2\|_{Y_j}$ intact. \square

Recall that for the convergence results stated in Chapter 3 we required $T_i u_0$ -continuity of D_i in f_i^\dagger for $i \in I^c$ (i.e. $D_i(T_i u_0, \cdot)$ is continuous in f_i^\dagger with respect to \mathcal{T}_{D_i}) and strong ψ_i -continuity of D_i on a set V_i in f_i^\dagger (modulus of continuity estimates in a surrounding of f_i^\dagger and on a set V_i). Hence, we next verify that these conditions are indeed satisfied for $j \in J$ where we use norm discrepancies.

Proposition 4.4. *Let Assumptions 4.2 be satisfied. For $j \in J$ with $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$, for every $f_j^\dagger \in Y_j$ and $v_0 \in Y_j$ the discrepancy D_j is v_0 -continuous in f_j^\dagger . Moreover, there is $c > 1$ such that with $\psi_j(t) = ct^{\frac{1}{p_j}}$ the function D_j is strongly ψ_j -continuous on $V_j = Y_j$ and in any $f_j^\dagger \in Y_j$.*

The constant $c > 0$ is not depending on f_j^\dagger or V_j , but solely on $\delta_0 > 0$ (recall $\psi_j: (0, \delta_0] \rightarrow [0, \infty)$, so δ_0 is a limit on the noise for which the modulus of continuity estimate needs to hold). This means that for $\|f_j - f_j^\dagger\|_{Y_j}^{p_j} = \delta_j < \delta_0$ and $v_j \in Y_j$ we obtain the modulus of continuity estimate

$$\left| \|v_j - f_j\|_{Y_j}^{p_j} - \|v_j - f_j^\dagger\|_{Y_j}^{p_j} \right| \leq c \delta_j^{\frac{1}{p_j}} (\|v_j - f_j^\dagger\|_{Y_j}^{p_j} + 1). \quad (102)$$

Proof. Let $j \in J$, $v_0, f_j, f_j^\dagger \in Y_j$. The v_0 -continuity of D_j for any $v_0 \in Y_j$ is imminent, since the norm is continuous due to the triangle inequality, i.e. for a sequence $(f_j^n)_n$ with

$$f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j^\dagger,$$

$$\left| \|T_j u - f_j^n\|_{Y_j} - \|T_j u - f_j^\dagger\|_{Y_j} \right| \leq \|f_j^n - f_j^\dagger\|_{Y_j} \rightarrow 0, \quad (103)$$

and composition with the continuous function $g(t) = t^{p_j}$ maintains the continuity. For $p_j = 1$ the modulus of continuity is already proven in the previous equation and restriction to $\delta_j < \delta_0$ is not necessary.

In order to show the modulus of continuity estimate for $p_j > 1$, we first estimate for $a, b, \beta \geq 0$ and $p, q > 1$ such that $\frac{1}{p} + \frac{1}{q} = 1$

$$|a + b|^p \leq a^p(1 + \beta^q)^{p-1} + b^p(1 + \beta^{-1})^{p-1} \quad (104)$$

in order to estimate $\|v_j - f_j\|_{Y_j}^{p_j} \leq (\|v_j - f_j\|_{Y_j} + \delta_j^{\frac{1}{p_j}})^{p_j}$ where $\delta_j = \|f_j - f_j^\dagger\|_{Y_j}^{p_j}$. Indeed, due to Hölder's Inequality applied to the standard \mathbb{R}^2 inner product

$$\begin{aligned} a + b &= a + \beta \frac{b}{\beta} = \left\langle \begin{pmatrix} a \\ \frac{b}{\beta} \end{pmatrix}, \begin{pmatrix} 1 \\ \beta \end{pmatrix} \right\rangle \leq \left\| \begin{pmatrix} a \\ \frac{b}{\beta} \end{pmatrix} \right\|_p \left\| \begin{pmatrix} 1 \\ \beta \end{pmatrix} \right\|_q = \sqrt[p]{a^p + \frac{b^p}{\beta^p}} \sqrt[q]{1 + \beta^q}, \\ (a + b)^p &\leq a^p(1 + \beta^q)^{\frac{p}{q}} + \left(\frac{b}{\beta}\right)^p(1 + \beta^q)^{\frac{p}{q}} = a^p(1 + \beta^q)^{p-1} + b^p(1 + \beta^{-q})^{p-1}. \end{aligned}$$

Next, we note that for β sufficiently small, there is $c > 0$ such that with $t = \beta^q$ and $h(t) = (1 + t)^{p-1}$,

$$1 - (1 + \beta^q)^{p-1} = h(0) - h(t) = h'(\xi)t \leq c\beta^q, \quad \text{and} \quad (1 + \beta^{-q})^{(p-1)} \leq c\beta^{-(p-1)q} \quad (105)$$

where we used the Taylor polynomial with intermediate point ξ , and that h' is bounded in a surrounding of 0.

Hence, with monotonicity of the function $g(t) = t^{p_j}$ and the equations (104) and (105) we estimate for β sufficiently small

$$\|v_j - f_j\|_{Y_j}^{p_j} \leq (\|v_j - f_j^\dagger\|_{Y_j} + \delta_j^{\frac{1}{p_j}})^{p_j} \leq \|v_j - f_j^\dagger\|_{Y_j}^{p_j} \underbrace{(1 + \beta^{q_j})^{p_j-1}}_{\leq 1 + c\beta^{q_j}} + \delta_j \underbrace{(1 + \beta^{-q_j})^{p_j-1}}_{\leq c\beta^{-q_j(p_j-1)}}.$$

Choosing $\beta = \delta_j^{\frac{1}{p_j q_j}}$ and δ_j sufficiently small therefore results in

$$\|v_j - f_j\|_{Y_j}^{p_j} \leq \|v_j - f_j^\dagger\|_{Y_j}^{p_j} (1 + c\delta_j^{\frac{1}{p_j}}) + c\delta_j^{\frac{1}{p_j}}. \quad (106)$$

Note that this is part of the estimate (102), we exchange the roles of f_j and f_j^\dagger in order

to get the other part, yielding

$$\|v_j - f_j^\dagger\|_{Y_j}^{p_j} \leq \|v_j - f_j\|_{Y_j}^{p_j} (1 + c\delta_j^{\frac{1}{p_j}}) + c\delta_1^{\frac{1}{p_j}}.$$

which when rearranged results in

$$\|v_j - f_j\|_{Y_j}^{p_j} \geq \|v_j - f_j^\dagger\|_{Y_j}^{p_j} - c\delta_j^{\frac{1}{p_j}} \left(\underbrace{\|v_j - f_j\|_{Y_j}^{p_j}}_{\leq c\|v_j - f_j^\dagger\|_{Y_j}^{p_j} + \delta_0^{\frac{1}{p_j}}} + 1 \right) \geq (1 - c\delta_j^{\frac{1}{p_j}}) \|v_j - f_j^\dagger\|_{Y_j}^{p_j} - c\delta_j^{\frac{1}{p_j}}. \quad (107)$$

Note that here $\delta_0 > 0$ is simply used to limit the amount of noise for which the estimates need to hold, i.e. $\delta_j \leq \delta_0$. Combining the estimates (106) and (107) yields the desired modulus of continuity estimate. \square

Remark 4.5. Note that in $\psi_j: [0, \delta_0) \rightarrow [0, \infty)$ with $\psi_j(\delta_j) = c\delta_j^{\frac{1}{p_j}}$, the constant c does not depend on f^\dagger , $v_j \in Y_j$ or even the specific norm, but solely on δ_0 and p_j .

So we see that all requirements for the theory of Part I are satisfied by norm discrepancies with only very basic assumptions, thus making approaches featuring norms possible. The application of such Tikhonov approaches with norm discrepancies is summarised in the following corollary.

Corollary 4.6. This corollary summarises the theory of Part I applied to norm discrepancies. We consider 4 statements: existence, convergence, rates and single-data results:

1. Let the Assumptions 4.2 hold for $j \in J$ such that $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$. For $i \in J^c$, let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ be a basic discrepancy. Further, let $(R_\alpha)_\alpha$ be a continuous family of regularisation functionals and with $\lambda = \mathbf{1}$ and some $\alpha = \alpha_0 \in \mathcal{A}$ let the Tikhonov functional

$$F_{\mathbf{1}, \alpha_0}(u, f) = \sum_{j \in J} \|T_j u - f_j\|_{Y_j}^{p_j} + \sum_{i \in J^c} D_i(T_i u, f_i) + R_{\alpha_0}(u) \quad (108)$$

be uniformly coercive. Then, for $f^\dagger \in Y$ the Problem $(N\text{-}MTIKH_{\lambda, \alpha}(f^\dagger))$ is either solvable or $F_{\lambda, \alpha}(\cdot, f^\dagger) \equiv \infty$ for all $\alpha \in \mathcal{A}$, $\lambda \in (0, \infty)^M$.

2. Additionally to point 1., let $I \subset \{1, \dots, M\}$, let parameter choice rules as in Theorem 3.9 be applied, and let an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u_0 to $Tu = f^\dagger$

exists such that for $i \in J^c \cap I^c$ the discrepancies D_i are $T_i u_0$ -continuous in f_i^\dagger . Let a sequence $(f^\delta)_\delta \subset Y$ be such that $f^\delta \xrightarrow{T_R} f^\dagger$ and denote the corresponding solutions to N -MTIKH $_{\lambda^\delta, \alpha^\delta}(f^\delta)$ by u^δ . Then, one obtains subsequential convergence of $(u^\delta)_\delta$ to $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solutions to $Tu = f^\dagger$.

3. Additionally to 1. and 2., let X be a normed space and $(\mathcal{A}, d_{\mathcal{A}})$ be a metric space, and let u^\dagger be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution to $Tu = f^\dagger$. Let R_α for all $\alpha \in \mathcal{A}$ and $D_i(T_i \cdot, f_i^\dagger)$ for all $i \in I^c$ be convex. Let $(f^\delta)_\delta \subset Y$ be a sequence of data, and denote by $\delta_i = D_i(f_i^\dagger, f_i^\delta)$. For $i \in J^c$ let the discrepancy function D_i be strongly ψ_i -continuous on $V_i \subset Y_i$ in f_i^\dagger and let the family $(R_\alpha)_\alpha$ be strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on $U \subset X$ in α^\dagger . Let $u^\dagger, u^\delta \in U$ and $T_i u^\dagger, T_i u^\delta \in V_i$ for $i \in J^c$ for $D_i(f_i^\dagger, f_i^\delta) = \delta_i < \delta_0$ with some constant $\delta_0 > 0$. Let there be constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that the following source condition holds: There is $\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ such that for u satisfying $R_{\alpha^\dagger, \lambda^\dagger, I}(u, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f_i^\dagger) \leq \epsilon_0$

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u, T_i u^\dagger), \quad (\text{SC3})$$

where for $j \in I \cap J$, the function $\phi_j(T_j u, T_j u^\dagger) = \|T_j u - T_j u^\dagger\|_{Y_j}$. Here, for $i \in I$, the function $\phi_i: Y_i \times Y_i \rightarrow [0, \infty]$ is such that for $v_i \in V_i$

$$\phi_i(v_i, f_i^\dagger) \leq \Phi_i(D_i(f_i^\dagger, f_i)) D_i(v_i, f_i) + \psi_i(D_i(f_i^\dagger, f_i)),$$

where $\Phi_i: [0, \infty] \rightarrow [0, \infty]$ is such that $\Phi_i(\delta_i) \leq \frac{1}{4\gamma_2} \lambda_i^\delta$ for δ_i sufficiently small.

Then, there are constants $c > 0$ and $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ such that for $\delta < \bar{\delta}$ and $j \in J \cap I$,

$$\begin{aligned} \|T_j u^\delta - f_j^\delta\|_{Y_j}^{p_j} &\leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \\ &\quad \left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right) \end{aligned} \quad (109)$$

holds. For $j \in I$:

$$D_j(T_j u^\delta, f_j^\delta) \leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \\ \left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right), \quad (110)$$

$$D_{R_{\alpha^\dagger, \lambda^\dagger, I}^\xi(\cdot, f^\dagger)}(u^\delta, u^\dagger) \leq c \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \\ \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right). \quad (111)$$

In particular, this constant c solely depends on $R_{\alpha^\dagger, \lambda^\dagger, f^\dagger}(u^\dagger, f^\dagger)$, γ_1 , γ_2 , λ^\dagger , α^\dagger , f^\dagger and $\bar{\delta}$, but not on the specific sequence $(u^\delta)_\delta$, $(f^\delta)_\delta$ or even $(\delta)_{\delta \in \Delta}$.

4. In the single-data case $M = 1$: Let R be \mathcal{T}_X -lower semi-continuous and for all $C > 0$, let the set $\{u \in X \mid R(u) + \|Tu - f\|_Y^p \leq C\}$ be \mathcal{T}_X -precompact and let $\text{dom}(R) \cap \text{dom}(T) \neq \emptyset$. Then, for $Tu = f^\dagger$, the single data Tikhonov regularisation

$$\min_{u \in X} \|Tu - f^\dagger\|_Y^p + \alpha R(u) \quad (112)$$

is solvable and stable, and the convergence results stated in Part I hold.

Proof. Application of Theorems 3.5, 3.9 and Theorem 3.21, whose assumptions are fulfilled due to Propositions 4.3, 4.4 and the assumptions made in this theorem. \square

Example 4.7. Let $M = 2$ and let $(Y_1, \|\cdot\|_{Y_1})$ and $(Y_2, \|\cdot\|_{Y_2})$ be normed spaces. We consider the Tikhonov functional $F_\lambda(u, f^\dagger) = \lambda_1 \|T_1 u - f_1^\dagger\|_{Y_1} + \lambda_2 \|T_2 u - f_2^\dagger\|_{Y_2}^2 + R_\alpha(u)$, i.e. with two norm discrepancies and $p_1 = 1$ and $p_2 = 2$. Let the Assumptions 4.2 for $J = \{1, 2\}$ hold, let $(R_\alpha)_\alpha$ be continuous families of functions. Let $I = \{1, 2\}$, let u^\dagger be an R -minimal solution and let $D(\cdot, f^\dagger)$ and R be convex. Let the Source Condition (SC3) of Theorem 4.6 for u with the same requirements be satisfied in u^\dagger and choose $\lambda^\delta = (\delta_1^{-(1-\epsilon)}, \delta_2^{\frac{-1}{2}})$ where $\delta_i = \|f_i^\dagger - f_i^\delta\|^{p_i}$. In particular, Theorem 3.21 is applicable when we use the Source Condition (SC3) with $\phi_i(v_i, f_i) = \|v_i - f_i\|_{Y_i}$. Then, one obtains

$$\|T_1 u^\delta - f_1^\delta\|_{Y_1} = O(\delta^{1-\epsilon} (\delta_1^\epsilon + \delta_2^{\frac{1}{2}})), \quad \|T_2 u^\delta - f_2^\delta\|_{Y_2}^2 = O(\delta^{\frac{1}{2}} (\delta_1^\epsilon + \delta_2^{\frac{1}{2}})), \\ D_R^\xi(u^\delta, u^\dagger) = O(\delta_1^\epsilon + \delta_2^{\frac{1}{2}}).$$

Note that the estimate for D_1 improves for ϵ closer to 0, however the estimates for D_2

and D_R^ξ potentially deteriorate unless δ_1 goes to 0 at a significantly higher speed than δ_2 .

If one changes the setting to $I = \{2\}$, changes all the corresponding conditions, and chooses $|\lambda_1^\dagger - \lambda_1^\delta| = O(\delta_1)$ for some $\lambda_1^\dagger \in (0, \infty)$, one obtains

$$\|T_2 u^\delta - f_2^\delta\|_{Y_2}^2 = O(\delta_2^{\frac{1}{2}} (\delta_2^{\frac{1}{2}} + \delta_1)), \quad D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) = O(\delta_2^{\frac{1}{2}} + \delta_1).$$

For this choice of parameter, we see that the noise level δ_2 has greater impact than δ_1 . In particular, when $\delta_1^2 \approx \delta_2$, i.e. $\|f_1^\dagger - f_1^\delta\|_{Y_1} \approx \|f_2^\dagger - f_2^\delta\|_{Y_2}$, the estimate is not obstructed by the problem for $i = 1$, and one obtains the same convergence rate, as one would if solving solely the problem for $i = 2$ with single-data Tikhonov regularisation.

4.2. Subnorms

We continue our discussion of norms as discrepancies in a slightly different setting. Sometimes the operator T maps onto a normed space Y , however a suitable discrepancy is a stronger norm, solely defined on a subspace $Z \subset Y$. A typical example is that $Y = L^2(\Omega)$ and T maps continuously onto L^2 , however, the suitable discrepancy is the Sobolev norm $\|\cdot\|_{H^1}$.

Definition 4.8. Let $(Y, \|\cdot\|_Y)$ and $(Z, \|\cdot\|_Z)$ be normed spaces. For an embedding $\iota: Z \hookrightarrow Y$ that is injective, linear and continuous with respect to the norm topologies, we define in slight abuse of notation

$$\|\cdot\|_Z: Y \rightarrow [0, \infty], \quad \|y\|_Z = \begin{cases} \|\iota^{-1}y\|_Z & \text{if } y \in \iota(Z), \\ \infty & \text{else,} \end{cases} \quad (113)$$

i.e. taking the norm in Z for suitable y , and penalising with ∞ otherwise.

In this chapter we use such subnorms as discrepancies, and the corresponding setting is summarised in the following.

Problem 4.9. Let (X, \mathcal{T}_X) , (Y_i, \mathcal{T}_{Y_i}) for $i \in \{1, \dots, M\}$ and $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ be Hausdorff spaces and let $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$ be continuous operators with respect to \mathcal{T}_X and \mathcal{T}_{Y_i} with closed domain. Moreover, let $J \subset \{1, \dots, M\}$ and for $j \in J$ let the space $(Y_j, \|\cdot\|_{Y_j})$ be a normed space and let $(Z_j, \|\cdot\|_{Z_j})$ be a normed space such that $\iota_j: Z_j \hookrightarrow Y_j$ linearly and continuously. For $j \in J$, let $p_j \in [1, \infty)$ and $D_j: Y_j \times Y_j \rightarrow [0, \infty]$ with $D_j(v_j, f_j) = \|v_j - f_j\|_{Z_j}^{p_j}$ as in (113). Let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ for $i \in J^c$ be functions, let $\lambda \in (0, \infty)^M$ and let $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha: X \rightarrow [0, \infty]$ be a family of functions. We say u^\dagger is a solution

to the Tikhonov problem (SN-MTIKH $_{\lambda,\alpha}(f^\dagger)$) regarding $Tu = f^\dagger$ with discrepancies D_i , weights λ_i and regularisation R_α with parameter $\alpha \in \mathcal{A}$, if

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda,\alpha}(u, f^\dagger) \text{ such that } F_{\lambda,\alpha}(u^\dagger, f^\dagger) < \infty \\ \text{with } F_{\lambda,\alpha}(u, f^\dagger) = \left(\sum_{j \in J} \|T_j u - f_j^\dagger\|_{Z_j}^{p_j} \right) + \left(\sum_{i \in J^c} D_i(T_i u, f_i^\dagger) \right) + R_\alpha(u). \end{cases} \quad (\text{SN-MTIKH}_{\lambda,\alpha}(f^\dagger))$$

So this problem is a multi-data Tikhonov approach where the discrepancies concerning $j \in J$ are subnorms of the differences taken to the p_j -th power, i.e. $D_j(v_j, f_j) = \|v_j - f_j\|_{Z_j}^{p_j}$.

Again we start by stating assumptions making $D_j(v_j, f_j) = \|v_j - f_j\|_{Z_j}^{p_j}$ basic discrepancy function.

Assumptions 4.10 (Subnorms). *Let $J \subset \{1, \dots, M\}$ such that $D_j(v_j, f_j) = \|v_j - f_j\|_{Y_j}^{p_j}$, and let the following hold for all $j \in J$:*

$\tilde{N}1$ *Let Y_j be a vector space with norm $\|\cdot\|_{Y_j}$ and let Z_j be a reflexive Banach space such that $Z_j \xrightarrow{\iota_j} Y_j$ linearly, densely and continuously with respect to the norm topologies.*

$\tilde{N}2$ *The topology \mathcal{T}_{Y_j} is such that for all $\xi \in Y_j^*$ the operation $\langle \xi, \cdot \rangle_{Y_j^* \times Y_j}$ is \mathcal{T}_{Y_j} -continuous, i.e. \mathcal{T}_{Y_j} is stronger than the weak topology on Y_j .*

$\tilde{N}3$ *\mathcal{T}_{D_j} is a topology on Y_j , such that for sequences $(v_j^n)_n, (f_j^n)_n \subset Y_j$,*

$$f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j \quad \Rightarrow \quad (f_j - f_j^n \in \iota_j(Z_j) \text{ and } \|f_j - f_j^n\|_{Z_j} \rightarrow 0). \quad (114)$$

We again use the product space notation $T = (T_1, \dots, T_M)$, $Y = Y_1 \times \dots \times Y_M$ with product topologies \mathcal{T}_Y and \mathcal{T}_D .

With these assumption, the subnorm discrepancy is indeed a reasonable discrepancy as confirmed in the following proposition.

Proposition 4.11. *With Assumption 4.10, for $j \in J$ the function $D_j: Y_j \times Y_j \rightarrow [0, \infty]$ with $D_j(v_j, f_j) = \|v_j - f_j\|_{Z_j}^{p_j}$ and some $p_j \in [1, \infty)$ is a basic discrepancy.*

Note here, that $D_j(v_j, f_j)$ is still defined on Y_j and not Z_j , so $f_j \notin \iota_j(Z_j)$ is allowed, thus it is not necessary that $v_j \in \iota_j(Z_j)$ either (as would not be expected for $v_j = T_j u$).

Proof. Analogously to the proof of Proposition 4.3, for $j \in J$ the conditions concerning the \mathcal{T}_{D_j} topology and positivity are satisfied (\mathcal{T}_{D_j} is stronger than D_j and D_j attains positive values for non-equal instances) due to the basic properties of norms and the general setting.

In order to ensure lower semi-continuity of D_j with respect to the $\mathcal{T}_{Y_j} \times \mathcal{T}_{D_j}$ topology, we first note that $\iota_j^*(Y_j^*) \subset Z_j^*$ densely. Indeed, by application of Hahn-Banach's Theorem, a subspace S of Z_j^* is dense, if and only if for $z^{**} \in Z_j^{**}$, $z^{**}(S) = 0$ implies $z^{**} = 0$. The canonical embedding $\tilde{\iota}_j: Z_j \hookrightarrow Z_j^{**}$ is surjective due to reflexivity, and hence for $z^{**} = \tilde{\iota}_j(z) \in Z_j^{**}$,

$$0 = z^{**}(\iota_j^* y^*) = \langle \tilde{\iota}_j z, \iota_j^* y^* \rangle_{Z_j^{**} \times Z_j^*} = \langle \iota_j^* y^*, z \rangle_{Z_j^* \times Z_j} = \langle y^*, \iota_j z \rangle_{Y_j^* \times Y_j} \quad \text{for all } y^* \in Y_j^* \quad (115)$$

if and only if $\iota_j z = 0$ which in turn implies $z = 0$ and $z^{**} = 0$ yielding the desired density property. Note, that for $z \in Z_j$ the norm is thus equivalently defined via

$$\|z\|_{Z_j} = \sup_{\substack{\xi \in Z_j^* \\ \|\xi\|_{Z_j^*} \leq 1}} \langle \xi, z \rangle_{Z_j^* \times Z_j} = \sup_{\substack{\xi \in \iota_j^*(Y_j^*) \\ \|\xi\|_{Z_j^*} \leq 1}} \langle \xi, z \rangle_{Z_j^* \times Z_j} = \sup_{\substack{\xi \in Y_j^* \\ \|\iota_j^* \xi\|_{Z_j^*} \leq 1}} \langle \xi, \iota_j z \rangle_{Y_j^* \times Y_j}, \quad (116)$$

where we took advantage of the continuity of $\langle \cdot, z \rangle_{Z_j^* \times Z_j}$ with respect to the Z_j^* norm and density of $\iota_j^*(Y_j^*)$. Thus, for $y \in Y_j$, such that $y \in \iota_j(Z_j)$,

$$\|y\|_{Z_j} = \sup_{\substack{\xi \in Y_j^* \\ \|\iota_j^* \xi\|_{Z_j^*} \leq 1}} \langle \xi, \iota_j^{-1} y \rangle_{Y_j^* \times Y_j} = \sup_{\substack{\xi \in Y_j^* \\ \|\iota_j^* \xi\|_{Z_j^*} \leq 1}} \langle \xi, y \rangle_{Y_j^* \times Y_j} \quad (117)$$

which is a weakly lower semi-continuous function as supremum of weakly continuous functions.

In order to show lower semi-continuity of D_j , let $v_j, f_j \in Y_j$, sequences $(v_j^n)_n, (f_j^n)_n \subset Y_j$ and we consider two cases: First, let $v_j - f_j \in \iota_j(Z_j)$, $v_j^n \xrightarrow{\mathcal{T}_{Y_j}} v_j$, $f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j$ and without loss of generality $v_j^n - f_j^n \in \iota_j(Z_j)$ for all $n \geq 1$. Hence, we are able to use the representation (117) which is weakly lower semi-continuous in Y_j and $v_j^n - f_j^n \rightarrow v_j - f_j$, resulting in $\|v_j - f_j\|_{Z_j} \leq \liminf_{n \rightarrow \infty} \|v_j^n - f_j^n\|_{Z_j}$.

For the second case, let $v_j - f_j \notin \iota_j(Z_j)$ and again denote by f_j^n, v_j^n the corresponding converging sequences such that $v_j^n - f_j^n \in \iota_j(Z_j)$. If there was a subsequence (with the same name) such that $\|v_j^n - f_j^n\|_{Z_j}$ was bounded, Alaoglu's Theorem in reflexive Z would imply a further subsequence such that $v_j^{n'} - f_j^{n'} = \iota_j(z_j^{n'})$ and $z_j^{n'} \rightarrow z_j \in Z_j$. By continuity of ι_j one obtains $\iota_j(z_j) = v_j - f_j$ contradicting the assumptions, thus $\|v_j^n - f_j^n\|_{Z_j} \rightarrow \infty = \|v_j - f_j\|_{Z_j}$. So in both cases a lower semi-continuity estimate holds, yielding desired lower semi-continuity. \square

Next, we show that $\|\cdot\|_{Z_j}$ still satisfies triangle inequalities in a certain sense that will

be required later on.

Lemma 4.12. *Let $j \in J$ and let Assumptions 4.10 hold. Let $a, b, c \in Y_j$ such that $b - c \in \iota_j(Z_j)$. Then the triangle inequality and inverse triangle inequality hold as follows:*

$$\begin{aligned} \|a - b\|_{Z_j} &\leq \|a - c\|_{Z_j} + \|b - c\|_{Z_j}, \\ \left| \|a - c\|_{Z_j} - \|b - c\|_{Z_j} \right| &\leq \|a - b\|_{Z_j}, \end{aligned} \tag{118}$$

where the values ∞ are allowed (with the rule $\infty \leq \infty$).

Proof. Note that $a - b \in \iota_j(Z_j)$ if and only if $a - c \in \iota_j(Z_j)$, and hence infinity can only occur on both sides of the inequalities simultaneously. In case $a - b \in \iota_j(Z)$ also $a - c \in \iota_j(Z)$ and thus the standard triangle inequality or inverse triangle inequality for $\|\cdot\|_{Z_j}$ on $a - b$ and $b - c$ lead to both stated inequalities. In the case $a - b \notin \iota_j(Z_j)$ also $a - c \notin \iota_j(Z_j)$, and consequently all inequalities remain true via $\infty \leq \infty + \|b - c\|_{Z_j}$ and $|\infty - \|b - c\|_{Z_j}| \leq \infty$. \square

Note that the triangle inequality would hold without the assumption $b - c \in \iota_j(Z_j)$, but the left side of the inverse triangle inequality would not be well-defined in case $\infty - \infty$.

With these results, we can investigate whether for $j \in J$ the discrepancy D_j is continuous and satisfies a modulus of continuity estimate in f^\dagger .

Proposition 4.13. *If Assumptions 4.10 are satisfied, for $j \in J$ such that $D_j(v_j, f_j) = \|v_1 - f_1\|_{Z_j}^{p_j}$ with $p_j \geq 1$, then for every $f_j^\dagger \in Y_j$ and $v_0 \in Y_j$ the discrepancy D_j is v_0 -continuous in f_j^\dagger .*

Moreover, for any $f_j^\dagger \in Y_j$ and $V_j = Y_j$, the discrepancy D_j is strongly ψ_j -continuous on V_j in f_j^\dagger , where $\psi_j: [0, \delta_0] \rightarrow [0, \infty)$ is $\psi_j(t) = ct^{\frac{1}{p_j}}$ with some constant $c > 1$ and $\delta_0 > 0$ limits the noise, i.e. $\delta_0 > \delta_j$. This means that for $\|f_j - f_j^\dagger\|_{Z_j}^{p_j} = \delta_j < \delta_0$ we obtain

$$\left| \|T_j u - f_j\|_{Z_j}^{p_j} - \|T_j u - f_j^\dagger\|_{Z_j}^{p_j} \right| \leq c \delta_j^{\frac{1}{p_j}} (\|T_j u - f_j^\dagger\|_{Z_j}^{p_j} + 1). \tag{119}$$

Proof. The continuity of $D_j(v_0, \cdot)$ with respect to \mathcal{T}_{D_j} is a direct consequence of the triangle inequalities which we just established, used on v_j, f_j^\dagger and $(f_j^\delta)_\delta$, where $f_j^\delta \rightarrow f_j^\dagger$ in \mathcal{T}_{D_j} implies the required condition for applicability of the triangle inequalities.

The proof of Proposition 4.4 concerning the strong ψ_j -continuity solely used basic results on convex analysis in finite dimensions and the inverse triangle inequality. Thus, a completely analogue proof can be made. \square

Hence, we see that also subnorms satisfy the conditions required for the Theory developed in Part I and the following corollary summarises the application of said theory.

Corollary 4.14. *This corollary summarises the theory of Part I applied to the Problem $(SN-MTIKH_{\lambda,\alpha}(f^\dagger))$. We again split into 4 statements, existence, convergence, rates and single-data:*

1. *Let the Assumptions 4.10 hold with J such that $D_j(v_j, f_j) = \|v_j - f_j\|_{Z_j}^{p_j}$ for $j \in J$, for $i \in J^c$ let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ be a basic discrepancy function. Further, let $(R_\alpha)_\alpha$ be a continuous family of functions and with $\lambda = \mathbf{1}$ and some $\alpha = \alpha_0 \in \mathcal{A}$ let the Tikhonov functional*

$$F_{\mathbf{1},\alpha_0}(u, f) = \left(\sum_{j \in J} \|T_j u - f_j\|_{Y_j}^{p_j} \right) + \left(\sum_{i \in I^c} D_i(T_i u, f_i) \right) + R_{\alpha_0}(u) \quad (120)$$

be uniformly coercive. Then, for $f^\dagger \in Y$ the Problem $(SN-MTIKH_{\lambda,\alpha}(f^\dagger))$ is either solvable or $F_{\lambda,\alpha}(\cdot, f^\dagger) \equiv \infty$ for all $\lambda \in (0, \infty)^M$, $\alpha \in \mathcal{A}$.

2. *Additionally to 1., let $I \subset \{1, \dots, M\}$, parameter choice rules as in Theorem 3.9 be applied, and let an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u_0 exists such that D_i is $T_i u_0$ -continuous in f_i^\dagger for all $i \in I^c \cap J^c$. Let $(f^\delta)_\delta$ be a sequence in Y such that $f^\delta \xrightarrow{T} f^\dagger$ and let the corresponding solutions to $SN-MTIKH_{\lambda^\delta, \alpha^\delta}(f^\delta)$ be denoted by u^δ . Then, one obtains subsequential convergence of $(u^\delta)_\delta$ to $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solutions to $Tu = f^\dagger$.*
3. *Additionally to 1. and 2., let X be a normed space and $(\mathcal{A}, d_{\mathcal{A}})$ be a metric space, and let u^\dagger be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution to $Tu = f^\dagger$. For $i \in J^c$ let the discrepancy D_i be strongly ψ_i -continuous on V_i in f_i^\dagger for some sets $V_i \subset Y_i$ and suitable functions ψ_i , and let there be a set $U \subset X$ and function $\psi_{R_{\alpha^\dagger}}$ such that the family $(R_\alpha)_\alpha$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on U in α^\dagger . Let R_{α^\dagger} and $D_i(T_i \cdot, f_i^\dagger)$ for $i \in I^c$ be convex. Also, let $u^\dagger, u^\delta \in U$ and $T_i u^\dagger, T_i u^\delta \in V_i$ for $i \in J^c$ and for $\delta_j < \delta_0$ with some constant $\delta_0 > 0$. Let there be constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that the following source condition holds: There is*

$\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ such that for u satisfying $R_{\alpha^\dagger, \lambda^\dagger, I}(u, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f_i^\dagger) \leq \epsilon_0$

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u, T_i u^\dagger), \quad (\text{SC3})$$

where in case $j \in I \cap J$, the function $\phi_j(T_j u, T_j u^\dagger) = \|T_j u - T_j u^\dagger\|_{Z_j}$. Here, for $i \in I$, the function $\phi_i: Y_i \times Y_i \rightarrow [0, \infty]$ is such that for $v_i \in Y_i$

$$\phi_i(v_i, f_i^\dagger) \leq \Phi_i(D_i(f_i^\dagger, f_i)) D_i(v_i, f_i) + \psi_i(D_i(f_i^\dagger, f_i)),$$

where $\Phi_i: [0, \infty] \rightarrow \mathbb{R}$ is such that $\Phi_i(\delta_i) \leq \frac{1}{4\gamma_2} \lambda_i^\delta$ for δ_i sufficiently small.

Then, there are constants $c > 0$ and $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M) \in (0, \infty)^M$ such that for $\delta < \bar{\delta}$ and $j \in I \cap J$,

$$\begin{aligned} \|T_j u^\delta - f_j^\delta\|_{Z_j}^{p_j} &\leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \\ &\quad \left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right). \end{aligned} \quad (121)$$

For $j \in I$:

$$\begin{aligned} D_j(T_j u^\delta, f_j^\delta) &\leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \\ &\quad \left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right), \end{aligned} \quad (122)$$

$$\begin{aligned} D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) &\leq c \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \\ &\quad \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right). \end{aligned} \quad (123)$$

In particular, this constant c solely depends on $R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger)$, γ_1 , γ_2 , λ^\dagger , α^\dagger , f^\dagger and $\bar{\delta}$, but not on the specific sequence $(u^\delta)_\delta$, $(f^\delta)_\delta$ or even $(\delta)_{\delta \in \Delta}$.

4. In the single-data case $M = 1$: Let $R: X \rightarrow [0, \infty)$ be \mathcal{T}_X -lower semi-continuous and for all $C > 0$, let the set $\{u \in X \mid R(u) + \|Tu - f\|_Z^p \leq C\}$ be \mathcal{T}_X -precompact

and let $\text{dom}(R) \cap \text{dom}(T) \neq \emptyset$. Then, for $Tu = f^\dagger$ the Tikhonov regularisation

$$\min_{u \in X} \|Tu - f^\dagger\|_Z^p + \alpha R(u) \quad (124)$$

is solvable and stable, and the convergence results stated in Part I hold.

Proof. Application of Theorems 3.5, 3.9 and Theorem 3.21, whose assumptions are fulfilled due to Propositions 4.11, 4.13 and the general setting. \square

5. Kullback-Leibler Divergence

5.1. Motivation

While using norms for the discrepancy function is often reasonable as described in the previous chapter, the discrepancy should always be suitable to the noise model one considers, and there are types of noise for which norms simply are not feasible discrepancy choices. In this chapter the Kullback-Leibler divergence is derived and its use for regularisation is considered. Using such a fidelity term is in particular reasonable when dealing with Poisson distributed noise, e.g. if $Y = L^1(\Omega)$, and every point contains noise which is Poisson distributed with the true value as expected value.

If X is a Poisson distributed random variable with parameter λ , then for $k \in \{0, 1, 2, \dots\}$

$$\mathbb{P}(X = k) = \frac{\lambda^k}{k!} e^{-\lambda}. \quad (125)$$

When we consider $v = (v_1, \dots, v_N)$ and $f = (f_1, \dots, f_N)$ such that f is a random-variable and f_i is Poisson distributed with expected value v_i , i.e. f is a version of v containing Poisson noise, then the likelihood function is $L(v, f) = \prod_{i=1}^N \frac{v_i^{f_i}}{f_i!} e^{-v_i}$, and consequently

$$\begin{aligned} \operatorname{argmax}_v (L(v, f)) &= \operatorname{argmin}_v (-\ln(L(v, f))) = \operatorname{argmin}_v \left(-\ln \left(\prod_{i=1}^N \frac{v_i^{f_i}}{f_i!} e^{-v_i} \right) \right) \\ &= \operatorname{argmin}_v \left(\sum_{i=1}^N -f_i \ln(v_i) + v_i + \ln(f_i!) \right) = \operatorname{argmin}_v \left(\sum_{i=1}^N v_i - f_i - f_i \ln \left(\frac{v_i}{f_i} \right) \right). \end{aligned}$$

It is well known that the likelihood function is a suitable discrepancy when trying to recover parameter (in our case v), and therefore $D(v, f) = \sum_{i=1}^N v_i - f_i - f_i \ln \left(\frac{v_i}{f_i} \right)$ is a reasonable measure of the discrepancy when dealing with Poisson distributed noise.

Understanding this as a special case for the counting measure, we generalise this concept to the Kullback-Leibler divergence.

Definition 5.1 (Kullback-Leibler divergence). *Let μ be a positive finite Radon measure and $(\Omega, \mathcal{A}, \mu)$ the corresponding measure space. Let $L_\mu^{1,+}(\Omega) = \{v \in L_\mu^1(\Omega) \mid v \geq 0 \text{ } \mu \text{ a.e.}\}$ and we define the Kullback-Leibler divergence (also I-divergence) as*

$$D_{KL}: L_\mu^{1,+}(\Omega) \times L_\mu^{1,+}(\Omega) \rightarrow [0, \infty], \quad D_{KL}(v, f) = \int_\Omega v - f - f \ln \left(\frac{v}{f} \right) d\mu,$$

where we understand the integrand $d(a, b) = a - b - \ln\left(\frac{a}{b}\right)$ such that $d(a, 0) = a$ for $a \geq 0$ and $d(0, b) = \infty$ for $b > 0$ and in particular $d(0, 0) = 0$.

Note that $L_\mu^{1,+}(\Omega)$ is not a vector space, but one could extend the Kullback-Leibler divergence with values ∞ onto the whole space $L_\mu^1(\Omega)$. Moreover, one can still consider concepts of convexity on $L_\mu^{1,+}(\Omega)$ as it is a convex subset of the vector space $L_\mu^1(\Omega)$. Moreover, we will in the following use the norm topology from L_μ^1 also on $L_\mu^{1,+}(\Omega)$ by considering the resulting subspace topology to which we also refer to as the L_μ^1 topology in slight abuse of notation.

5.2. Basic Properties

First of all, let us consider some of the basic properties of the Kullback-Leibler divergence, in particular its analytic properties relevant to the application as a discrepancy in Part I. We will therefore in the following assume that a finite measure space $(\Omega, \mathcal{A}, \mu)$ as in Definition 5.1 exists in the background without further mention.

Lemma 5.2. *For $v, f \in L_\mu^{1,+}(\Omega)$, the mapping $(v, f) \mapsto D_{KL}(v, f)$ is convex. Also, the positive definiteness property*

$$D_{KL}(v, f) \geq 0, \quad \text{and} \quad D_{KL}(v, f) = 0 \Leftrightarrow v = f \quad \mu \text{ a.e. in } \Omega, \quad (126)$$

holds. Furthermore, $D_{KL}(\cdot, f)$ is strictly convex, if and only if $f > 0$ μ almost everywhere.

Proof. We consider the function $d: [0, \infty) \times [0, \infty) \rightarrow \mathbb{R}$ such that for $a, b \geq 0$, $d(a, b) = a - b - b \ln\left(\frac{a}{b}\right)$, i.e. the integrand in D_{KL} as in Definition 5.1 with the same special cases. Many computations and consideration concerning the Kullback-Leibler divergence can be reduced to point-wise considerations with regard to d . Since $\text{dom}(D_{KL}) \subset L_\mu^{1,+}(\Omega) \times L_\mu^{1,+}(\Omega)$ which is a convex subset of $L_\mu^1(\Omega) \times L_\mu^1(\Omega)$, it is sufficient to consider $v, f \geq 0$ and $v, f < \infty$ μ a.e., in order to investigate convexity or positivity.

Convexity: We aim to show that $d: [0, \infty) \times [0, \infty)$ is a convex function as this immediately implies the convexity of D_{KL} . In $a, b > 0$,

$$\nabla d = \begin{pmatrix} 1 - \frac{a}{b} \\ -\ln\left(\frac{a}{b}\right) \end{pmatrix}, \quad \nabla^2 d = \begin{pmatrix} \frac{b}{a^2} & -\frac{1}{a} \\ -\frac{1}{a} & \frac{1}{b} \end{pmatrix} \quad \text{and} \quad \det(\nabla^2 d) = \frac{b}{a^2} \frac{1}{b} - \frac{1}{a} \frac{1}{a} = 0 \quad (127)$$

implying that d is convex on $(0, \infty) \times (0, \infty)$.

So it remains to show that convexity holds even if one of the variables possesses the value 0. Let therefore $a_1, a_2, b_1, b_2 \geq 0$ and for some $\alpha \in (0, 1)$ let $\bar{a} = \alpha a_1 + (1 - \alpha)a_2$ and $\bar{b} = \alpha b_1 + (1 - \alpha)b_2$. We need to show that $d(\bar{a}, \bar{b}) \leq \alpha d(a_1, b_1) + (1 - \alpha)d(a_2, b_2)$.

The cases left to consider revolve around at least one of the instances a_1, a_2, b_1, b_2 being zero, however, the cases $a_i = 0$ but $b_i > 0$ for some $i \in \{1, 2\}$ are trivial as then $d(a_i, b_i) = \infty$ and the convexity estimate would hold trivially. Therefore, also in the case $a_1 = 0$ and $a_2 = 0$ the convexity estimates hold as either $d(a_i, b_i) = \infty$ for at least one i , or $a_1 = a_2$ and $b_1 = b_2$.

So trivial cases are taken care of and the cases with one $b_i = 0$ remain, i.e. $b_2 = 0$, $a_1 \geq 0$, $b_1 \geq 0$ and $a_2 \geq 0$ (and the same with the roles $i = 1$ and $i = 2$ exchanged).

We further split this up into the case $a_2 = 0$, $b_2 = 0$, $a_1 > 0$, $b_1 \geq 0$ and the case $b_2 = 0$, $b_1 \geq 0$, $a_1 \geq 0$, $a_2 > 0$ (and the cases exchanging roles $i = 1$ with $i = 2$). For the first case, i.e. that $a_2 = 0$ and $b_2 = 0$ we see via computation that $d(\bar{a}, \bar{b}) = \alpha d(a_1, b_1)$ which implies the convexity estimate as $d(a_2, b_2) = 0$. In the second case, i.e. $a_i > 0$ for $i \in \{1, 2\}$ and $b_2 = 0$, since $\bar{a} \geq \alpha a_1$ we obtain

$$\begin{aligned} d(\bar{a}, \bar{b}) &= \alpha \left(a_1 - b_1 - b_1 \ln \left(\frac{\bar{a}}{\alpha b_1} \right) \right) + (1 - \alpha) \left(a_2 - b_2 - \underbrace{b_2 \ln \left(\frac{a_2}{b_2} \right)}_{=0} \right) \\ &\leq \alpha \left(a_1 - b_1 - b_1 \ln \left(\frac{\alpha a_1}{\alpha b_1} \right) \right) + (1 - \alpha) \left(a_2 - b_2 - b_2 \ln \left(\frac{a_2}{b_2} \right) \right) \\ &= \alpha d(a_1, b_1) + (1 - \alpha) d(a_2, b_2), \end{aligned}$$

which holds true even if $b_1 = 0$. Hence, the function $d: [0, \infty) \times [0, \infty) \rightarrow \mathbb{R}^\infty$ is indeed convex.

Apparently, $D_{KL}(v, f) = \int_{\Omega} d(v(x), f(x)) \, d\mu(x)$ and it is well-known, that the integral of convex functions (with an unsigned measure) is again convex.

Positivity: To confirm that $D_{KL}(v, f) \geq 0$ and equality holds if and only if $v = f$, we compute for fixed $f \in L_{\mu}^{1,+}(\Omega)$ what the infimum value $\inf_{v \in L_{\mu}^{1,+}(\Omega)} D_{KL}(v, f)$ is. We will see that these infima are always zero, and the infimum is only attained by $v = f$ μ a.e., consequently confirming the positivity statements.

In order to find the infimum, we consider $\min_{a \geq 0} d(a, b)$ for fixed $b \geq 0$ since integrating point-wise minimal functions will lead to minimal integrals. The first order optimality condition in the case $a > 0$, $b > 0$ is satisfied by $a = b$ which obviously yields $d(a, b) = 0$. In case $a > 0$, $b = 0$, the value $d(a, b) = a > 0$, which is not optimal, since $d(0, 0) = 0$. The case $a = 0$, $b > 0$ implies $d(a, b) = \infty$, while $d(b, b) = 0$. Consequently, in any

case $a = b$ minimises the functional $d(\cdot, b)$. By monotonicity of the integral operator and since $d(v(x), f(x)) = 0$ is minimal only for $v(x) = f(x)$, we obtain that it is both necessary and sufficient for the minimiser v of $D_{KL}(\cdot, f)$ that $v = f$ μ almost everywhere in Ω and in particular $D_{KL}(v, f) \geq 0$ for any $v \in L_\mu^{1,+}(\Omega)$.

Strict convexity: The strict convexity of the functional with respect to the first component is again obtained from considering the point-wise function d . For $b = 0$, $d(a, b) = a$ is linear, and consequently not strictly convex. Hence, for $\tilde{\Omega} = \{x \in \Omega \mid f(x) = 0\}$ the characteristic function $\chi_{\tilde{\Omega}}$ such that $\chi_{\tilde{\Omega}}(x) = 1$ if $x \in \tilde{\Omega}$ and zero otherwise has the property

$$D_{KL}(\chi_{\tilde{\Omega}}, f) = \int_{\tilde{\Omega}} 1 \, dx = |\tilde{\Omega}| = \frac{1}{3}|\tilde{\Omega}| + \frac{2}{3}|\tilde{\Omega}| = \frac{1}{2}D_{KL}\left(\frac{2}{3}\chi_{\tilde{\Omega}}, f\right) + \frac{1}{2}D_{KL}\left(\frac{4}{3}\chi_{\tilde{\Omega}}, f\right), \quad (128)$$

which shows that $D_{KL}(\cdot, f)$ is not strictly convex if $|\tilde{\Omega}| > 0$. In the case that $f > 0$ a.e. on Ω , $d(\cdot, f(x))$ is strictly convex for μ almost all $x \in \Omega$ (as $v(x) \mapsto -f(x) \ln(v(x))$ is for $f(x) > 0$), resulting in $D_{KL}(\cdot, f) = \int_{\Omega} d(\cdot(x), f(x)) \, d\mu$ being strictly convex. \square

As we have seen in Part I, the topological properties of the discrepancy term D are important in order to establish technical results concerning stability and convergence of the regularised solutions. Therefore, we next consider what properties D_{KL} possesses with regard to the L_μ^1 topology.

Under some additional assumptions, the functional D_{KL} induces a topology stronger than the L_μ^1 norm topology.

Lemma 5.3. *For $v, f \in L_\mu^{1,+}(\Omega)$, the inequality*

$$\|v - f\|_{L_\mu^1(\Omega)}^2 \leq \left(\frac{2}{3}\|f\|_{L_\mu^1} + \frac{4}{3}\|v\|_{L_\mu^1} \right) D_{KL}(v, f) \quad (129)$$

holds. In particular, for sequences $(v^n)_n$ and $(f^n)_n$ bounded in L_μ^1 , we have

$$\lim_{n \rightarrow \infty} D_{KL}(v^n, f^n) = 0 \quad \Rightarrow \quad \lim_{n \rightarrow \infty} \|v^n - f^n\|_{L_\mu^1} = 0. \quad (130)$$

Proof: [see e.g. [30, 9].] For $a, b \in \mathbb{R}$ with $a > 0$ and $b \geq 0$, we first show the scalar inequality

$$(a - b)^2 \leq \left(\frac{2}{3}b + \frac{4}{3}a \right) \left(-b \ln\left(\frac{a}{b}\right) + a - b \right). \quad (131)$$

In order to do so, we consider $g(t) = \left(\frac{4}{3} + \frac{2}{3}t \right) \left(t \ln(t) - t + 1 \right) - (t - 1)^2$. Note that for $t = \frac{b}{a} \geq 0$, $a^2 g(t)$ is the difference of the two sides of (131), and hence we aim to show

$g(t) \geq 0$ for all $t > 0$. One can compute, that

$$\frac{\partial g}{\partial t}(t) = \frac{4}{3}(-2t + (t+1)\ln(t) + 2) \quad \text{and} \quad \frac{\partial^2 g}{\partial t^2}(t) = \frac{4}{3}\left(-2 + \frac{t+1}{t} + \ln(t)\right). \quad (132)$$

The value $t = 1$ is a solution to the first order optimality condition of g , and $\frac{\partial^2 g}{\partial t^2}(t) > 0$ for $t \neq 1$ (since $\frac{1}{t} + \ln(t) > 1$ for $t \neq 1$) implying that $t = 1$ is the unique solution to the first order condition as g is strictly convex. Therefore the minimum value of g can only be attained in $t = 1$, and since $g(1) = 0$, also $g(t) \geq 0$ for all $t > 0$, which implies (131) as multiplication with a^2 will not change the sign.

Now, we can turn to the D_{KL} estimate and note, that for $v(x) = 0$ only $f(x) = 0$ (in an μ a.e. sense) is reasonable, since otherwise $D_{KL}(v, f) = \infty$ and the estimate would be trivially fulfilled. Consequently, we assume without loss of generality, that $v > 0$ μ almost everywhere. Then, application of the scalar estimate, as well as the Cauchy-Schwarz Inequality yield

$$\begin{aligned} \left(\int_{\Omega} |v - f| \, d\mu\right)^2 &\stackrel{(131)}{\leq} \left(\int_{\Omega} \sqrt{\left(\frac{2}{3}f + \frac{4}{3}v\right)} \sqrt{-f \ln\left(\frac{v}{f}\right) + v - f} \, d\mu\right)^2 \\ &\stackrel{\text{C.S.I.}}{\leq} \int_{\Omega} \left(\frac{2}{3}|f| + \frac{4}{3}|v|\right) \, d\mu \int_{\Omega} \left(-f \ln\left(\frac{v}{f}\right) + v - f\right) \, d\mu \stackrel{\text{def.}}{=} \left(\frac{2}{3}\|f\|_{L^1_{\mu}} + \frac{4}{3}\|v\|_{L^1_{\mu}}\right) D_{KL}(v, f). \end{aligned}$$

□

The topology induced by the Kullback-Leibler divergence is in a way stronger than the L^1_{μ} norm. Next we discuss how the D_{KL} functional react to L^1_{μ} convergence of its arguments in terms of continuity, and how a Topology $\mathcal{T}_{D_{KL}}$ implying D_{KL} convergence might look like.

5.3. Continuity Results

In this chapter we investigate suitable topologies and assumptions such that continuity of D_{KL} is achieved in reasonable settings.

Lemma 5.4. *Let $f^{\dagger} \in L^1_{\mu^+}(\Omega)$. For fixed $\delta_0 > 0$, there is a constant $c > 0$ such that if $D_{KL}(f^{\dagger}, f^{\delta}) \leq \delta_0$ for $f^{\delta} \in L^1_{\mu^+}(\Omega)$, also $\|f^{\delta}\|_{L^1_{\mu}} < c$. This means that small distance with respect to D_{KL} implies boundedness in L^1_{μ} . Note that the constant c does depend on $\|f^{\dagger}\|_{L^1_{\mu}}$ and δ_0 .*

Proof. Let $f^{\delta} \in L^1_{\mu^+}(\Omega)$ with $D_{KL}(f^{\dagger}, f^{\delta}) < \delta_0$. Then using the estimate (129) in

Lemma 5.3 (stating an estimate between $\|f - f^\dagger\|_{L_\mu^1}$ and $D_{KL}(f^\dagger, f)$) one computes

$$(\|f^\delta\|_{L_\mu^1} - \|f^\dagger\|_{L_\mu^1})^2 \leq \|f^\dagger - f^\delta\|_{L_\mu^1}^2 \stackrel{(129)}{\leq} 2(\|f^\dagger\|_{L_\mu^1} + \|f^\delta\|_{L_\mu^1})D_{KL}(f^\dagger, f^\delta).$$

Reformulating by putting all $\|f^\delta\|_{L_\mu^1}$ on the left side, applying the binomial formula and using that $D_{KL}(f^\dagger, f^\delta) \leq \delta_0$, one obtains the equivalent inequality

$$\|f^\delta\|_{L_\mu^1}(\|f^\delta\|_{L_\mu^1} - 2\delta_0 - 2\|f^\dagger\|_{L_\mu^1}) + \|f^\dagger\|_{L_\mu^1}^2 \leq 2\|f^\dagger\|_{L_\mu^1}\delta_0.$$

Now, if $\|f^\delta\|_{L_\mu^1} > 4\|f^\dagger\|_{L_\mu^1} + 2\delta_0$ were to hold and omitting the term $\|f^\dagger\|_{L_\mu^1}^2 \geq 0$, one sees

$$\|f^\delta\|_{L_\mu^1} \leq \delta_0$$

contradicting $\|f^\delta\|_{L_\mu^1} > 4\|f^\dagger\|_{L_\mu^1} + 2\delta_0$. So we obtain that

$$\|f^\delta\|_{L_\mu^1} \leq 4\|f^\dagger\|_{L_\mu^1} + 2\delta_0. \quad (133)$$

□

So we see that there indeed are uniform bounds on the L_μ^1 norm for small D_{KL} distance. This will later be useful in order to connect the L_μ^1 topology with a topology stronger than D_{KL} .

Lemma 5.5. *The mapping $(u, v) \mapsto D_{KL}(u, v)$ in $L_\mu^{1,+}(\Omega) \times L_\mu^{1,+}(\Omega)$ is lower semi-continuous with respect to the $L_\mu^1 \times L_\mu^1$ norm topology.*

Proof. In order to prove the lower semi-continuity, we employ the Lemma of Fatou. Again, only functions with non-negative finite values need to be considered and we do the proof by contradiction. We assume that D_{KL} is not lower semi-continuous and therefore there are sequences $(v^n)_n$ and $(f^n)_n$ in $L_\mu^{1,+}(\Omega)$ such that $v^n \rightarrow v$ in L_μ^1 and $f^n \rightarrow f$ in L_μ^1 , but

$$\lim_{n \rightarrow \infty} D_{KL}(v^n, f^n) < D_{KL}(v, f). \quad (134)$$

It is well known, that every convergent sequence in L_μ^1 admits a subsequence which converges point-wise μ almost everywhere. Hence, we can select a subsequence indexed by n' for which $v^{n'}(x) \rightarrow v(x)$ μ a.e. and $f^{n'}(x) \rightarrow f(x)$ μ a.e.. In particular $v < \infty$ and $f < \infty$ μ a.e., and thus the cases $v(x) = \infty$ or $f(x) = \infty$ are negligible. Therefore, we show that the integrand function d with $d(a, b) = a - b - b \ln\left(\frac{a}{b}\right)$ is lower semi-continuous on $[0, \infty) \times [0, \infty)$ as preparation for Fatou's Lemma. All parts of $d(a, b)$

other than $g(a, b) = -b \ln\left(\frac{a}{b}\right)$, with the conventions as in the definition of D_{KL} are obviously lower semi-continuous, so our focus will lie on this part of d . Let $(a^n)_n$ and $(b^n)_n$ be convergent non-negative valued sequences with respective limits $a, b \in [0, \infty)$. If $a > 0$ and $b > 0$, the function d is continuous in (a, b) as the composition of continuous functions. The case $b = 0$ and $a > 0$ does not pose any problems either, since $\ln(a^n)$ is bounded, implying $\lim_{n \rightarrow \infty} g(a^n, b^n) = 0 = g(a, b)$ due to our conventions. This leaves the case $a = 0$, and either $b = 0$ or $b > 0$. In the former, $d(a, b) = 0 \leq d(a^n, b^n)$ and therefore the lower semi-continuity estimate holds, while for the latter, obviously $g(a, b) = \infty = \lim_{n \rightarrow \infty} g(a^n, b^n)$.

Hence, $d(v(x), f(x)) \leq \liminf_{n' \rightarrow 0} d(v^{n'}(x), f^{n'}(x))$ and $d(v(x), f(x)) \geq 0$ for μ almost every $x \in \Omega$, thus Fatou's Lemma is applicable and results in

$$\begin{aligned} D_{KL}(v, f) &= \int_{\Omega} d(v(x), f(x)) \, d\mu(x) \\ &\leq \liminf_{n' \rightarrow \infty} \int_{\Omega} d(v^{n'}(x), f^{n'}(x)) \, d\mu(x) = \lim_{n \rightarrow \infty} D_{KL}(v^n, f^n), \end{aligned}$$

contradicting the assumptions stating existence of sequences $(v^n)_n, (f^n)_n$ such that $\lim_{n \rightarrow \infty} D_{KL}(v^n, f^n) < D_{KL}(v, f)$, and consequently D_{KL} is lower semi-continuous. \square

Recall that being a basic discrepancy requires a topology \mathcal{T}_D which is stronger than the discrepancy, and yields $\mathcal{T}_Y \times \mathcal{T}_D$ -lower semi-continuity. Next we try to find such a topology and show its properties.

Definition 5.6. *We define the topology $\mathcal{T}_{D_{KL}}$ on $L_{\mu}^{1,+}(\Omega)$ as the topology created by the subbasis $S \subset \mathcal{P}(L_{\mu}^{1,+}(\Omega))$ (the smallest topology containing S , constructed by arbitrary unions of finite intersections of elements in S), where*

$$\begin{aligned} S &= \left\{ B_{\epsilon}(f^{\dagger}) \mid \epsilon \in (0, \infty), f^{\dagger} \in L_{\mu}^{1,+}(\Omega) \right\} \quad \text{with} \\ B_{\epsilon}(f^{\dagger}) &= \{ f \in L_{\mu}^{1,+}(\Omega) \mid D_{KL}(f^{\dagger}, f) < \epsilon \}, \end{aligned} \tag{135}$$

i.e. the topology induced by level sets with regard to the function $D_{KL}(f^{\dagger}, \cdot)$. Note that this construction indeed is a topology, and this topology will serve as the \mathcal{T}_{D_i} topology for the Tikhonov theory if the discrepancy $D_i = D_{KL}$.

Lemma 5.7. *For a sequence $(f^n)_n \subset L_{\mu}^{1,+}(\Omega)$ and $f^{\dagger} \in L_{\mu}^{1,+}(\Omega)$, convergence $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f^{\dagger}$ holds if and only if for any $f \in L_{\mu}^{1,+}(\Omega)$,*

$$\lim_{n \rightarrow \infty} D_{KL}(f, f^n) = D_{KL}(f, f^{\dagger}). \tag{136}$$

In particular, $\mathcal{T}_{D_{KL}}$ is stronger than the L_μ^1 norm topology and $\mathcal{T}_{D_{KL}}$ is also a Hausdorff topology.

Proof. First we assume that $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f^\dagger$ and show that (136) holds for any $f \in L_\mu^{1,+}(\Omega)$. This convergence of $f^n \rightarrow f^\dagger$ is equivalently defined via: for any neighbourhood U of $f^\dagger \in L_\mu^{1,+}(\Omega)$ there is $n_0 > 0$ such that $f^n \in U$ for $n \geq n_0$. It is however sufficient to consider $U = \bigcap_{i=1}^N B_{\epsilon_i}(f_i)$ for arbitrary $f_1, \dots, f_N \in L_\mu^{1,+}(\Omega)$ and $\epsilon_1, \dots, \epsilon_N > 0$ such that $D_{KL}(f_i, f^\dagger) < \epsilon_i$, i.e. finite intersections of elements of the subbasis containing f^\dagger . This in turn means that for such f_1, \dots, f_N and $\epsilon_1, \dots, \epsilon_N$ there is a $n_0 > 0$ such that for $n > n_0$

$$D_{KL}(f_i, f^n) \leq \epsilon_i.$$

When choosing $N = 1$, $f_1 = f^\dagger$ and $\epsilon_1 > 0$ arbitrarily small, this implies the convergence $D_{KL}(f^\dagger, f^n) \rightarrow 0$ and due to Lemma 5.4 the norm $\|f^n\|_{L_\mu^1}$ is bounded and thus also $f^n \xrightarrow{L_\mu^1} f^\dagger$ due to Lemma 5.3, showing that indeed $\mathcal{T}_{D_{KL}}$ is stronger than the L_μ^1 topology.

Also, choosing $N = 1$ and $f \in L_\mu^{1,+}(\Omega)$ arbitrary, we see that

$$\begin{aligned} \limsup_{n \rightarrow \infty} D_{KL}(f, f^n) &\leq \inf \{ \epsilon > 0 \mid D_{KL}(f, f^\dagger) < \epsilon \} \\ &= D_{KL}(f, f^\dagger). \end{aligned}$$

Hence, we see that $\limsup_{n \rightarrow \infty} D_{KL}(f, f^n) \leq D_{KL}(f, f^\dagger)$. However, as $\mathcal{T}_{D_{KL}}$ is stronger than L_μ^1 , Lemma 5.5 implies that $D_{KL}(f, f^\dagger) \leq \liminf_{n \rightarrow \infty} D_{KL}(f, f^n)$, which together yields the claimed convergence statement.

For the converse implication, let $D_{KL}(f, f^n) \rightarrow D_{KL}(f, f^\dagger)$ for all $f \in L_\mu^{1,+}$. Then it is easy to see that indeed $f^n \in U$ for any neighbourhood U after finitely many n and consequently $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f^\dagger$.

That this is a Hausdorff topology follows immediately from the fact that $\mathcal{T}_{D_{KL}}$ is stronger than the Hausdorff topology induced by $\|\cdot\|_{L_\mu^1}$. \square

Lemma 5.8. *The function D_{KL} is $\mathcal{T}_{L_\mu^1, W} \times \mathcal{T}_{D_{KL}}$ lower semi-continuous, i.e. for sequences $(v^n)_n$ and $(f^n)_n$ in $L_\mu^{1,+}(\Omega)$,*

$$\left(v^n \xrightarrow{L_\mu^1} v, f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f \right) \Rightarrow D_{KL}(v, f) \leq \liminf_{n \rightarrow \infty} D_{KL}(v^n, f^n). \quad (137)$$

In particular $D_{KL}: L_\mu^{1,+}(\Omega) \times L_\mu^{1,+}(\Omega) \rightarrow [0, \infty]$ is a basic discrepancy with respect to $\mathcal{T}_{L_\mu^1, W}$ and $\mathcal{T}_{D_{KL}}$, where again in slight abuse of notation $\mathcal{T}_{L_\mu^1, W}$ will denote the subtopology

of the weak L_μ^1 topology on $L_\mu^{1,+}(\Omega)$. Moreover, for any $v_0, f^\dagger \in L_\mu^{1,+}(\Omega)$ the Kullback-Leibler divergence is v_0 -continuous in f^\dagger .

Proof. Lemma 5.5 shows the lower semi-continuity on $L_\mu^1 \times L_\mu^1$, and D_{KL} is convex, thus Lemma 1.43 implies that D_{KL} is even $\mathcal{T}_{L_\mu^1, W} \times \mathcal{T}_{L_\mu^1, W}$ lower semi-continuous. Strictly speaking one would require a vector space for this lemma, however $L_\mu^{1,+}(\Omega)$ is a convex, weakly closed subset and the same argument can be made to D_{KL} by extending D_{KL} with ∞ onto $L_\mu^1(\Omega)$. In particular, $\mathcal{T}_{D_{KL}}$ is stronger than the weak topology on L_μ^1 due to Lemma 5.7, and thus convergence in $\mathcal{T}_{D_{KL}}$ implies convergence in $\mathcal{T}_{L_\mu^1, W}$, ensuring the desired lower semi-continuity property. In particular, the other conditions for being a basic discrepancy with respect to $\mathcal{T}_{L_\mu^1(\Omega)}$ and $\mathcal{T}_{D_{KL}}$ are fulfilled (positivity and topology \mathcal{T}_D stronger than D), so D_{KL} is indeed a basic discrepancy. That $D_{KL}(v_0, \cdot)$ is continuous in f^\dagger with respect to $\mathcal{T}_{D_{KL}}$ is immanent due to Lemma 5.7 \square

Remark 5.9. *The previous lemma ensures that in a Tikhonov approach the discrepancy $D = D_{KL}$ with $Y = L_\mu^{1,+}(\Omega)$, $\mathcal{T}_Y = \mathcal{T}_{L_\mu^1, W}$ and $\mathcal{T}_D = \mathcal{T}_{D_{KL}}$ (Definition 5.6), the function D_{KL} is a suitable choice for a discrepancy function.*

We wish to investigate the topology further, in order to find conditions allowing to verify convergence more easily than considering $D_{KL}(f, f^n)$ for all $f \in L_\mu^{1,+}(\Omega)$ and identify sets V suitable for strong continuity of D_{KL} . The following example illustrates, that it is not sufficient that $D_{KL}(f^\dagger, f^n) \rightarrow 0$ to obtain convergence in $\mathcal{T}_{D_{KL}}$.

Example 5.10. *We show an example of functions v_0, f^\dagger and a sequence of function $(f^n)_n$ in $L_\mu^{1,+}$ such that $D_{KL}(f^\dagger, f^n) \rightarrow 0$ does not imply $D_{KL}(v_0, f^n) \rightarrow D_{KL}(v_0, f^\dagger)$ and consequently f^n does not converge with respect to $\mathcal{T}_{D_{KL}}$. To do so, we consider $\Omega = [0, 1]$ and μ is the standard Lebesgue measure. When we consider $v_0, f^\dagger \in L^{1,+}(\Omega)$ such that for $x \in \Omega$, $v_0(x) = e^{\frac{-1}{x^2}} x^{\frac{3}{2}}$ and $f^\dagger(x) = x^{\frac{3}{2}}$, then*

$$D_{KL}(v_0, f^\dagger) = \int_0^1 v_0 - f^\dagger - x^{\frac{3}{2}} \ln(e^{\frac{-1}{x^2}}) dx = \int_0^1 \underbrace{v_0 - f^\dagger}_{\leq 1} + x^{\frac{3}{2}} \frac{1}{x^2} dx < \infty.$$

For the sequence of functions $(f^n)_n \subset L^{1,+}(\Omega)$ with $f^n(x) = x^{\frac{3}{2}} + \frac{1}{n}x$ for $n \geq 1$, we

see that

$$\begin{aligned} D_{KL}(f^\dagger, f^n) &= \int_0^1 x^{\frac{3}{2}} - x^{\frac{3}{2}} - \frac{1}{n}x - (x^{\frac{3}{2}} + \frac{1}{n}x) \ln \left(\frac{x^{\frac{3}{2}}}{x^{\frac{3}{2}} + \frac{1}{n}x} \right) dx \\ &= -\frac{1}{n} \int_0^1 x dx + \int_0^1 \underbrace{-(x^{\frac{3}{2}} + \frac{1}{n}x)}_{\leq 2x \leq 2} \underbrace{\ln \left(\frac{x^{\frac{3}{2}}}{x^{\frac{3}{2}} + \frac{1}{n}x} \right)}_{\xrightarrow{n \rightarrow \infty} 0} dx. \end{aligned}$$

Obviously the first integral will vanish for $n \rightarrow \infty$, while for the second we find a majorant $g(x) = -x \ln \left(\frac{x}{2} \right)$, and thus Lebesgue's Theorem implies that the second integral vanishes as well, thus yielding $D_{KL}(f^\dagger, f^n) \rightarrow 0$. However,

$$\begin{aligned} D_{KL}(v_0, f^n) &= \int_0^1 v_0 - f^n - (x^{\frac{3}{2}} + \frac{1}{n}x) \ln \left(e^{\frac{-1}{x^{\frac{3}{2}}}} \frac{x^{\frac{3}{2}}}{x^{\frac{3}{2}} + \frac{1}{n}x} \right) dx \\ &= \underbrace{\int_0^1 v_0 - f^n dx}_{\leq c} + \underbrace{\int_0^1 (x^{\frac{3}{2}} + \frac{1}{n}x) \frac{1}{x^2} dx}_{=\infty} - \underbrace{\int_0^1 (x^{\frac{3}{2}} + \frac{1}{n}x) \ln \left(\frac{x^{\frac{3}{2}}}{x^{\frac{3}{2}} + \frac{1}{n}x} \right) dx}_{\xrightarrow{n \rightarrow \infty} 0} = \infty, \end{aligned}$$

where the first integral is bounded, the second is essentially $\int_0^1 x^{-1} dx$ which is infinite, and the last integral was estimated before. Hence, for this v_0 and this f^\dagger ,

$$D_{KL}(v_0, f^\dagger) < \infty = \lim_{\delta \rightarrow 0} D_{KL}(v_0, f^\delta),$$

implying that f^n does not converge in $\mathcal{T}_{D_{KL}}$ to f^\dagger . In particular we note that all occurring functions are even bounded in $L_\mu^\infty(\Omega)$, so convergence might require even stronger assumptions.

Theorem 5.11. *Let $f^\dagger, v_0 \in L_\mu^{1,+}(\Omega)$ such that $D_{KL}(v_0, f^\dagger) < \infty$, and let $(f^n)_n \subset L_\mu^{1,+}(\Omega)$ be a sequence with $D_{KL}(f^\dagger, f^n) \rightarrow 0$. Then*

$$\lim_{n \rightarrow \infty} D_{KL}(v_0, f^n) = D_{KL}(v_0, f^\dagger) \iff \lim_{n \rightarrow \infty} \int_{\{v_0 \neq 0, f^\dagger \neq 0\}} \ln \left(\frac{v_0}{f^\dagger} \right) (f^\dagger - f^n) d\mu = 0. \quad (138)$$

In particular, if a sequence $(f^n)_n$ in $L_\mu^{1,+}(\Omega)$ is such that there is a constant $c > 0$ with $f^n(x) \leq c f^\dagger(x)$ and $f^n(x) \rightarrow f^\dagger(x)$ for almost every $x \in \Omega$, then $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f^\dagger$. Also, $f \in L_\mu^{1,+}(\Omega)$ is isolated with respect to the $\mathcal{T}_{D_{KL}}$ topology if and only if $f \equiv 0$.

Proof. Note that if $D_{KL}(v, f) = \int_\Omega d(v(x), f(x)) d\mu(x) < \infty$, also $d(v(x), f(x)) < \infty$ μ a.e. and hence $v(x) = 0$ implies $f(x) = 0$. Therefore, in a μ a.e. sense $v_0(x) = 0$

implies $f^\dagger(x) = 0$ and $f^\dagger(x) = 0$ implies $f^n(x) = 0$ for n sufficiently large since both $D_{KL}(v_0, f^\dagger) < \infty$ and $D_{KL}(f^\dagger, f^n) < \infty$ for n sufficiently large.

For $a, b, c \in [0, \infty)$, such that $a = 0 \Rightarrow b = 0$ and $b = 0 \Rightarrow c = 0$, with the conventions concerning $d(a, b) = a - b - \ln(\frac{a}{b})$, we compute

$$\begin{aligned} d(a, c) - d(a, b) - d(b, c) &= -c \ln\left(\frac{a}{c}\right) + b \ln\left(\frac{a}{b}\right) + c \ln\left(\frac{b}{c}\right) \\ &= (\ln(a) - \ln(b))(b - c). \end{aligned} \quad (139)$$

Indeed, if $a > 0, b > 0, c > 0$ this is basic a computation with logarithms, in case $c = 0$ and a, b not, the first and last term vanish, leaving solely $b(\ln(a) - \ln(b))$ which is again correct. In case $a = 0$ or $b = 0$, also $b = c = 0$ holds, and thus obviously the equation holds with the values 0. Using linearity of integrals and (139),

$$\left| D_{KL}(v_0, f^n) - D_{KL}(v_0, f^\dagger) - D_{KL}(f^\dagger, f^n) \right| = \left| \int_{\{v_0 \neq 0, f^\dagger \neq 0\}} \ln\left(\frac{v_0}{f^\dagger}\right) (f^\dagger - f^n) d\mu \right|, \quad (140)$$

and since $D_{KL}(f^\dagger, f^n) \rightarrow 0$, the convergence of $D_{KL}(v_0, f^n)$ is equivalent to the stated integral's convergence.

Next we show that for a sequence $(f^n)_n$ with $f^n \leq cf^\dagger$ and $f^n \rightarrow f^\dagger$ point-wise μ almost everywhere, also $D_{KL}(v_0, f^\dagger) = \lim_{n \rightarrow \infty} D_{KL}(v_0, f^n)$ since then Lemma 5.7 implies convergence in $\mathcal{T}_{D_{KL}}$.

To show the convergence of $D(v_0, f^n)$, we may assume $D_{KL}(v_0, f^\dagger) < \infty$, as otherwise, the convergence is implied by lower semi-continuity in L_μ^1 as stated in Lemma 5.5. Thus we can apply the first statement of this theorem which reduces the proof to showing that the right side of (138) holds. Therefore, we consider

$$\int_{\{v_0 \neq 0, f^\dagger \neq 0\}} \ln\left(\frac{v_0}{f^\dagger}\right) (f^n - f^\dagger) d\mu = \int_{\{v_0 \neq 0, f^\dagger \neq 0\}} \chi_{\{f^\dagger \neq f^n\}} f^\dagger \ln\left(\frac{v_0}{f^\dagger}\right) \left(1 - \frac{f^n}{f^\dagger}\right) d\mu, \quad (141)$$

where in an almost everywhere sense $f^\dagger(x) = 0$ implies $f^n(x) = 0$ for n sufficiently large (independent of x) and therefore division by 0 does not occur. Furthermore, $f^\dagger \ln\left(\frac{v_0}{f^\dagger}\right) \in L_\mu^1(\Omega)$ since $D_{KL}(v_0, f^\dagger) < \infty$, and the function $\left|1 - \frac{f^n}{f^\dagger}\right| < c + 1$ and converges subsequentially point-wise μ a.e. towards 0. Hence, application of Lebesgue's Theorem ensures convergence of the integral on the right side of (141) towards 0. Thus, $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f$ due to Lemma 5.7.

In particular, for any $f \in L_\mu^{1,+}(\Omega)$ with f not constant zero, there is a sequence of

functions $(f^n)_n$ (e.g. $(1 + \frac{1}{n})f$) such that $f^n \xrightarrow{\mathcal{T}_{D_{KL}}} f$, so f is not isolated. On the other hand, $D_{KL}(0, f) = \infty$ for all $f \in L_\mu^{1,+}$ and therefore the only open neighbourhood of $f \equiv 0$ is $\{f \equiv 0\}$. \square

Remark 5.12. *Note that the conditions $f^n \leq cf^\dagger$ and point-wise convergence almost everywhere are sufficient conditions which can be verified more easily, but not necessarily an equivalent formulation of the convergence induced by the topology. However, the condition in (138) for convergence is close to an L_μ^∞ convergence of $\frac{f^n}{f^\dagger}$ towards constant 1, more precisely the condition appears similar to convergence in a topology pre-dual to L_μ^1 .*

Next, for $f^\dagger \in L_\mu^{1,+}$ we wish to identify a set $V \subset L_\mu^{1,+}(\Omega)$ and a function $\psi: [0, \infty) \rightarrow [0, \infty)$ such that the discrepancy D_{KL} is strongly ψ -continuous on V in f^\dagger , i.e. whether for $v_0 \in V$ a modulus of continuity estimate in f^\dagger holds.

Theorem 5.13. *Let $f^\dagger, v_0 \in L_\mu^{1,+}(\Omega)$ such that*

$$\ln\left(\frac{v_0}{f^\dagger}\right) \in L_\mu^\infty(\{f^\dagger \neq 0, v_0 \neq 0\}). \quad (142)$$

Then, for fixed $f^\delta \in L_\mu^1(\Omega)$ with $D_{KL}(f^\dagger, f^\delta) = \delta$ the following estimate holds:

$$|D_{KL}(v_0, f^\dagger) - D_{KL}(v_0, f^\delta)| \leq 2 \left\| \ln\left(\frac{v_0}{f^\dagger}\right) \right\|_{L_\mu^\infty(\{f^\dagger \neq 0, v_0 \neq 0\})} (\|f^\dagger\|_{L_\mu^1} + \|f^\delta\|_{L_\mu^1})^{\frac{1}{2}} \delta^{\frac{1}{2}} + \delta. \quad (143)$$

In particular, for constant $c_1 > 0$ and for

$$V = \left\{ v \in L_\mu^{1,+}(\Omega) \mid \ln\left(\frac{v}{f^\dagger}\right) < c_1 \right\} \quad (144)$$

there is constant $c > 1$ such that for $\psi: [0, \delta_0) \rightarrow [0, \infty)$ with $\psi(t) = ct^{\frac{1}{2}}$ the discrepancy D_{KL} is strongly ψ -continuous on V in f^\dagger . Here, δ_0 limits the noise, for which the modulus of continuity estimate is required to hold.

One gets the even slightly stronger statement that there is $c > 0$ such that for $f^\delta \in L_\mu^{1,+}(\Omega)$ with $D_{KL}(f^\dagger, f^\delta) = \delta < \delta_0$ and $v_0 \in V$ one obtains the estimate

$$|D_{KL}(v_0, f^\delta) - D_{KL}(v_0, f^\dagger)| \leq c\delta^{\frac{1}{2}}, \quad (145)$$

i.e. D_{KL} is locally Hölder-continuous in the $\mathcal{T}_{D_{KL}}$ topology.

Proof. Note that again $v_0(x) = 0$ implies $f^\dagger(x) = 0$ and $f^\dagger(x) = 0$ implies $f^\delta(x) = 0$ for

almost every $x \in \Omega$. Obviously, points $x \in \Omega$ with $f^\dagger(x) = f^\delta(x)$ do not contribute to the integrals defining the difference $D_{KL}(v_0, f^\dagger) - D_{KL}(v_0, f^\delta)$, and therefore the points x with $f^\dagger(x) = 0$ or $v_0(x) = 0$ do not have any impact on the following considerations. The estimate (140) implies

$$|D_{KL}(v_0, f^\dagger) - D_{KL}(v_0, f^\delta)| \leq \left\| \ln \left(\frac{v_0}{f^\dagger} \right) \right\|_{L^\infty(\{f^\dagger \neq 0, v_0 \neq 0\})} \|f^\delta - f^\dagger\|_{L^1_\mu(\Omega)} + \delta, \quad (146)$$

with $\delta = D_{KL}(f^\dagger, f^\delta)$. Furthermore, Lemma 5.3 implies $\|f^\dagger - f^\delta\|_{L^1_\mu(\Omega)}^2 \leq 2 \sup_\delta (\|f^\dagger\|_{L^1_\mu} + \|f^\delta\|_{L^1_\mu}) \delta$ yielding the desired estimate.

The strong ψ -continuity is an immediate consequence, as $\delta^{\frac{1}{2}}$ goes slower to 0 than δ , $\|f^\delta\|_{L^1_\mu}$ is uniformly bounded due to Lemma 5.4 and $\left\| \ln \left(\frac{v_0}{f^\dagger} \right) \right\|_\infty \leq c_1$ by assumption on v_0 , and as stated even a locally Hölder-continuity estimate holds. \square

5.4. Applicability as a Discrepancy

With these results in mind, we can propose suitable assumptions to use the Kullback-Leibler divergence as a discrepancy. The corresponding setting is summarised in the following problem, featuring the Kullback-Leibler divergence as discrepancy functions.

Problem 5.14. *Let (X, \mathcal{T}_X) , (Y_i, \mathcal{T}_{Y_i}) for $i \in \{1, \dots, M\}$ and $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ be Hausdorff spaces and let $T_i: \text{dom}(T_i) \subset X \rightarrow Y_i$ be continuous operators with respect to \mathcal{T}_X and \mathcal{T}_{Y_i} with closed domain. Moreover, let $J \subset \{1, \dots, M\}$ and for $j \in J$ let $(\Omega_j, \mathcal{A}_j, \mu_j)$ be a finite measure space and $(Y_j, \mathcal{T}_{Y_j}) = (L^1_{\mu_j}(\Omega_j), \mathcal{T}_{L^1_{\mu_j}(\Omega_j), W})$, and let $D_j: Y_j \times Y_j \rightarrow [0, \infty]$ be such that $D_j(v_j, f_j) = D_{KL}(v_j, f_j)$ as in Definition 5.1. Let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ for $i \in J^c$ be functions, let $\lambda \in (0, \infty)^M$ and let $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha: X \rightarrow [0, \infty]$ be a family of functions. We say u^\dagger is a solution to the Tikhonov regularisation (KL-MTIKH $_{\lambda, \alpha}(f^\dagger)$) with regards to $Tu = f^\dagger$ with discrepancies D_i , weights λ_i and regularisation R_α with parameter $\alpha \in \mathcal{A}$, if*

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda, \alpha}(u, f^\dagger) \text{ such that } F_{\lambda, \alpha}(u^\dagger, f^\dagger) < \infty \\ \text{with } F_{\lambda, \alpha}(u, f^\dagger) = \left(\sum_{j \in J} D_{KL}(T_j u, f_j^\dagger) \right) + \left(\sum_{i \in J^c} D_i(T_i u, f_i^\dagger) \right) + R_\alpha(u). \end{cases} \quad (\text{KL-MTIKH}_{\lambda, \alpha}(f^\dagger))$$

So this problem is a multi-data Tikhonov approach where Kullback-Leibler divergence discrepancies $D_j(v_j, f_j) = D_{KL}(v_j, f_j)$ are used. Strictly speaking one would require the notation for D_{KL} to also reflect the corresponding measure space, as its definition would depend on it. However, for the sake of readability, we will not use such notation as it

will be clear from context which space to use, and we implicitly use the D_{KL} functional fitting the arguments.

Assumptions 5.15 (Kullback-Leibler divergence). *Let $J \subset \{1, \dots, M\}$ be such that for $j \in J$, $D_j = D_{KL}$. Then for $j \in J$ let the following hold:*

KL Let $\mathcal{T}_{D_j} = \mathcal{T}_{D_{KL}}$ be the topology stated in Definition 5.6 for the respective space $L_{\mu_j}^1(\Omega_j)$. In particular, then for sequences $(f_j^n)_n \subset Y_j$ and $f_j^\dagger \in Y_j$

$$f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j^\dagger \quad \Rightarrow \quad \lim_{n \rightarrow \infty} D_{KL}(f_j, f_j^n) = D_{KL}(f_j, f_j^\dagger) \text{ for all } f_j \in L_{\mu_j}^{1,+}(\Omega_j). \quad (147)$$

We again use the product space notation $T = (T_1, \dots, T_M)$, $Y = Y_1 \times \dots \times Y_M$ with product topologies \mathcal{T}_Y and \mathcal{T}_D . Also, recall that $f_j^n \leq c f_j^\dagger$ and $f_j^n(x) \rightarrow f_j^\dagger(x)$ for μ almost all $x \in \Omega$ implies $f_j^n \xrightarrow{\mathcal{T}_{D_j}} f_j^\dagger$.

Proposition 5.16. *Let Assumptions 5.15 hold. Then, for $j \in J$ the function $D_j = D_{KL}$ is basic discrepancies, which is v_0 -continuous in f_j^\dagger for all $v_0, f_j^\dagger \in L_{\mu_j}^{1,+}(\Omega_j)$. Moreover, for $f_j^\dagger \in L_{\mu_j}^{1,+}(\Omega_j)$ the discrepancy D_j is strongly ψ_j -continuous on V_j in f_j^\dagger , where*

$$V_j = \left\{ v_j \in L_{\mu_j}^{1,+}(\Omega_j) \mid \ln \left(\frac{v_j}{f_j^\dagger} \right) < c_j \right\} \quad (148)$$

for any $c_j > 0$, and $\psi_j: [0, \delta_0) \rightarrow [0, \infty)$ is $\psi_j(t) = ct^{\frac{1}{2}}$ for some constant $c \geq 1$, more precisely $D_{KL}(v_j, \cdot)$ is even locally Hölder-continuous for $v_j \in V_j$.

Theorem 5.17. *This theorem summarises the theory of Part I for the specific problem $(KL-MTIKH_{\lambda,\alpha}(f^\dagger))$. We consider 3 statements, existence, convergence and rates:*

1. *Let the Assumptions 5.15 hold for $j \in J$ with $D_j(v_j, f_j) = D_{KL}(v_j, f_j)$. For $i \in J^c$, let $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ be a basic discrepancy function on Y_i with topologies \mathcal{T}_{Y_i} and \mathcal{T}_{D_i} . Further, let $(R_\alpha)_\alpha$ be a continuous family of functions, and with $\lambda = \mathbf{1}$ and some $\alpha = \alpha_0 \in \mathcal{A}$ let the Tikhonov functional*

$$F_{\mathbf{1},\alpha_0}(u, f) = \left(\sum_{j \in J} D_{KL}(T_j u, f_j) \right) + \left(\sum_{i \in J^c} D_i(T_i u, f_i) \right) + R_{\alpha_0}(u) \quad (149)$$

be uniformly coercive. Then, for $f^\dagger \in Y$ the Problem $(KL-MTIKH_{\lambda,\alpha}(f^\dagger))$ is either solvable or $F_{\lambda,\alpha}(\cdot, f^\dagger) \equiv \infty$.

2. Additionally to 1., let $I \subset \{1, \dots, M\}$, let a parameter choice rules as in Theorem 3.9 be applied, and let there be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution u_0 such that for $i \in J^c$ the discrepancy D_i is $T_i u_0$ -continuous in f_i^\dagger . Let a sequence $(f^\delta)_\delta \subset Y$ such that $f^\delta \xrightarrow{TR} f^\dagger$, and denote corresponding solutions to $(KL-MTIKH_{\lambda^\delta, \alpha^\delta}(f^\delta))$ by u^δ . Then, one obtains subsequential convergence of $(u^\delta)_\delta$ to $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solutions to $Tu = f^\dagger$.
3. Additionally to 1., 2., let X be a normed space and $(\mathcal{A}, d_{\mathcal{A}})$ be a metric space, and let u^\dagger be an $R_{\alpha^\dagger, \lambda^\dagger, I}$ -minimal I -partial solution to $Tu = f^\dagger$. For a sequence $(f^\delta)_\delta \in Y$ denote with $\delta = (\delta_1, \dots, \delta_M)$ and $D_i(f_i^\dagger, f_i^\delta) = \delta_i$. Let there be sets $U \subset X$ and $V_i \subset Y_i$ and functions $\psi_i, \psi_{R_{\alpha^\dagger}}$ for $i \in J^c$ such that for $i \in J^c$ the discrepancy D_i is strongly ψ_i -continuous on V_i in f^\dagger and the family $(R_\alpha)_\alpha$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on U in α^\dagger (modulus of continuity estimates hold on the discrepancies and regularisation). Furthermore, for $j \in J$ let V_j and ψ_j be as in Lemma 5.16, and let $u^\dagger, u^\delta \in U$ and $T_i u^\dagger, T_i u^\delta \in V_i$ for $i \in \{1, \dots, M\}$ and $\delta_i < \delta_0$ with some constant $\delta_0 > 0$. Let R_{α^\dagger} and $D_i(T_i \cdot, f_i^\dagger)$ be convex functions. Let there be constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that the following source condition holds: There is $\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ such that for u satisfying $R_{\alpha^\dagger, \lambda^\dagger, I}(u, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f_i^\dagger) \leq \epsilon_0$

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u, T_i u^\dagger), \quad (\text{SC3})$$

where in case $j \in J \cap I$, the function $\phi_j(T_j u, T_j u^\dagger) = \|T_j u - T_j u^\dagger\|_{L_\mu^1}$. Here, for $i \in I$, the function $\phi_i: Y_i \times Y_i \rightarrow [0, \infty]$ is such that for $v_i = Y_i$

$$\phi_i(v_i, f_i^\dagger) \leq \Phi_i(D_i(f_i^\dagger, f_i)) D_i(v_i, f_i) + \psi_i(D_i(f_i^\dagger, f_i)),$$

where $\Phi_i: [0, \infty] \rightarrow \mathbb{R}$ is such that $\Phi_i(\delta_i) \leq \frac{1}{4\gamma_2} \lambda_i^\delta$ for δ_i sufficiently small.

Then, there are constants $c > 0$ and $\bar{\delta} = (\bar{\delta}_1, \dots, \bar{\delta}_M)$ such that for $\delta < \bar{\delta}$ and $j \in I \cap J$

$$D_{KL}(T_j u^\delta, f_j^\delta) \leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \\ \left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right). \quad (150)$$

For $j \in I$:

$$D_j(T_j u^\delta, f_j^\delta) \leq c \left((\lambda_j^\delta)^{-1} \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \right. \quad (151)$$

$$\left. \left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right) \right),$$

$$D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) \leq c \left(\sum_{i \in I} (\lambda_i^\delta \delta_i + \psi_i(\delta_i)) \right. \quad (152)$$

$$\left. + \sum_{i \in I^c} (\psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta|) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right).$$

In particular, this constant c solely depends on $R_{\alpha^\dagger, \lambda^\dagger, f^\dagger}(u^\dagger, f^\dagger)$, γ_1 , γ_2 , c_j for $j \in J$ and $\bar{\delta}$, but not on the specific sequence $(f^\delta)_\delta$ or even $(\delta)_{\delta \in \Delta}$ and the general setting.

Proof. Application of Theorems 3.5, 3.9 and Theorem 3.21, whose assumptions are fulfilled due to Propositions 5.16 and the general setting. \square

Example 5.18. Let $M = 2$, let $(Y_1, \|\cdot\|_{Y_1})$ be a normed space and $Y_2 = L_\mu^{1,+}(\Omega)$ for $\Omega \subset \mathbb{R}$ bounded and μ the Lebesgue measure and $D_1(v_1, f_1) = \|v_1 - f_1\|_{Y_1}$ and $D_2(v_2, f_2) = D_{KL}(v_2, f_2)$. Let Assumptions 4.2 for $j = 1$ and Assumptions 5.15 for $j = 2$ hold and let $(R_\alpha)_\alpha$ be a strongly $\psi_{R_{\alpha^\dagger}}$ -continuous family of functions. Let $(f^\delta)_\delta \subset Y = Y_1 \times Y_2$ such that $D_i(f^\dagger, f^\delta) = \delta_i$ and let the sequence of solutions $(u^\delta)_\delta$ and u^\dagger concerning $(f^\delta)_\delta$ and f^\dagger . Let $u^\delta, u^\dagger \in U$ and $T_2 u^\dagger, T_2 u^\delta \in V_2$ with V_2 as in Proposition 5.16. Let the Source Condition (SC3) hold and the same requirements as in Theorem 5.17. For $I = \{2\}$, $\lambda_2^\delta = \delta_2^{\frac{1}{2}}$ and $|\lambda_1^\delta - \lambda_1^\dagger| = \delta_1$ one obtains the convergence rates

$$D_{KL}(T u, f^\delta) = O(\delta_2^{\frac{1}{2}}(\delta_2^{\frac{1}{2}} + \delta_1)), \quad D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) = O(\delta_2^{\frac{1}{2}} + \delta_1).$$

Note that the Kullback-Leibler divergence yields the same convergence as norm discrepancy with power $p_j = 2$. However, unlike in the norm case V_j is not the entire space and $T_j u^\delta \in V_j$ is a condition that can not be checked a-priori.

For the single-data case, we present an alternative source condition, solely dependent on u^\dagger . This different source condition in the single data case allows to avoid the need for sets V_j and corresponding conditions, and can be seen as a different approach using an other type of source conditions.

Theorem 5.19. Let $(X, \|\cdot\|_X)$ be a normed space, $T: X \rightarrow L_\mu^{1,+}(\Omega)$ be a linear continuous operator for a finite measure space $(\Omega, \mathcal{A}, \mu)$. Let $(f^\delta)_\delta \subset L_\mu^{1,+}(\Omega)$ and $f^\dagger \in L_\mu^{1,+}(\Omega)$

such that $f^\delta \xrightarrow{\mathcal{T}_{D_{KL}}} f^\dagger$. Further, let $f^\dagger \in \text{Rg}(T)$ and u^\dagger be an R -minimal solution. Let an $\xi \in X^*$ satisfy the source condition:

$$\text{there is } \omega \in L_\mu^\infty(\Omega) \text{ such that } T^*\omega = \xi \in \partial R(u^\dagger), \quad (\text{SC4})$$

where $T^*: L_\mu^\infty(\Omega) \rightarrow X^*$ denotes the adjoint operator of $T: X \rightarrow L_\mu^1(\Omega)$. Further, let $D_{KL}(Tu, f) + R(u)$ be uniformly coercive.

Choosing α such that $c\delta^{\frac{1}{2}} \leq \alpha(\delta) \leq C\delta^{\frac{1}{2}}$ for some constant $c, C > 0$ where $D_{KL}(f^\dagger, f^\delta) = \delta$ and denoting with u_α^δ solutions to

$$\underset{u \in X}{\text{argmin}} D_{KL}(Tu, f^\delta) + \alpha(\delta)R(u)$$

yields

$$D_R^\xi(u_\alpha^\delta, u^\dagger) = O(\delta^{\frac{1}{2}}), \text{ and } D_{KL}(Tu_\alpha^\delta, f^\delta) = O(\delta). \quad (153)$$

Proof. Similarly to the proof of Theorem 2.15, one obtains due to optimality and via rearranging

$$D_{KL}(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta - \alpha(\delta)\langle \xi, u_\alpha^\delta - u^\dagger \rangle_{X^* \times X}.$$

Since $\xi = T^*\omega$, one obtains

$$D_{KL}(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta - \alpha(\delta)\langle \omega, Tu_\alpha^\delta - f^\delta \rangle_{L^\infty \times L^1} + \alpha(\delta)\langle \omega, f^\dagger - f^\delta \rangle_{L^\infty \times L_\mu^1}. \quad (154)$$

Estimating the occurring dual pairings where c_{f^\dagger} denotes the constant such that $\|f - f^\dagger\|_{L_\mu^1}^2 \leq c_{f^\dagger} D_{KL}(f^\dagger, f)$ in Lemma 5.3, yields

$$\begin{aligned} \langle \omega, f^\delta - f \rangle_{L_\mu^\infty \times L_\mu^1} &\leq \|\omega\|_{L_\mu^\infty} \|f - f^\delta\|_{L_\mu^1} \leq \|\omega\|_{L_\mu^\infty} c_{f^\dagger} \sqrt{D_{KL}(f, f^\delta)} \leq c_{f^\dagger} \sqrt{\delta}, \\ |\alpha(\delta)\langle \omega, Tu_\alpha^\delta - f^\delta \rangle_{L_\mu^\infty \times L_\mu^1}| &\leq \alpha(\delta)\|\omega\|_{L_\mu^\infty} \|Tu_\alpha^\delta - f^\delta\|_{L_\mu^1} \stackrel{\text{Young}}{\leq} \alpha(\delta)^2 \frac{\|\omega\|_{L_\mu^\infty}^2}{\tilde{c}} + \tilde{c}\|Tu_\alpha^\delta - f^\delta\|_{L_\mu^1}^2 \\ &\leq \alpha(\delta)^2 \frac{\|\omega\|_{L_\mu^\infty}^2}{\tilde{c}} + c_{f^\dagger}^2 \tilde{c} D_{KL}(Tu_\alpha^\delta, f^\delta), \end{aligned}$$

and where $\tilde{c} > 0$ is arbitrary and Young's inequality was applied. Inserting these estimates into (154) yields

$$(1 - c_{f^\dagger}^2 \tilde{c}) D_{KL}(Tu_\alpha^\delta, f^\delta) + \alpha(\delta)D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta + \alpha(\delta)c_{f^\dagger} \delta^{\frac{1}{2}} + \alpha(\delta)^2 \frac{\|\omega\|_{L_\mu^\infty}^2}{\tilde{c}}, \quad (155)$$

which when choosing $\tilde{c} = \frac{c^2}{2}$ results in

$$c_1 D_{KL}(Tu_\alpha^\delta, f^\delta) + \alpha(\delta) D_R^\xi(u_\alpha^\delta, u^\dagger) \leq \delta + \alpha(\delta) c_2 \delta^{\frac{1}{2}} + \alpha(\delta)^2 c_3 \|\omega\|_{L^\infty}^2 \quad (156)$$

with $c_1, c_2, c_3 > 0$ suitable. The desired convergence estimates are an immediate consequence of this estimate when choosing $\alpha \approx \delta^{\frac{1}{2}}$. \square

Part III.

Regularisation Functionals

Although some requirements concerning the families of regularisation functionals $(R_\alpha)_\alpha$ were needed in the theory of Part I, we did not yet address how possible regularisations look like and this chapter tries to exemplarily answer this. The focus in the requirements of Part I lay more heavily on the discrepancy functionals D_i and those were addressed exemplarily in Part II. The family of regularisation functional $(R_\alpha)_{\alpha \in \mathcal{A}}$ is only required to be a continuous family of functions, i.e. $\mathcal{T}_X \times \mathcal{T}_\mathcal{A}$ -lower semi-continuous, continuous in $\mathcal{T}_\mathcal{A}$ and topologically equivalent $R_\alpha \leq c(\alpha, \beta)R_\beta$. Moreover, the function resulting as the sum of the discrepancies and the family of regularisation functionals must be uniformly coercive. Thus, a wide range of regularisation functionals is applicable, but typically the regularisation functionals are chosen in a way that penalises undesired properties so as to make solutions to the Tikhonov problems suitable. In this part we first motivate a general approach using norms of closed operators in Banach spaces, while afterwards we introduce Total Deformation (TD) and Total Generalised Variation (TGV) regularisation functionals which are commonly used in regularisation of imaging problems. They are known to penalise local fluctuation while allowing for jump discontinuities, and thus when used as regularisation preserve edges while reducing noise.

6. Regularisation with Norms and Closed Operators

In a normed space setting the norm is usually the measure of choice as it is easily applicable and is adapted to the linear structure. Thus it would also make sense to use a norm as a regularisation function when X has vector space structure. As the norm should be suitable to penalise undesired properties, such a norm might lie in a different space, and thus one considers the family $(R_\alpha(u))_{\alpha \in (0, \infty)}$ with $R_\alpha = \alpha \|Au\|$ for a linear operator A transporting into the suitable space and emphasising certain properties.

Problem 6.1. *Let $(X, \|\cdot\|_X)$ be a Banach space, let $(Y_i, \|\cdot\|_{Y_i})$ for $i \in \{1, \dots, M\}$ and $(U, \|\cdot\|_U)$ be normed spaces and let $T_i: X \rightarrow Y_i$ be linear and continuous with respect to the weak-weak topology and $T = (T_1, \dots, T_M)$. Further, let $A: \text{dom}(A) \subset X \rightarrow U^*$ be a linear operator where U^* denotes the dual space of U .*

For $\lambda \in (0, \infty)^M$, $\alpha \in (0, \infty)$ and $p_i \in [1, \infty)$, we consider the following Tikhonov

regularisation approach to $Tu = f^\dagger$ for $f^\dagger \in Y$:

$$\begin{cases} x^\dagger \in \min_{x \in X} F_{\lambda, \alpha}(x, f^\dagger), & \text{with} \\ F_{\lambda, \alpha}(x) = \sum_{i=1}^M \lambda_i \|T_i x - f_i^\dagger\|_{Y_i}^{p_i} + \alpha \|Ax\|_{U^*} \end{cases} \quad (\text{A-Tikh})$$

where regularisation is applied via the family $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha(x) = \alpha \|Ax\|_{U^*}$ and $\mathcal{A} = (0, \infty)$ equipped with the standard topology induced by $|\cdot|$. We consider the following topologies in context of this problem: we use weak topologies $\mathcal{T}_X = \mathcal{T}_{X, W}$, $\mathcal{T}_{Y_i} = \mathcal{T}_{Y_i, W}$, and \mathcal{T}_{D_i} is the topology induced by the norm in Y_i . Moreover, \mathcal{T}_Y and \mathcal{T}_D denote the respective product topologies.

In this chapter we will consider the situation described in Problem 6.1, and note that the stated topologies are natural for this setting.

Remark 6.2. One chooses A such that Ax highlights undesired properties in the U^* norm. Common choices for A are derivative operators in order to promote smoothness and penalise strong fluctuations.

Note that in this setting $D_i(v_i, f_i) = \|v_i - f_i\|_{Y_i}^{p_i}$ is a strongly continuous discrepancy on Y_i in all f_i^\dagger . Thus all potential requirements for the discrepancy terms are fulfilled, so we can focus on the regularisation functional. Also other discrepancy functions would be possible.

This chapter will in particular serve as a blueprint for application of other regularisation functionals, namely TD and TGV. Relevant questions are how such a functional fits into the theory of regularisers (in this specific linear setting), and what necessary assumptions might be.

Lemma 6.3. Let the setting in Problem 6.1 hold. Let $A: \text{dom}(A) \subset X \rightarrow U^*$ be weak-weak* closed. Then $x \mapsto \|Ax\|_{U^*}$ is \mathcal{T}_X -lower semi-continuous (i.e. weakly l.s.c.). Moreover, if A is injective, the mapping $A^{-1}: \text{Rg}(A) \rightarrow X$ is continuous with respect to the norm topologies, if and only if $\text{Rg}(A)$ is closed in the $\|\cdot\|_{U^*}$ topology.

Proof. We show lower semi-continuity by direct proof. Let $(x^n)_n \subset X$ be a sequence with $x^n \rightharpoonup x$, and we may further assume that Ax^n is bounded in U^* . Banach Alaoglu's Theorem implies $Ax^n \overset{*}{\rightharpoonup} \xi$ for some $\xi \in U^*$ subsequentially, and using closedness one obtains $Ax = \xi$ and thus $Ax^n \overset{*}{\rightharpoonup} Ax$. The norm $\|\cdot\|_{U^*}$ is a dual norm and thus lower semi-continuous with respect to the weak* topology on U^* , which yields $\|Ax\|_{U^*} \leq \liminf_n \|Ax^n\|_{U^*}$.

To show continuous invertibility of A in case $\text{Rg}(A)$ is closed, let $\text{Rg}(A)$ be closed, let a sequence $(y^n)_n \subset \text{Rg}(A)$ be such that $y^n \xrightarrow{*} y$, and let $(x^n)_n \subset X$ be such that $Ax^n = y^n$ and $x^n \rightharpoonup x$. By closedness of A , $x \in \text{dom}(A)$ and $Ax = y$ or looking at it conversely $y \in \text{dom}(A^{-1})$ and $A^{-1}y = x$. Hence, A^{-1} is a closed operator originating from a Banach space (since $\text{Rg}(A)$ is closed) and is thus continuous with respect to the respective norms due to the Closed Graph Theorem.

Conversely, if A^{-1} was continuous, then for a sequence $(y^n)_n \subset \text{Rg}(A)$ with $y^n \rightarrow y$ in $\|\cdot\|_{U^*}$, the sequence $(x^n)_n$ in X with $x^n = A^{-1}y^n$ would be a Cauchy sequence in X , and thus closedness would imply $y = Ax \in \text{Rg}(A)$ and consequently $\text{Rg}(A)$ would be closed. \square

Corollary 6.4. *Let the assumptions in Lemma 6.3 hold. Then, the family of functions $(R_\alpha)_{\alpha \in (0, \infty)}$ with $R_\alpha(x) = \alpha \|Ax\|_{U^*}$ is a continuous family of functions (i.e. $(x, \alpha) \mapsto R_\alpha(x)$ is $\mathcal{T}_X \times \mathcal{T}_\mathcal{A}$ -lower semi-continuous, $\alpha \mapsto R_\alpha(x)$ is continuous and there is a constant $c(\alpha, \beta)$ such that $R_\alpha(x) \leq c(\alpha, \beta)R_\beta(x)$ for any x , see Definition 3.2).*

Proof. In order to show continuity of the family $(R_\alpha)_{\alpha \in (0, \infty)}$, note that $\mathcal{A} = (0, \infty)$ with the standard $|\cdot|$ topology is a Hausdorff space. Moreover, $(x, \alpha) \mapsto R_\alpha(x)$ is $\mathcal{T}_X \times \mathcal{T}_\mathcal{A}$ -lower semi-continuous as $\|Ax\|_{U^*}$ is \mathcal{T}_X -lower semi-continuous and multiplication with non-negative numbers is monotone and continuous. For $\alpha, \beta \in \mathcal{A}$, $R_\alpha(x) = \frac{\alpha}{\beta}R_\beta(x)$ for all $x \in X$, so $c(\alpha, \beta) = \frac{\alpha}{\beta}$ which remains bounded for $\alpha \rightarrow \alpha^\dagger \in (0, \infty)$ and in particular $R_\alpha(x) \rightarrow R_{\alpha^\dagger}(x)$ for all $x \in X$ holds. \square

Lemma 6.5. *Let the assumptions from Lemma 6.3 hold. Let $(X, \|\cdot\|_X)$ be a reflexive Banach space. Let linear $A: X \rightarrow U^*$ be a weak-weak*-closed operator with closed range and finite-dimensional kernel and let $T_i: X \rightarrow Y_i$ be continuous with respect to $\mathcal{T}_{X, W}$ and $\mathcal{T}_{Y_i, W}$ and linear with $T = (T_1, \dots, T_M)$ such that $\text{Ker}(T) \cap \text{Ker}(A) = \{0\}$. Then the functional $F_{1,1}$ in Problem 6.1 is uniformly coercive with respect to the weak topology on X and the \mathcal{T}_D topology on Y , i.e. for $(f^n)_n \subset Y$ with $f^n \xrightarrow{\mathcal{T}_D} f^\dagger$ and for any constant $C > 0$, the set $\bigcup_{n=1}^\infty \left\{x \in X \mid F_{1,1}(x, f^n) < C\right\}$ is \mathcal{T}_X -precompact.*

Proof. We aim at using Banach-Alaoglu's Theorem to show precompactness with respect to the weak topology. Thus we first show that for a sequence $(f^n)_n \subset Y$ with $f^n \xrightarrow{\mathcal{T}_D} f^\dagger$ and $C > 0$, a sequence $(x^n)_n \subset X$ with $F_{1,1}(x^n, f^n) < C$ is bounded in $\|\cdot\|_X$.

Since $\text{Ker}(A)$ is finite-dimensional, there is a projection $P: X \rightarrow \text{Ker}(A)$ and consequently we use the representation $x = Px + (id - P)x = v + w$. Let a sequence $(x^n)_n = (v^n)_n + (w^n)_n \subset X$ with $C \geq \|Ax^n\|_{U^*}$. Due to the continuity of $A^{-1}: \text{Rg}(A) \rightarrow$

$(id - P)(U^*)$ established in Lemma 6.3, also $C \geq \|Aw^n\|_{U^*} \geq c\|w^n\|_X$ and thus we see that w^n is bounded in $\|\cdot\|_X$. So it remains to show that also v^n is bounded. Since $T = (T_1, \dots, T_M)$ is injective and continuous on $\text{Ker}(A)$, T is continuously invertible on $T(\text{Ker}(A))$ onto $\text{Ker}(A)$ by finite-dimensionality. As $C \geq \|T(v^n + w^n) - f^n\|_Y \geq \|Tv^n\|_Y - \|Tw^n - f^n\|_Y$ where $\|f\|_Y = \sum \|f_i\|_{Y_i}$, the boundedness of Tv^n implies boundedness of v^n , and therefore also x^n is bounded in $\|\cdot\|_X$. Due to the Banach-Alaoglu Theorem $(x^n)_n$ admits a weak convergent subsequence thus confirming the coercivity claim. \square

Remark 6.6. *We note that the condition $\text{Ker}(T) \cap \text{Ker}(A) = \{0\}$ is a technical one which can always be satisfied by considering a suitable factor space since factorising with respect to this kernel does not alter the function values, completeness or reflexivity.*

Corollary 6.7. *Let the assumptions of Lemma 6.5 hold. Let for $i \in \{1, \dots, M\}$ the functions $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ be basic discrepancies with respect to $\mathcal{T}_Y = \mathcal{T}_{Y,W}$ and a topology \mathcal{T}_D . We consider*

$$\left\{ x^\dagger \in \min_{x \in X} \tilde{F}_\lambda, \alpha(x, f^\dagger). \quad \text{with} \quad \tilde{F}_{\lambda, \alpha}(x) = \sum_{i=1}^M \lambda_i D_i(T_i x, f_i^\dagger) + \alpha \|Ax\|_{U^*}. \right.$$

Further, let D_i be such that for a sequence $(f^n)_n$ in Y with $f^n \xrightarrow{\mathcal{T}_D} f$, the estimate

$$D_i(v, f_i^n) \geq \phi_{(f^n)_n}(\|v - f_i^n\|_{Y_i}) \tag{157}$$

holds, where the function $\phi_{(f^n)_n}: [0, \infty] \rightarrow [0, \infty]$ is coercive and continuous in 0 with $\phi_{(f^n)_n}(0) = 0$. Then $\tilde{F}_{1,1}$ is uniformly coercive with respect to \mathcal{T}_X and \mathcal{T}_D .

This simply means that the coercivity statement extends when using discrepancies which are coercive with respect to the norm topologies.

7. Total Deformation

Many inverse problems are posed on function spaces like $L^p(\Omega)$ spaces with the standard Lebesgue measure, and regularisation functionals are used to promote smoothness in a suitable sense. Using the previous chapter, one could consider regularisation by penalising the norm of a derivative operator (these are typically closed and have closed range in the correct setting). Using Sobolev spaces and the corresponding derivative operators for regularisation is quite common, although not always suitable. These Sobolev approaches typically lead to smooth solutions, which do not allow for jump discontinuities.

But, in imaging and other scientific fields, one would expect hard transitions and jump discontinuities from solutions, and thus these Sobolev approaches might not be ideal. Hence, we introduce the Total Deformation, which works similarly in a slightly different functional analytic setting in order to allow jump discontinuities while still penalising fluctuating functions.

7.1. Symmetric Tensor Fields

Before we can start with the actual definition of the Total Deformation, we need to introduce and investigate suitable spaces and operations to build upon. Spaces of multilinear functions will serve as this foundation, since derivatives can also be understood to be multilinear operations, leading to a consistent and elegant notion of differentiation.

Definition 7.1. For $d \in \mathbb{N}$ and $k \in \mathbb{N}_0$, a function $\xi: \underbrace{\mathbb{R}^d \times \dots \times \mathbb{R}^d}_{k \text{ times}} \rightarrow \mathbb{R}$ is called multilinear, if for $\tilde{a}, a_1, \dots, a_k \in \mathbb{R}^d$ and $\lambda \in \mathbb{R}$,

$$\begin{aligned} \xi(a_1, \dots, a_{i-1}, a_i + \lambda \tilde{a}, a_{i+1}, \dots, a_k) &= \xi(a_1, \dots, a_{i-1}, a_i, a_{i+1}, \dots, a_k) \\ &\quad + \lambda \xi(a_1, \dots, a_{i-1}, \tilde{a}, a_{i+1}, \dots, a_k), \end{aligned}$$

where for $k = 0$, ξ is a real number. Moreover, ξ is called symmetric if for any permutation $\sigma: \{1, 2, \dots, k\} \rightarrow \{1, 2, \dots, k\}$ (i.e. σ bijective. We also say $\sigma \in S_k$),

$$\xi(a_1, a_2, \dots, a_k) = \xi(a_{\sigma_1}, a_{\sigma_2}, \dots, a_{\sigma_k}).$$

Furthermore, we denote by

$$\begin{aligned} \mathcal{T}^{k,d} &= \left\{ \xi: \underbrace{\mathbb{R}^d \times \dots \times \mathbb{R}^d}_{k \text{ times}} \rightarrow \mathbb{R} \mid \xi \text{ is multilinear} \right\}, \\ \text{Sym}^{k,d} &= \left\{ \xi \in \mathcal{T}^{k,d} \mid \xi \text{ is symmetric} \right\}, \end{aligned}$$

the spaces of multilinear functions and symmetric multilinear functions respectively.

In the following we will always assume k and d to be suitable and will not further comment on them unless there is relevance to their properties.

Remark 7.2. When endowing the space $\mathcal{T}^{k,d}$ with the standard algebra for function spaces, i.e. point-wise addition and point-wise multiplication with scalars, the resulting structure is a finite-dimensional vector space. A basis of $\mathcal{T}^{k,d}$ is given by considering for

$p \in \{1, \dots, d\}^k$ the corresponding multilinear forms e_p with $e_p(a_1, \dots, a_k) = \prod a_{i,p_i}$, and in particular the space $\mathcal{T}^{k,d}$ has the dimension d^k . Also, the space $\text{Sym}^{k,d}$ is a subspace of $\mathcal{T}^{k,d}$ when equipped with the same algebraic operations.

Due to their specific structure, these spaces can further be equipped with natural operations to combine multilinear forms and to compute products or norm of multilinear forms.

Definition 7.3. For $k, l \geq 0$, we define

$$\otimes: \mathcal{T}^{k,d} \times \mathcal{T}^{l,d} \rightarrow \mathcal{T}^{l+k,d} \quad \text{with} \quad \xi \otimes \eta(a_1, \dots, a_{k+l}) = \xi(a_1, \dots, a_k) \eta(a_{k+1}, \dots, a_{k+l}),$$

for $a_1, \dots, a_{k+l} \in \mathbb{R}^d$ and $\xi \in \mathcal{T}^{k,d}$, $\eta \in \mathcal{T}^{l,d}$. We define the trace of multilinear forms with $k \geq 2$ as

$$\text{tr}: \mathcal{T}^{k,d} \rightarrow \mathcal{T}^{k-2,d} \quad \text{with} \quad \text{tr}(\xi)(a_1, \dots, a_{k-2}) = \sum_{i=1}^d \xi(e_i, a_1, \dots, a_{k-2}, e_i), \quad (158)$$

where e_i denotes the i -th standard unit vector in \mathbb{R}^d . Further, we define for $\xi, \eta \in \mathcal{T}^{k,d}$ the inner product

$$\xi \cdot \eta = \text{tr}^k(\bar{\xi} \otimes \eta) = \sum_{i_1=1}^d \sum_{i_2=1}^d \cdots \sum_{i_k=1}^d \xi(e_{i_1}, \dots, e_{i_k}) \eta(e_{i_1}, \dots, e_{i_k}), \quad (159)$$

where $\text{tr}^k = \text{tr} \circ \text{tr}^{k-1}$ is the trace operation iterated k times, and the multilinear form $\bar{\xi}$ satisfies $\bar{\xi}(a_1, \dots, a_k) = \xi(a_k, a_{k-1}, \dots, a_1)$, i.e. is the multilinear form with switched order of arguments.

It is an easy exercise to verify that these definitions induce a finite-dimensional Hilbert space $\mathcal{T}^{k,d}$. In particular, this allows us to find a suitable projection onto $\text{Sym}^{k,d}$ and thus we are also able to find a basis for $\text{Sym}^{k,d}$.

Proposition 7.4. We define the linear symmetrisation operation $|||: \mathcal{T}^{k,d} \rightarrow \text{Sym}^{k,d}$, such that for $\xi \in \mathcal{T}^{k,d}$

$$|||\xi(a_1, \dots, a_k) = \frac{1}{k!} \sum_{\sigma \in S_k} \xi(a_{\sigma_1}, \dots, a_{\sigma_k}) \quad (160)$$

for $a_1, \dots, a_k \in \mathbb{R}^d$. Then $|||$ is well defined and is the orthogonal projection onto $\text{Sym}^{k,d}$ in $\mathcal{T}^{k,d}$.

Proof. We do the proof in two steps, first we show that application of the symmetrisation operation yields a symmetric multilinear form, and afterwards we compute that it is indeed a projection.

Well-defined: Indeed, for a multilinear form $\xi \in \mathcal{T}^{k,d}$, a permutation $\pi \in S_k$ and vectors $a_1, \dots, a_k \in \mathbb{R}^d$, one sees

$$\begin{aligned} |||\xi(a_{\pi_1}, \dots, a_{\pi_k}) &= \frac{1}{k!} \sum_{\sigma \in S_k} \xi(a_{\pi(\sigma_1)}, \dots, a_{\pi(\sigma_k)}) = \frac{1}{k!} \sum_{\tilde{\sigma} \in S_k} \xi(a_{\tilde{\sigma}_1}, \dots, a_{\tilde{\sigma}_k}) \\ &= |||\xi(a_1, \dots, a_k), \end{aligned}$$

where we transformed $\sigma \mapsto \tilde{\sigma}$ on S_k bijectively by $\tilde{\sigma} = \pi \circ \sigma$, and therefore $|||\xi \in \text{Sym}^{k,d}$ and the operation $|||$ is well-defined. Moreover, that $|||$ is linear follows immediately from its definition.

Projection: Obviously, for $\xi \in \text{Sym}^{k,d}$, $|||\xi = \xi$ since the summands in the definition of the operation do not depend on σ , and there are $k!$ summands. Also, for $\xi \in \text{Sym}^{k,d}$ and $\eta \in \mathcal{T}^{k,d}$, we compute

$$\begin{aligned} \xi \cdot (|||\eta) &= \sum_{i_1=1, \dots, i_k=1}^d (\xi(e_{i_1}, \dots, e_{i_k}) |||\eta(e_{i_1}, \dots, e_{i_k})) \\ &= \sum_{i_1=1, \dots, i_k=1}^d (\xi(e_{i_1}, \dots, e_{i_k}) \frac{1}{k!} \sum_{\sigma \in S_k} \eta(e_{\sigma(i_1)}, \dots, e_{\sigma(i_k)})) \\ &\stackrel{\text{Sym.}}{=} \frac{1}{k!} \sum_{\sigma \in S_k} \sum_{i_1=1, \dots, i_k=1}^d \xi(e_{\sigma(i_1)}, \dots, e_{\sigma(i_k)}) \eta(e_{\sigma(i_1)}, \dots, e_{\sigma(i_k)}) = \frac{1}{k!} \sum_{\sigma \in S_k} \xi \cdot \eta = \xi \cdot \eta. \end{aligned}$$

Thus the inner product is invariant under application of $|||$ for $\xi \in \text{Sym}^{k,d}$, and consequently $|||$ is an orthogonal projection with respect to this inner product. \square

From this proposition, it is easy to find a basis of $\text{Sym}^{k,d}$ as the symmetrisation of the basis of $\mathcal{T}^{k,d}$.

Proposition 7.5. *We consider the mapping $\sigma: \{1, \dots, d\}^k \rightarrow \{\beta \in \mathbb{N}_0^d \mid |\beta| = k\}$ such that $\sigma(p)_i = |\{j \in \{1, \dots, k\} \mid p_j = i\}|$ for $p \in \{1, \dots, d\}^k$. The set*

$$\{e_\beta = k! |||e_p \mid p \in \{1, \dots, d\}^k, \beta = \sigma(p)\} \quad (161)$$

is an orthonormal basis of $\text{Sym}^{k,d}$.

This allows for a different interpretation and notation on $\text{Sym}^{k,d}$. Since every $\xi \in \text{Sym}^{k,d}$ is the linear combination of the basis-vectors, we define the corresponding basis representation indexed by multiindices $\beta \in \mathbb{N}_0^d$ with $|\beta| = k$ such that

$$\xi = \sum_{\beta \in \mathbb{N}_0^d, |\beta|=k} \xi_\beta e_\beta, \quad (162)$$

where the corresponding coefficients for $\beta = \sigma(p)$ are $\xi_\beta = \xi(e_{p_1}, \dots, e_{p_k}) \in \mathbb{R}$. With this new notation, some operations can be rewritten in a more compact manner as depicted in the following corollary.

Corollary 7.6. *The operators introduced in Definition 7.3, can be described in the multiindices notation as follows: For $\xi \in \text{Sym}^{k,d}$, $\eta \in \text{Sym}^{l,d}$, and $\alpha, \beta, \gamma \in \mathbb{N}_0^d$ with $|\beta| = k, |\gamma| = l, |\alpha| = k - l$,*

$$(\xi \otimes \eta)_{(\beta,\gamma)} = \xi_\beta \eta_\gamma, \quad \text{tr}^l(\xi \otimes \eta)_\alpha = \sum_{\gamma \in \mathbb{N}_0^d, |\gamma|=l} \frac{l!}{\gamma!} \xi_{\alpha+\gamma} \eta_\gamma \quad (163)$$

Proof. Straight forward computation. □

Now that we have a deeper understanding of the space $\text{Sym}^{k,d}$, we wish to use it as a basis for the definition of $\text{Sym}^{k,d}$ -valued function spaces. In this context, we note that with the basis representation, one could understand the following as functions onto \mathbb{R}^N for some $N > 0$, but we use this specific structure as it will allow a more elegant definition of derivative operations.

Definition 7.7. *Let Ω be a bounded Lipschitz domain equipped with the standard Lebesgue measure, and equip $\text{Sym}^{k,d}$ with the Borel algebra corresponding to its Hilbert space topology. For $p \in [1, \infty]$ the spaces $L^p(\Omega, \text{Sym}^{k,d})$ are defined analogously to Definition 1.25 as spaces of functions integrable to the p -th power, i.e*

$$L^p(\Omega, \text{Sym}^{k,d}) = \left\{ \xi: \Omega \rightarrow \text{Sym}^{k,d} \mid \xi \text{ measurable, } \|\xi\|_p < \infty \right\}, \quad \text{with} \quad (164)$$

$$\|\xi\|_p = \left(\int_{\Omega} |\xi(x)|^p dx \right)^{\frac{1}{p}} \text{ for } 1 \leq p < \infty, \quad \text{and} \quad \|\xi\|_\infty = \text{ess-sup}_{x \in \Omega} |\xi(x)|,$$

where $|\xi| = (\xi \cdot \xi)^{\frac{1}{2}}$. Furthermore, $\mathcal{C}(\Omega, \text{Sym}^{k,d})$ denotes the $\text{Sym}^{k,d}$ -valued functions that are continuous with respect to the topology induced by the norm on $\text{Sym}^{k,d}$ and is

equipped with the supremum norm. Moreover,

$$\mathcal{C}_c(\bar{\Omega}, \text{Sym}^{k,d}) = \{f \in \mathcal{C}(\Omega, \text{Sym}^{k,d}) \mid \text{support of } \xi \text{ is compact in } \Omega\}, \quad (165)$$

and $\mathcal{C}_0(\Omega, \text{Sym}^{k,d})$ denotes its closure with respect to $\|\cdot\|_\infty$. The space of $\text{Sym}^{k,d}$ -valued, signed Radon measures is denoted by $\mathcal{M}(\Omega, \text{Sym}^{k,d})$.

In the following we will assume that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain equipped with Borel algebra and the Lebesgue measure.

Knowing the dual space of a normed space gives more insight into said space, and recall that for $p, p^* \in [1, \infty)$ and $\frac{1}{p} + \frac{1}{p^*} = 1$ isometric bijections $(L^p)^* \cong L^{p^*}$ and $(\mathcal{C}_0)^* \cong \mathcal{M}$ exist for classical function onto \mathbb{R} . Analogue results hold for $\text{Sym}^{k,d}$ -valued functions as depicted in the following proposition.

Proposition 7.8. *Let $p \in [1, \infty)$ and p^* be such that $\frac{1}{p} + \frac{1}{p^*} = 1$ with $p^* = \infty$ for $p = 1$. Then, the dual space of $L^p(\Omega, \text{Sym}^{k,d})$ and $\mathcal{C}_0(\Omega, \text{Sym}^{k,d})$ satisfy the isometric bijections $(L^p(\Omega, \text{Sym}^{k,d}))^* \cong L^{p^*}(\Omega, \text{Sym}^{k,d})$ and $(\mathcal{C}_0(\Omega, \text{Sym}^{k,d}))^* \cong \mathcal{M}(\Omega, \text{Sym}^{k,d})$. Moreover, the corresponding dual pairings for $\rho \in L^p(\Omega, \text{Sym}^{k,d})$, $\eta \in L^{p^*}(\Omega, \text{Sym}^{k,d})$, $\xi \in \mathcal{C}_0(\Omega, \text{Sym}^{k,d})$ and $\mu = \lambda|\mu| \in \mathcal{M}(\Omega, \text{Sym}^{k,d})$ are defined via*

$$\langle \eta, \rho \rangle_{L^{p^*}, L^p} = \int_{\Omega} \eta \cdot \rho \, dx \quad \text{and} \quad \langle \mu, \xi \rangle_{\mathcal{M}, \mathcal{C}_0} = \int_{\Omega} \xi(x) \, d\mu(x) = \int_{\Omega} \xi(x) \cdot \lambda(x) \, d|\mu|(x),$$

where \cdot denotes the inner product on $\text{Sym}^{k,d}$ and $\lambda: \Omega \rightarrow \text{Sym}^{k,d}$ is the density of μ with respect to $|\mu|$ and is in particular $|\mu|$ measurable. Recall, the semi variation measure is

$$|\mu| = \sup \left\{ \sum_{i=1}^N |\mu(B_i)| \mid B_1, \dots, B_N \subset \Omega \text{ measurable, } \bigcup_{i=1}^N B_i = \Omega, B_i \cap B_j = \emptyset \text{ for } i \neq j \right\}.$$

Next, we want to consider a notion of differentiability to such spaces, which are adapted to this specific structure.

Definition 7.9. *We call $\xi \in \mathcal{C}(\bar{\Omega}, \text{Sym}^{k,d})$ differentiable if the coefficient ξ_β is differentiable for all multiindices $\beta \in \mathbb{N}_0^d$ with $|\beta| = k$. We then define for $a_1, \dots, a_{k+1} \in \mathbb{R}^d$,*

$$\begin{aligned} \nabla \otimes \xi(x)(a_1, \dots, a_{k+1}) &= [D\xi(x)(a_1)](a_2, \dots, a_{k+1}) = \sum_{i=1}^d a_{1,i} \frac{\partial \xi}{\partial x_i}(a_2, \dots, a_{k+1}) \\ \xi \otimes \nabla(x)(a_1, \dots, a_{k+1}) &= [D\xi(x)(a_{k+1})](a_1, \dots, a_k), \end{aligned}$$

where $D\xi(x) \in \mathcal{L}(\mathbb{R}^d, \text{Sym}^{k,d})$ denotes the derivative of ξ . In particular, $\frac{\partial \xi(a_2, \dots, a_{k+1})}{\partial x_i}$ can be computed via standard analysis in \mathbb{R} , and thus one can use the coefficient representation to compute $[D\xi_\beta(x)(e_i)] = [(D\xi(x))_\beta(e_i)]$.

With this definition of differentiability we can introduce spaces of differentiable functions of higher order, and on those define the differential operations \mathcal{E} and div and their iterates.

Definition 7.10. *We define*

$$\mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k,d}) = \left\{ \xi \in \mathcal{C}(\bar{\Omega}, \text{Sym}^{k,d}) \mid \xi \text{ differentiable and } \nabla \otimes \xi \in \mathcal{C}(\bar{\Omega}, \mathcal{T}^{k+1,d}) \right\}.$$

The space $\mathcal{C}^l(\bar{\Omega}, \text{Sym}^{k,d})$ for $l \in \mathbb{N}$ with $l \geq 2$ is then defined inductively as

$$\mathcal{C}^l(\bar{\Omega}, \text{Sym}^{k,d}) = \left\{ \xi \in \mathcal{C}^{l-1}(\bar{\Omega}, \text{Sym}^{k,d}) \mid \nabla^{l-1} \otimes \xi \text{ differentiable and } \nabla^l \otimes \xi \in \mathcal{C}(\bar{\Omega}, \mathcal{T}^{k+l,d}) \right\},$$

where $\nabla^l \otimes \xi = \nabla \otimes (\nabla^{l-1} \otimes \xi)$ denotes the iterated derivation operation. Furthermore, we define the symmetrised derivative \mathcal{E} for $k \geq 0$, via

$$\mathcal{E}: \mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k,d}) \rightarrow \mathcal{C}(\bar{\Omega}, \text{Sym}^{k+1,d}) \quad \text{such that} \quad \mathcal{E}\xi = |||(\nabla \otimes \xi) = |||(\xi \otimes \nabla)$$

for $\xi \in \mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k,d})$, which unlike $\nabla \otimes \xi$ is again symmetric. We further define the divergence operator for $k \geq 1$ via

$$\text{div}: \mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k,d}) \rightarrow \mathcal{C}(\bar{\Omega}, \text{Sym}^{k-1,d}), \quad \text{such that} \quad \text{div} \xi = \text{tr}(\nabla \otimes \xi).$$

In particular, for multiindices $\beta \in \mathbb{N}_0^d$ such that $|\beta| = k - 1$ and $a_1, \dots, a_{k-1} \in \mathbb{R}^d$, one computes

$$\text{div} \xi_\beta = \sum_{i=1}^d \frac{\partial \xi_{\beta+e_i}}{\partial x_i} \quad \text{and} \quad \text{div} \xi(a_1, \dots, a_{k-1}) = \sum_{j=1}^d \frac{\partial \xi}{\partial x_j}(a_1, \dots, a_{k-1}, e_j).$$

We illustrate with small examples how these technical definitions play out in relevant situations, i.e., how occurring operations and spaces look like.

Example 7.11. *For $k = 0, 1, 2$ the corresponding spaces $\text{Sym}^{k,d}$ are*

$$\text{Sym}^{0,d} \cong \mathbb{R}, \quad \text{Sym}^{1,d} \cong \mathbb{R}^d \quad \text{and} \quad \text{Sym}^{2,d} \cong \{A \in \mathbb{R}^{d \times d} \mid A \text{ is symmetric} \}.$$

So for $k = 0$ the space of symmetric multilinear forms contains reals, for $k = 1$ it contains vectors, and for $k = 2$ the elements correspond to symmetric matrices. In particular when interpreting this in the multiindices notation for $d = 2$ one obtains for $u \in \text{Sym}^{0,2}$, $\xi \in \text{Sym}^{1,2}$ and $\eta \in \text{Sym}^{2,2}$, that

$$u \approx u_{0,0}, \quad \xi \approx \begin{pmatrix} \xi_{1,0} \\ \xi_{0,1} \end{pmatrix} \approx \begin{pmatrix} \xi_x \\ \xi_y \end{pmatrix}, \quad \text{and} \quad \eta \approx \begin{pmatrix} \eta_{2,0} & \eta_{1,1} \\ \eta_{1,1} & \eta_{0,2} \end{pmatrix} \approx \begin{pmatrix} \eta_{xx} & \eta_{xy} \\ \eta_{xy} & \eta_{yy} \end{pmatrix}.$$

When computing the corresponding differential operators, and denoting with x, y the respective axes, one sees

$$\begin{aligned} \mathcal{E}u &\approx \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{pmatrix} = \nabla u, & \mathcal{E}\xi &\approx \begin{pmatrix} \frac{\partial \xi_{1,0}}{\partial x} & \frac{1}{2} \left(\frac{\partial \xi_{1,0}}{\partial y} + \frac{\partial \xi_{0,1}}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial \xi_{1,0}}{\partial y} + \frac{\partial \xi_{0,1}}{\partial x} \right) & \frac{\partial \xi_{0,1}}{\partial y} \end{pmatrix}, \\ \text{div } \xi &\approx \frac{\partial \xi_{1,0}}{\partial x} + \frac{\partial \xi_{0,1}}{\partial y}, & \text{div } \eta &\approx \begin{pmatrix} \frac{\partial \eta_{2,0}}{\partial x} + \frac{\partial \eta_{1,1}}{\partial y} \\ \frac{\partial \eta_{0,2}}{\partial y} + \frac{\partial \eta_{1,1}}{\partial x} \end{pmatrix}. \end{aligned}$$

So we see that indeed these operations workout analogously to their well-known counterparts in classical analysis. In particular, for a symmetric matrix, its divergence is simply the classical divergence applied to its rows and the symmetrised derivative of a vector is the symmetrised Jacobian matrix.

We see that this notion of differentiability is similar to the classical one when interpreted in the correct way, and hence one would expect many of the properties of classical derivatives to remain valid in this setting.

Proposition 7.12 (see [12]). *If $u \in \mathcal{C}^{k+1}(\Omega, \text{Sym}^{k,d})$ satisfies $\mathcal{E}u = 0$, then also $\nabla^{k+1} \otimes u = 0$. If additionally Ω is a domain, then u is a $\text{Sym}^{k,d}$ -valued polynomial, i.e. there are $A_l \in \text{Sym}^{l,d} \otimes \text{Sym}^{k,d}$ for $l = 0, \dots, k$, such that for $x \in \Omega$ and $y_1, \dots, y_k \in \mathbb{R}^d$,*

$$u(x)(y_1, \dots, y_k) = \sum_{l=0}^k A_l(\underbrace{x, \dots, x}_{l \text{ times}}, y_1, \dots, y_k) = \sum_{l=0}^k \sum_{|\beta|=l} A_{l\beta}(y_1, \dots, y_k) x^\beta.$$

In classical analysis the operators $-\nabla$ and div are adjoint operators given suitable boundary conditions, as can be observed via a divergence theorem. Similarly, we show a divergence theorem for multilinear forms.

Lemma 7.13 (see [14]). *Let $\xi \in \mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k+1,d})$ and $\eta \in \mathcal{C}^1(\bar{\Omega}, \text{Sym}^{k,d})$ with Ω a*

bounded Lipschitz domain. Then the following integration by parts formula holds:

$$\int_{\Omega} \operatorname{div} \xi \cdot \eta \, dx = \int_{\partial\Omega} \xi \cdot \llbracket (\eta \otimes \nu) \, d\mathcal{H}^{d-1} - \int_{\Omega} \xi \mathcal{E} \eta \, dx, \quad (166)$$

where ν denotes the outer normal vector and \mathcal{H}^{d-1} denotes the $(d-1)$ -dimensional Hausdorff measure.

Proof. Using the multiindices notation, we apply the standard integration by parts formula for real-valued functions resulting in

$$\begin{aligned} \int_{\Omega} \operatorname{div} \xi \cdot \eta \, dx &= \int_{\Omega} \operatorname{tr}^k ((\operatorname{div} \xi) \otimes \eta) = \int_{\Omega} \operatorname{tr}^k \left(\sum_{i=1}^d \frac{\partial \xi}{\partial x_i} (\cdot, \dots, \cdot, e_i) \otimes \eta \right) dx \\ &= \int_{\Omega} \sum_{i=1}^d \sum_{\beta \in \mathbb{N}_0^d, |\beta|=k} \frac{k!}{\beta!} \frac{\partial \xi_{\beta+e_i}}{\partial x_i} \eta_{\beta} \, dx \\ &\stackrel{\text{Integration by parts}}{=} \sum_{i=1}^d \sum_{\beta \in \mathbb{N}_0^d, |\beta|=k} \frac{k!}{\beta!} \left(\int_{\partial\Omega} \xi_{\beta+e_i} \eta_{\beta} \nu_i \, d\mathcal{H}^{d-1} - \int_{\Omega} \xi_{\beta+e_i} \frac{\partial \eta_{\beta}}{\partial x_i} \, dx \right) \\ &= \sum_{i=1}^d \sum_{\beta \in \mathbb{N}_0^d, |\beta|=k} \frac{k!}{\beta!} \left(\int_{\partial\Omega} \xi_{\beta+e_i} (\eta \otimes \nu)_{\beta, e_i} \, d\mathcal{H}^{d-1} - \int_{\Omega} \xi_{\beta+e_i} (\nabla \otimes \eta)_{e_i, \beta} \, dx \right) \\ &= \int_{\partial\Omega} \xi \cdot (\eta \otimes \nu) \, d\mathcal{H}^{d-1} - \int_{\Omega} \xi \cdot (\nabla \otimes \eta) \, dx \\ &= \int_{\partial\Omega} \xi \cdot \llbracket (\eta \otimes \nu) \, d\mathcal{H}^{d-1} - \int_{\Omega} \xi \cdot \llbracket (\nabla \otimes \eta) \, dx, \end{aligned}$$

where the last equality holds due to the symmetrisation being an orthogonal projection and ξ being symmetric. \square

Note that again under suitable boundary conditions, this divergence formula implies that $-\mathcal{E}$ is adjoint to div . In particular, on $\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k,d})$ the duality $-\mathcal{E}^* = \operatorname{div}$ holds and consequently we can obtain a distributional symmetric derivative operator from the operation div on \mathcal{C}_c^{∞} .

Definition 7.14. We define the distributional symmetrised derivative operator \mathcal{E} via

$$\begin{aligned} \mathcal{E} : (\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k,d}))^* &\rightarrow (\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k+1,d}))^* \quad \text{with} \\ \mathcal{E} T(\phi) &= -T(\operatorname{div} \phi), \quad \text{for } \phi \in \mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k+1,d}), \quad T \in (\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k,d}))^* \end{aligned} \quad (167)$$

where div denotes the divergence operation defined for continuously differentiable functions.

In the following we will use this distributional symmetric derivative operator as the closed operator for regularisation as in Chapter 6, thus introducing Total Deformation.

7.2. Tensor Fields of Bounded Deformation

With these technicalities out of the way, we can define Total Deformation with the help of continuous functions on $\operatorname{Sym}^{k,d}$. As motivated before, the Total Deformation is the norm of a derivative operator, however, we start with the more commonly used variational definition.

Definition 7.15. *Let Ω be a bounded Lipschitz domain, let $k \geq 0$ and $d \geq 1$. For a function $u \in L^1(\Omega, \operatorname{Sym}^{k,d})$ the Total Deformation of u is*

$$\operatorname{TD}(u) = \sup \left\{ \int_{\Omega} u \cdot \operatorname{div} \psi \, dx \mid \psi \in \mathcal{C}_c^1(\Omega, \operatorname{Sym}^{k+1,d}) \text{ with } \|\psi\|_{\infty} \leq 1 \right\}. \quad (168)$$

Moreover, we say $u \in L^1(\Omega, \operatorname{Sym}^{k,d})$ has bounded deformation if $\operatorname{TD}(u) < \infty$, and denote by

$$\operatorname{BD}(\Omega, \operatorname{Sym}^{k,d}) = \left\{ u \in L^1(\Omega, \operatorname{Sym}^{k,d}) \mid \operatorname{TD}(u) < \infty \right\} \quad (169)$$

the set of functions with bounded deformation. We equip $\operatorname{BD}(\Omega, \operatorname{Sym}^{k,d})$ with the norm $\|u\|_{\operatorname{BD}} = \|u\|_{L^1} + \operatorname{TD}(u)$.

This variational definition is indeed equivalent to the norm of the derivative operator \mathcal{E} in the space of Radon measures as can be seen in the following Lemma.

Lemma 7.16. *Let $u \in L^1(\Omega, \operatorname{Sym}^{k,d})$. Then $u \in \operatorname{BD}(\Omega, \operatorname{Sym}^{k,d})$ holds, if and only if $\mathcal{E} u \in (\mathcal{C}_0(\Omega, \operatorname{Sym}^{k+1,d}))^* \cong \mathcal{M}(\Omega, \operatorname{Sym}^{k+1,d})$, and in this case $\operatorname{TD}(u) = \|\mathcal{E} u\|_{\mathcal{M}(\Omega, \operatorname{Sym}^{k+1,d})}$ holds.*

Proof. For $u \in \operatorname{BD}(\Omega, \operatorname{Sym}^{k,d})$, the distributional derivative $\mathcal{E} u$ is linear and continuous on $\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k,d})$ by definition. Also, $\mathcal{E} u$ is continuous with respect to the supremum norm $\|\cdot\|_{\infty}$ on $\mathcal{C}_c^{\infty}(\Omega, \operatorname{Sym}^{k,d})$, as

$$\mathcal{E} u(\phi) = \int_{\Omega} u \cdot \operatorname{div} \phi \, dx \leq \operatorname{TD}(u) \|\phi\|_{\infty} < \infty. \quad (170)$$

Hence, by density $\mathcal{E} u$ can be uniquely extended to a function $\tilde{\mathcal{E}} u \in \left(\mathcal{C}_0(\Omega, \text{Sym}^{k+1,d})\right)^*$, and by the Riesz Theorem $\mathcal{E} u$ possesses a representation as a Radon measure. In particular, by definition of the dual norm we obtain $\|\mathcal{E} u\|_{\mathcal{M}(\Omega, \text{Sym}^{k+1,d})} = \text{TD}(u)$.

Conversely, if $\mathcal{E} u \in \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$, then

$$\left| \int_{\Omega} u \cdot \text{div} \phi \, dx \right| = \left| \int_{\Omega} \phi \, d_{\mathcal{E} u}(x) \right| \leq \|\mathcal{E} u\|_{\mathcal{M}} \|\phi\|_{\infty}, \quad (171)$$

which implies $\text{TD}(u) < \infty$. □

Remark 7.17. *We recall that in the motivation in chapter 6 the operator A used as regularisation was required to be weak-weak* closed, to have finite-dimensional kernel and closed range. Thus in the following we investigate these topological properties of \mathcal{E} .*

The operator A being closed was an important tool for the theory of Section 6 which raises the question whether \mathcal{E} is closed. The following lemma answers this closedness question for $\mathcal{E}: \text{dom}(\mathcal{E}) \subset L^1(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$.

Lemma 7.18. *The distributional symmetric derivation operator $\mathcal{E}: \text{BD}(\Omega, \text{Sym}^{k,d}) \subset L^1(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$ is weak-weak* closed, i.e. if a sequence $(u_n)_{n \in \mathbb{N}}$ in $L^1(\Omega, \text{Sym}^{k,d})$ satisfies $u_n \xrightarrow{\mathcal{T}_{L^1}} u$ for $u \in L^1(\Omega, \text{Sym}^{k,d})$, and $\mathcal{E} u_n \xrightarrow{*} \eta$ in $\mathcal{M}(\Omega, \text{Sym}^{k+1,d})$, then $\mathcal{E} u = \eta$.*

Proof. Due to weak* convergence, for $\psi \in \mathcal{C}_c^1(\Omega, \text{Sym}^{k+1,d})$

$$\mathcal{E} u_n(\psi) = \int_{\Omega} \psi \, d_{\mathcal{E} u_n} \rightarrow \int_{\Omega} \psi \, d_{\eta} = \eta(\psi), \quad (172)$$

and due to weak L^1 convergence and $\text{div} \psi$ being bounded,

$$\text{div} \psi(u_n) = \int_{\Omega} u_n \cdot \text{div} \psi \, dx \rightarrow \int_{\Omega} u \cdot \text{div} \psi \, dx = \text{div} \psi(u). \quad (173)$$

By definition of \mathcal{E} , this results in

$$\int_{\Omega} \psi \, d_{\mathcal{E} u} \stackrel{\text{per def.}}{=} \int_{\Omega} u \cdot \text{div} \psi \, dx = \int_{\Omega} \psi \, d_{\eta}, \quad (174)$$

and by uniqueness of such a measure, $\mathcal{E} u = \eta$. □

Proposition 7.19. *The space $\text{BD}(\Omega, \text{Sym}^{k,d})$ is complete.*

Indeed, since both $L^1(\Omega, \text{Sym}^{k,d})$ and $\mathcal{M}(\Omega, \text{Sym}^{k+1,d})$ are Banach spaces and the symmetric differentiation operator $\mathcal{E}: \text{BD}(\Omega, \text{Sym}^{k,d}) \subset L^1(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$ is closed, $\text{BD}(\Omega, \text{Sym}^{k,d})$ is complete as well.

Proposition 7.20. *Let $\mathcal{E}: \text{BD}(\Omega, \text{Sym}^{k,d}) \subset L^1(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$ and let $\mathcal{A} = (0, \infty)$ and $\mathcal{T}_{\mathcal{A}}$ be the standard $|\cdot|$ topology on \mathcal{A} . Then the family $(R_{\alpha})_{\alpha \in \mathcal{A}}$ with $R_{\alpha}(u) = \alpha \|\mathcal{E}u\|_{\mathcal{M}} = \alpha \text{TD}(u)$ is a continuous family of functions.*

Moreover, this family is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on $\text{BD}(\Omega, \text{Sym}^{k,d})$ in any $\alpha^\dagger \in \mathcal{A}$ with $\psi_{R_{\alpha^\dagger}}(t) = t$.

Proof. Apply Corollary 6.4 with \mathcal{E} as the linear closed operator A , which is closed due to Lemma 7.18. The strong continuity claim is obviously fulfilled. \square

Recall that the only other requirement on R_{α} was that it ensures coercivity of the Tikhonov functional. When using norm discrepancies and a linear setting, we showed in Section 6 that this coercivity holds if X is reflexive and \mathcal{E} has closed range and finite kernel.

However, $X = L^1(\Omega, \text{Sym}^{k,d})$ is not reflexive, and we avoid this difficulty by switching to other L^p spaces thanks to the following embedding theorem.

Theorem 7.21 (see [12]). *For a bounded Lipschitz domain Ω , there is a continuous embedding*

$$\text{BD}(\Omega, \text{Sym}^{l,d}) \hookrightarrow L^{d/(d-1)}(\Omega, \text{Sym}^{l,d}), \quad (175)$$

as well as a compact embedding for $1 \leq p < d/(d-1)$, such that

$$\text{BD}(\Omega, \text{Sym}^{l,d}) \hookrightarrow L^p(\Omega, \text{Sym}^{l,d}), \quad (176)$$

where in case $d = 1$ we understand $\frac{d}{d-1} = \infty$.

In particular, we can consider $(X, \mathcal{T}_X) = (L^p(\Omega, \text{Sym}^{l,d}), \mathcal{T}_{L^p, W})$ for $1 < p < \frac{d}{d-1}$ instead of L^1 , which is reflexive and has a topology stronger than weak L^1 , so all continuity statements remain valid.

It is left to show that $\text{Rg}(\mathcal{E})$ is closed in $\mathcal{M}(\Omega, \text{Sym}^{k+1,d})$ and has finite kernel, and consequently \mathcal{E} is continuously invertible in a suitable setting.

Theorem 7.22 (see [12]). *Let Ω be a bounded Lipschitz domain. The kernel of the operation $\mathcal{E}: L^d(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k,d})$ is a finite-dimensional subspace, and thus there is a continuous projection from $L^{(d/d-1)}$ onto $\text{Ker}(\mathcal{E})$. Furthermore, for any such*

projection $P: L^{d/(d-1)}(\Omega, \text{Sym}^{k,d}) \rightarrow \text{Ker}(\mathcal{E})$, there is a constant $c > 0$ such that for $u \in \text{BD}(\Omega, \text{Sym}^{k,d})$

$$\|u - Pu\|_{d/(d-1)} \leq c \|\mathcal{E}u\|_{\mathcal{M}}. \quad (177)$$

Remark 7.23. Hence \mathcal{E} is continuously invertible on $\text{Rg}(\mathcal{E})$ (modulo finite-dimensional kernel).

Proposition 7.24. Let Ω be a bounded Lipschitz domain, let $(Y, \|\cdot\|_Y)$ be a normed space and let for some $1 < p \leq \frac{d}{d-1}$ the operation $T: L^p(\Omega, \text{Sym}^{k,d}) \rightarrow Y$ be linear and continuous with respect to the respective weak topologies. Then the function $F_{1,1}: L^p(\Omega, \text{Sym}^{k,d}) \times Y \rightarrow [0, \infty]$ with $F_{1,1}(u, f) = \|Tu - f\|_Y^q + \text{TD}(u)$ is uniformly coercive with respect to the topologies $\mathcal{T}_{L^p, W}$ and the norm topology on Y . In fact, for $1 \leq p < \frac{d}{d-1}$ the uniform coercivity also holds for the L^p norm topology instead of the weak topology on L^p .

Proof. Lemma 6.5 applied to this situation with $A = \mathcal{E}: \text{BD}(\Omega, \text{Sym}^{k,d}) \subset L^p(\Omega, \text{Sym}^{k,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k+1,d})$, whose assumptions on the operator A are fulfilled due to previous statements in this section. In the case $p < \frac{d}{d-1}$, we can apply the compact embedding instead of the continuous one, and thus get precompactness of the level set with respect to the L^p norm topology. \square

When starting the theory of TD, we aimed at obtaining a regularisation that penalises non-smoothness but allows for jump-discontinuities. The following examples show that we succeeded in doing so.

Example 7.25. Let $\Omega' \subset \Omega \subset \mathbb{R}^2$ be a Lipschitz domain such that Ω' has positive distance to the boundary of Ω . We consider the function $u = \mathcal{I}_{\Omega'}$ with $\mathcal{I}_{\Omega'}(x) = 1$ if $x \in \Omega'$ and 0 otherwise. We can compute for $\phi \in \mathcal{C}_c^\infty(\Omega, \text{Sym}^{1,2})$ that

$$\int_{\Omega} u \cdot \text{div} \phi \, dx = \int_{\Omega} \mathcal{I}_{\Omega'} \cdot \text{div} \phi \, dx = \int_{\Omega'} \text{div} \phi \, dx = \int_{\partial\Omega'} \phi \cdot \nu \, d\mathcal{H}^1 = \int_{\Omega} \phi \, d\mathcal{E}u.$$

Consequently $\mathcal{E}u = \nu \mathcal{H}^1$ where \mathcal{H}^1 denotes the Hausdorff measure on $\partial\Omega'$, which is not a function but in $\mathcal{M}(\Omega, \mathbb{R}^2)$. So we see that $u \in \text{BD}(\Omega, \text{Sym}^{0,2})$ and in particular $\text{TD}(u) = \|\mathcal{E}u\|_{\mathcal{M}} = \int_{\partial\Omega'} 1 \, d\mathcal{H}^1$, so jump discontinuities are allowed, and will be penalised by TD corresponding to the height and the perimeter of the jump.

Example 7.26. We consider functions over $\Omega = [-1, 1] \subset \mathbb{R}$ for the sake of simplicity, and note that similar principles can be applied for higher space-dimensions. Let

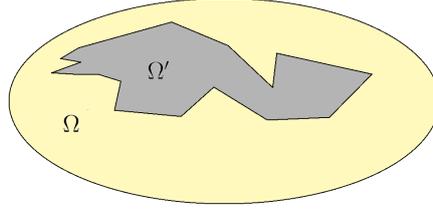


Figure 1: Exemplary illustration of Ω, Ω' in Example 7.25.

$u, v: \Omega \rightarrow \mathbb{R}$ be such that

$$u(x) = \begin{cases} -0.5 & \text{for } -1 \leq x \leq -0.5, \\ x & \text{for } -0.5 \leq x \leq 0.5, \\ 0.5 & \text{for } 0.5 \leq x \leq 1. \end{cases} \quad v(x) = \begin{cases} -0.5 & \text{for } -1 \leq x \leq 0, \\ 0.5 & \text{for } 0 < x \leq 1. \end{cases} \quad (178)$$

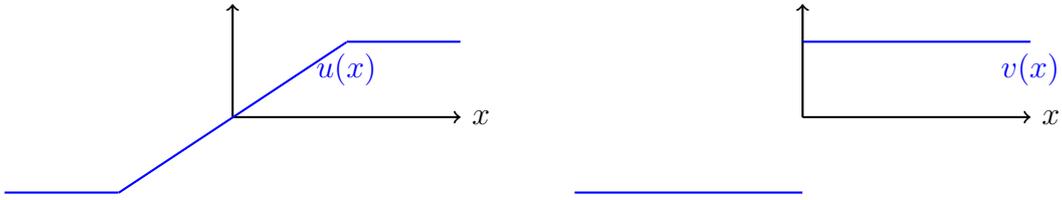


Figure 2: Illustration of functions u, v in Example 7.26.

It is easy to compute that $\text{TD}(u) = 1 < \infty$ and in particular the contribution to TD made on $(-0.5, 0.5)$ is 1 which is the raising in the segment $[-0.5, 0.5]$. When instead considering the Heaviside function v the same contribution 1 is made and thus $\text{TD}(v) = 1$. Indeed any monotonically increasing function w on $[-1, 1]$ with Dirichlet boundary conditions $w(-1) = -0.5, w(1) = 0.5$ (same as u or v) will lead to $\text{TD}(w) = 1$.

In particular, there is no function w with the same Dirichlet boundary conditions on $(-1, 1)$ that would have $\text{TD}(w) < 1$, and a function w which is not monotonically increasing would have $\text{TD}(w) > 1$, i.e. a higher deformation value.

Remark 7.27. The previous examples show how the TD functional penalises local fluctuations and jump discontinuities. In particular, when fixing the value of u on the right and left endpoint with the value 0, the only function attaining $\text{TD}(u) = 0$ is the constant zero-function.

Hence, one expects when using TD as a regulariser, that solutions are piece-wise constant in order to flatten fluctuations otherwise increasing the TD functional. This indeed allows for hard transitions, however one has to wonder whether piece-wise constant solutions are indeed desirable and suit the application.

8. Total Generalised Variation

In many applications such as imaging, one would like a regularisation method which does not solely promote piece-wise constant solutions, but also piece-wise polynomials of higher order. Often, approximating functions with piece-wise polynomials becomes more suitable for higher orders polynomials, and thus piece-wise polynomial solutions appear more natural. Therefore, we introduce Total Generalised Variation (TGV), a functional based on TD which is capable of promoting piece-wise polynomial solutions while maintaining the jump-discontinuity properties of the Total Deformation.

8.1. Basic Properties

In order to find such a regularisation method we generalise the variational definition of TD. We again assume throughout the chapter that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain.

Definition 8.1. *Let $l \in \mathbb{N}_0$, $k \in \mathbb{N}$ and weights $\alpha = (\alpha_0, \dots, \alpha_{k-1}) \in (0, \infty)^k$. Then we define the Total Generalised Variation for $u \in L^1(\Omega, \text{Sym}^{l,d})$, as*

$$\text{TGV}_\alpha^k(u) = \sup \left\{ \int_\Omega u \cdot \text{div}^k \phi \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d}) \right. \quad (179)$$

$$\left. \text{with } \|\text{div}^j \phi\|_\infty \leq \alpha_j \text{ for } j \in \{0, \dots, k-1\} \right\}.$$

Furthermore, we consider the space and norm

$$\text{BGV}_\alpha^k(\Omega, \text{Sym}^{l,d}) = \{u \in L^1(\Omega, \text{Sym}^{l,d}) \mid \text{TGV}_\alpha^k(u) < \infty\},$$

$$\text{with } \|u\|_{\text{BGV}_\alpha^k} = \|u\|_{L^1} + \text{TGV}_\alpha^k(u) \quad \text{for } u \in \text{BGV}_\alpha^k(\Omega, \text{Sym}^{l,d}).$$

We will in the following assume α , k and l to be appropriate as in Definition 8.1, and Ω to be a bounded Lipschitz domain and will not further comment on them.

Lemma 8.2. *Let $\alpha, \beta \in (0, \infty)^k$. Then $\text{BGV}_\alpha^k(\Omega, \text{Sym}^{l,d}) = \text{BGV}_\beta^k(\Omega, \text{Sym}^{l,d})$, and there is a constant $c(\alpha, \beta)$ such that for $u \in \text{BGV}_\alpha^k(\Omega, \text{Sym}^{l,d})$, the estimate $\text{TGV}_\alpha^k(u) \leq$*

$c(\alpha, \beta) \text{TGV}_\beta^k(u)$ is satisfied. In particular, for $\alpha^n \rightarrow \alpha^\dagger$ the constant $c(\alpha^n, \beta)$ remains bounded.

Proof. Let the set of admissible ϕ in (179) be denoted by $S(\alpha)$ and denote by $\bar{\alpha} = \max_{i=0, \dots, k-1} \alpha_i$ and $\underline{\alpha} = \min_{i=0, \dots, k-1} \alpha_i$ and analogously for β .

$$\text{TGV}_\alpha^k(u) = \sup_{\phi \in S(\alpha)} \int_{\Omega} u \cdot \text{div} \phi \, dx = \frac{\bar{\alpha}}{\underline{\beta}} \sup_{\phi \in S(\frac{\bar{\alpha}}{\underline{\beta}})^{-1}} \int_{\Omega} u \cdot \text{div} \phi \, dx \leq \frac{\bar{\alpha}}{\underline{\beta}} \text{TGV}_\beta^k(u), \quad (180)$$

where we used that $S(\alpha(\frac{\bar{\alpha}}{\underline{\beta}})^{-1}) \subset S(\beta)$. \square

Remark 8.3. We see that the set BGV_α^k and its topology does not depend on α , and therefore we will in the following omit the α and simply talk about BGV^k .

We start by showing some basic analytic properties of TGV_α^k and BGV^k which will later be relevant.

Lemma 8.4. *The following hold:*

1. TGV_α^k is a semi-norm on BGV^k , and $\|\cdot\|_{\text{BGV}_\alpha^k}$ is indeed a norm on $\text{BGV}^k(\Omega, \text{Sym}^{l,d})$.
2. The function $\text{TGV}_\alpha^k: L^1(\Omega, \text{Sym}^{l,d}) \rightarrow \mathbb{R}^\infty$ is lower semi-continuous with respect to the L^1 norm topology.
3. The normed space $(\text{BGV}^k, \|\cdot\|_{\text{BGV}_\alpha^k})$ is complete.

Proof. That TGV_α^k is a semi-norm follows from straight forward computation. Indeed, for $u, v \in \text{BGV}^k(\Omega, \text{Sym}^{l,d})$ and $\beta \in \mathbb{R}$, when choosing $\phi = 0$ in the supremum defining TGV_α^k we see $\text{TGV}_\alpha^k(u) \geq 0$, and $|\beta| \text{TGV}_\alpha^k(u) = \text{TGV}_\alpha^k(\beta u)$ as the set $S(\alpha)$ over which the supremum is taken satisfies $S(\alpha) = -S(\alpha)$ and due to the linearity of the integral. Also, due to the standard computation rules for suprema and the linearity $\int_{\Omega} (u+v) \text{div}^k \psi \, dx = \int_{\Omega} u \text{div}^k \psi \, dx + \int_{\Omega} v \text{div}^k \psi \, dx$, the triangle inequality holds. It follows immediately that $\|\cdot\|_{\text{BGV}_\alpha^k}$ is a norm.

To show lower semi-continuity, for fixed $\phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d})$ we consider the mapping

$$T_\phi: L^1(\Omega, \text{Sym}^{l,d}) \rightarrow \mathbb{R} \quad \text{with} \quad T_\phi u = \int_{\Omega} u \cdot \text{div}^k \phi \, dx \quad \text{for } u \in L^1(\Omega, \text{Sym}^{l,d}).$$

Since $\text{div}^k \phi \in L^\infty(\Omega, \text{Sym}^{l,d}) = \left(L^1(\Omega, \text{Sym}^{l,d})\right)^*$, T_ϕ is continuous with respect to the L^1 topology. Because the supremum of continuous functions is lower semi-continuous, also the function TGV_α^k is lower semi-continuous.

To prove completeness, consider a Cauchy sequence $(u_n)_{n \in \mathbb{N}}$ in $\text{BGV}^k(\Omega, \text{Sym}^{l,d})$ with respect to the $\|\cdot\|_{\text{BGV}^k}$ norm, i.e. for $m > n$, $\|u_n - u_m\|_{\text{BGV}^k} < \epsilon_n$ for a sequence $(\epsilon_n)_n$ in $(0, \infty)$ with $\epsilon_n \rightarrow 0$. Therefore u_n is a Cauchy sequence in L^1 , and hence there is $u \in L^1(\Omega, \text{Sym}^{l,d})$ such that $\|u_n - u\|_{L^1} \rightarrow 0$, and also $\text{TGV}_\alpha^k(u_n - u_m) \leq \epsilon_n$ for $m > n$. By lower semi-continuity, $\text{TGV}_\alpha^k(u_n - u) \leq \liminf_m \text{TGV}_\alpha^k(u_n - u_m) < \epsilon_n$, and therefore $\lim_{n \rightarrow \infty} \|u_n - u\|_{\text{BGV}^k} = 0$ implying completeness. \square

Next, we aim to show an equivalent representation of TGV, as an infimal convolution which allows for a different interpretation and more concrete application. In order to do so, we first need a simple lemma.

Lemma 8.5. *For $j \in \mathbb{N}_0$ let $w_j \in \mathcal{C}_0^j(\Omega, \text{Sym}^{l+j,d})$. Then*

$$\|\mathcal{E} w_{j-1} - w_j\|_{\mathcal{M}} = \sup \left\{ \langle w_{j-1}, \text{div } \phi \rangle + \langle w_j, \phi \rangle \mid \phi \in \mathcal{C}_c^j(\Omega, \text{Sym}^{l+j,d}) \text{ with } \|\phi\|_\infty \leq 1 \right\}. \quad (181)$$

In particular, $\mathcal{E} w_{j-1} - w_j \in \mathcal{M}(\Omega, \text{Sym}^{l+j,d})$ if and only if the supremum is finite.

Proof. It is well known that for a dense subset $U \subset V$ of a normed space $(V, \|\cdot\|_V)$, one can continuously extend a linear continuous functional $f: U \rightarrow \mathbb{R}$ to a functional $F \in V^*$, if and only if

$$\sup_{\substack{\phi \in U \\ \|\phi\|_V \leq 1}} \langle f, \phi \rangle < \infty.$$

With this in mind, note that the subspace $\mathcal{C}_c^\infty(\Omega, \text{Sym}^{j+l,d}) \subset \mathcal{C}_c^j(\Omega, \text{Sym}^{j+l,d})$ is dense in $\mathcal{C}_0(\Omega, \text{Sym}^{l+j,d})$, and hence, $\mathcal{E} w_{j-1} - w_j$ can be continuously extended onto $\mathcal{C}_0(\Omega, \text{Sym}^{l+j,d})$, if and only if

$$\sup_{\substack{\phi \in \mathcal{C}_c^\infty(\Omega, \text{Sym}^{l+j,d}) \\ \|\phi\|_\infty \leq 1}} (\langle \mathcal{E} w_{j-1} - w_j, \phi \rangle) = \sup_{\substack{\phi \in \mathcal{C}_c^\infty(\Omega, \text{Sym}^{l+j,d}) \\ \|\phi\|_\infty \leq 1}} (\langle w_j, \phi \rangle + \langle w_{j-1}, \text{div } \phi \rangle) < \infty. \quad (182)$$

Therefore $\mathcal{E} w_{j-1} - w_j$ is continuous on $\mathcal{C}_0(\Omega, \text{Sym}^{l+j,d})$ with respect to $\|\cdot\|_\infty$, i.e. by duality $\mathcal{E} w_{j-1} - w_j \in \mathcal{M}(\Omega, \text{Sym}^{l+j,d})$, if and only if the supremum in (181) is finite. The alternative formulation of the norm as the supremum follows from (182). \square

Theorem 8.6 (see [14]). *For $u \in \text{BGV}^k(\Omega, \text{Sym}^{l,d})$, TGV_α^k is equivalently defined via*

$$\text{TGV}_\alpha^k(u) = \inf \left\{ \sum_{j=1}^k \alpha_{k-j} \|w_j - \mathcal{E} w_{j-1}\|_{\mathcal{M}} \right. \\ \left. \mid w_j \in \text{BD}(\Omega, \text{Sym}^{l+j,d}) \text{ for } j = 0, 1, \dots, k, \text{ with } w_0 = u, w_k = 0 \right\}. \quad (183)$$

In particular, $u \in \text{BGV}^k(\Omega, \text{Sym}^{l,d})$ if and only if the infimum is finite and $\text{BD}(\Omega, \text{Sym}^{l,d}) = \text{BGV}^k(\Omega, \text{Sym}^{l,d})$. In case $\text{TGV}_\alpha^k(u) < \infty$, the minimum in (183) is attained for some w_1, \dots, w_{k-1} .

Proof. Let $u \in L^1(\Omega, \text{Sym}^{l,d})$ with $\text{TGV}_\alpha^k(u) < \infty$. We aim to reformulate TGV_α^k in a way, that enables us to use duality arguments. We consider the product spaces

$$\begin{aligned} X &= \mathcal{C}_0^1(\Omega, \text{Sym}^{l+1,d}) \times \dots \times \mathcal{C}_0^k(\Omega, \text{Sym}^{l+k,d}), \\ Y &= \mathcal{C}_0^1(\Omega, \text{Sym}^{l+1,d}) \times \dots \times \mathcal{C}_0^{k-1}(\Omega, \text{Sym}^{l+k-1,d}). \end{aligned}$$

On those, we define

$$F: X \rightarrow \mathbb{R}^\infty \quad \text{such that} \quad v \mapsto -\langle u, \text{div } v_1 \rangle + \sum_{j=1}^k \chi_{\{\|\cdot\|_\infty \leq \alpha_{k-j}\}}(v_j), \quad (184)$$

where v_j denotes the j -th projection of v ,

$$G: Y \rightarrow \mathbb{R}^\infty \quad \text{such that} \quad w \mapsto \chi_{(0,\dots,0)}(w), \quad (185)$$

and the linear and continuous function

$$\Lambda: X \rightarrow Y, \quad \text{with} \quad (\Lambda v)_j = -v_j - \text{div } v_{j+1}. \quad (186)$$

Then one can rewrite

$$\text{TGV}_\alpha^k(u) = \sup_{v \in X} -F(v) - G(\Lambda v). \quad (187)$$

Indeed, in this equation, v_j represents $\text{div}^{k-j} \phi (-1)^{k-j}$ in the definition of TGV_α^k when understanding $v_k = \phi$, since the characteristic function in $G \circ \Lambda$ enforces $\text{div } v_j = -v_{j-1}$ and in particular $\text{div } v_1 = (-1)^k \text{div}^k \phi$. Finally, the characteristic function in F enforces the condition $\|v^{k-j}\|_\infty = \|\text{div}^j \phi\|_\infty \leq \alpha_j$, and thus the alternative representation is indeed equivalent to TGV . We aim to apply Theorem 1.46 (recall: this states that $\inf_v F(v) + G(Tv) = \min_w F(-T^*w) + G^*(w)$, if $Y = \bigcap_{\lambda > 0} \lambda(\text{dom}(G) - T \text{dom}(F))$). Therefore, we need to show

$$Y = \bigcup_{\lambda > 0} \lambda \left(\text{dom}(G) - \Lambda \text{dom}(F) \right), \quad (188)$$

where the operations are understood element-wise, $\text{dom}(G) = \{0\}$ and $\text{dom}(F) =$

$B(0, \alpha_k) \times \cdots \times B(0, \alpha_1)$. For $y \in Y$, one can recursively define $v_k = 0$, $v_j = y_j - \operatorname{div} v_{j+1}$, i.e. $-\Lambda v = y$. Hence, there is a constant λ such that $\lambda^{-1}v \in \operatorname{dom}(F)$, and consequently $y = \lambda(0 - \Lambda v)$, confirming Condition (188). Thus, application of Theorem 1.46 to the maximisation problem in (187) yields

$$\operatorname{TGV}_\alpha^k(u) = \min_{w^* \in Y^*} F^*(-\Lambda^* w^*) + G^*(w^*), \quad (189)$$

and the minimum is indeed attained. A simple computation shows $G^*(w^*) = 0$ and per Proposition 1.44 $F^*(\xi) = \sup_{v \in X} \langle \xi, v \rangle - F(v)$, thus setting $w_0 = u$ and $w_k = 0$ results in

$$\begin{aligned} F^*(-\Lambda^* w^*) + G^*(w^*) &= - \sup_{v \in X} \langle \Lambda^* w^*, v \rangle + \langle u, \operatorname{div} v_1 \rangle - \sum_{j=1}^k \chi_{\{\|\cdot\|_\infty \leq \alpha_{k-j}\}}(v_j) \\ &= \sup_{v \in X, \|v_j\|_\infty \leq \alpha_{k-j}} \sum_{j=1}^k \langle w_j, v_j + \operatorname{div} v_{j+1} \rangle + \langle u, \operatorname{div} v_1 \rangle \\ &\stackrel{w_k=0}{=} \sup_{w_0=u} \sup_{v \in X, \|v_j\|_\infty \leq \alpha_{k-j}} \sum_{j=1}^k \langle w_j - \mathcal{E} w_{j-1}, v_j \rangle \\ &\stackrel{(181)}{=} \sum_{j=1}^k \alpha_{k-j} \| \mathcal{E} w_{j-1} - w_j \|_{\mathcal{M}}, \end{aligned}$$

where the third line is true due to $w_0 = u$ and $w_k = 0$. Now taking the minimum, together with (189) shows the desired representation. In particular, this minimum is finite for $u \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l,d})$, by setting $w_j = 0$ for $j \geq 1$ and the fact that $\mathcal{E} u \in \mathcal{M}(\Omega, \operatorname{Sym}^{l+1,d})$. Conversely, a finite sum for $u \in L^1(\Omega, \operatorname{Sym}^{l,d})$ implies finite TGV yielding $u \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l,d})$. \square

Remark 8.7. Thanks to the representation in (183), one can define $\operatorname{TGV}_\alpha^k$ recursively for $u \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l,d})$, via

$$\operatorname{TGV}_\alpha^{k+1}(u) = \min_{w \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l+1,d})} \alpha_k \| \mathcal{E} u - w \|_{\mathcal{M}} + \operatorname{TGV}_{\tilde{\alpha}}^k(w), \quad (190)$$

where $\tilde{\alpha} = (\alpha_0, \dots, \alpha_{k-1})$. In particular, the minimum is attained for some $w \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l+1,d})$.

From this it is effortless to see that $\operatorname{Ker}(\operatorname{TGV}_\alpha^k) = \operatorname{Ker}(\mathcal{E}^k) \subset L^1(\Omega, \operatorname{Sym}^{l,d})$. In the case that $l = 0$, i.e. considering real valued functions, we can further describe the

elements of the kernel as follows.

Proposition 8.8 (see [14]). *In the case $l = 0$, the kernel of $\mathcal{E}^k: \text{BD}(\Omega, \text{Sym}^{0,d}) \rightarrow \mathcal{M}(\Omega, \text{Sym}^{k,d})$ consists of $\text{Sym}^{0,d}$ -valued polynomials of degree less than k . In particular $\text{Ker}(\text{TGV}_\alpha^k) = \text{Ker}(\mathcal{E}^k)$ consists solely of such polynomials.*

With this knowledge concerning the TGV_α^k functional, we can deduce that the TGV_α^k functionals constitute a suitable family of regularisations. Recall, that we needed to assume for families of regularisation functionals $(R_\alpha)_{\alpha \in \mathcal{A}}$ with a Hausdorff space $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ that they are continuous families of functions, i.e. $(u, \alpha) \mapsto R_\alpha(u)$ is $\mathcal{T}_X \times \mathcal{T}_\mathcal{A}$ -lower semi-continuous, $\alpha \mapsto R_\alpha(u)$ is continuous for fixed $u \in X$, and $R_\alpha(u) \leq c(\alpha, \beta)R_\beta(u)$. Also strongly $\psi_{R_{\alpha^\dagger}}$ -continuity on a set $U \subset X$ in $\alpha^\dagger \in \mathcal{A}$ was required, which meant that $(\mathcal{A}, \mathcal{T}_\mathcal{A})$ is a metric space with metric $d_\mathcal{A}$, and a modulus of continuity estimate holds such that for $u \in U$,

$$|R_\alpha(u) - R_{\alpha^\dagger}(u)| < \psi_{R_{\alpha^\dagger}}(d_\mathcal{A}(\alpha, \alpha^\dagger))(R_{\alpha^\dagger}(u) + 1)$$

for $\alpha \in \mathcal{A}$ with $d_\mathcal{A}(\alpha, \alpha^\dagger)$ sufficiently small.

The following proposition shows that indeed all these requirements are satisfied by the TGV_α^k family of regularisations.

Proposition 8.9. *For $k \geq 1$, let $\mathcal{A} = (0, \infty)^k$ equipped with the topology $\mathcal{T}_\mathcal{A}$ induced by $|\cdot|$. Then the family of functions $(R_\alpha)_{\alpha \in \mathcal{A}}$ with $R_\alpha(u) = \text{TGV}_\alpha^k(u)$ for $u \in \text{BD}(\Omega, \text{Sym}^{l,d})$ is a continuous family of functions with respect to $\mathcal{T}_{L^1, W}$ and $\mathcal{T}_\mathcal{A}$.*

Moreover, for $\alpha^\dagger \in \mathcal{A}$ there is a constant $c > 1$ such that with $\psi_{R_{\alpha^\dagger}}(t) = ct$, the family $(R_\alpha)_{\alpha \in \mathcal{A}}$ is strongly $\psi_{R_{\alpha^\dagger}}$ -continuous on $L^1(\Omega, \text{Sym}^{l,d})$ in α^\dagger when using $d_\mathcal{A}(\alpha, \alpha^\dagger) = \|\alpha - \alpha^\dagger\|_\infty$.

Proof. Note that in Lemma 8.2 the claim concerning the constants such that $R_\alpha \leq c(\alpha, \beta)R_\beta$ was already discussed.

We first show an estimate needed for the modulus of continuity statement, as it will reduce the effort needed to show the remaining statements.

Let $\alpha, \alpha^\dagger \in (0, \infty)^k$ be such that $2|\alpha - \alpha^\dagger| < \underline{\alpha}^\dagger = \min_{i=0, \dots, k-1} \alpha_i^\dagger$ and let $u \in \text{BD}(\Omega, \text{Sym}^{l,d})$. Recall the infimal convolution representation of TGV in Theorem 8.6 and that there are w_j for $j = 0, \dots, k$ such that this infimum is indeed attained. We

denote by w_j^\dagger for $j = 0, \dots, k$ these infimising instances for $\text{TGV}_{\alpha^\dagger}^k(u)$. Therefore,

$$\begin{aligned}
\text{TGV}_\alpha^k(u) &= \inf \left\{ \sum_{j=1}^k \alpha_{k-j} \|w_j - \mathcal{E} w_{j-1}\|_{\mathcal{M}} \right. \\
&\quad \left. \mid w_j \in \text{BD}(\Omega, \text{Sym}^{l+j,d}) \text{ for } j = 0, 1, \dots, k, \text{ with } w_0 = u, w_k = 0 \right\} \\
&\leq \sum_{j=1}^k \alpha_{k-j} \|w_j^\dagger - \mathcal{E} w_{j-1}^\dagger\|_{\mathcal{M}} \\
&= \text{TGV}_{\alpha^\dagger}^k(u) + \sum_{j=1}^k (\alpha_{k-j} - \alpha_{k-j}^\dagger) \|w_j^\dagger - \mathcal{E} w_{j-1}^\dagger\|_{\mathcal{M}} \\
&\leq \text{TGV}_{\alpha^\dagger}^k(u) \left(1 + \frac{\|\alpha^\dagger - \alpha\|_\infty}{\underline{\alpha}^\dagger} \right). \tag{191}
\end{aligned}$$

Interchanging the rules of α and α^\dagger also yields

$$\text{TGV}_{\alpha^\dagger}^k(u) \leq \text{TGV}_\alpha^k(u) \left(1 + \frac{\|\alpha^\dagger - \alpha\|_\infty}{\underline{\alpha}} \right) \leq \text{TGV}_\alpha^k(u) \left(1 + 2 \frac{\|\alpha^\dagger - \alpha\|_\infty}{\underline{\alpha}^\dagger} \right). \tag{192}$$

So from (191) and (192), it becomes obvious that $\alpha \mapsto R_\alpha(u)$ is continuous and also the strong $\psi_{R_{\alpha^\dagger}}$ -continuity estimate is immanent with $\psi_{R_{\alpha^\dagger}}(t) = ct$ with $c = 2 \frac{1}{\underline{\alpha}^\dagger}$ when using the supremum metric on \mathcal{A} .

It is left to show, that $(u, \alpha) \mapsto R_\alpha(u)$ is $\mathcal{T}_{L^1, W} \times \mathcal{T}_{\mathcal{A}}$ -lower semi-continuous. Let sequences $(\alpha^n)_n \subset \mathcal{A}$ and $(u^n)_n \subset L^1(\Omega, \text{Sym}^{l,d})$ be such that $u^n \rightharpoonup u$ and $\alpha^n \rightarrow \alpha^\dagger$. We further may assume $\liminf_{n \rightarrow \infty} \text{TGV}_{\alpha^n}^k(u^n) < \infty$ and note that due to the estimates (191) and (192) $\text{TGV}_{\alpha^n}^k(u^n) - \text{TGV}_{\alpha^\dagger}^k(u^n) \rightarrow 0$. Then, we compute

$$\begin{aligned}
\liminf_{n \rightarrow \infty} \text{TGV}_{\alpha^n}^k(u^n) &= \liminf_{n \rightarrow \infty} \text{TGV}_{\alpha^n}^k(u^n) - \text{TGV}_{\alpha^\dagger}^k(u^n) + \text{TGV}_{\alpha^\dagger}^k(u^n) \\
&= \liminf_{n \rightarrow \infty} \text{TGV}_{\alpha^\dagger}^k(u^n) \stackrel{\text{l.s.c.}}{\geq} \text{TGV}_{\alpha^\dagger}^k(u),
\end{aligned}$$

confirming the lower semi-continuity claim where for the last inequality we used lower semi-continuity of $\text{TGV}_{\alpha^\dagger}^k$ for fixed α^\dagger . \square

8.2. Topological Properties

We know that BGV^k and BD are equivalent in a bijective sense, but we are not yet aware in which relation the respective topologies stand. Thus, we investigate the topological properties of BGV^k and consequently TGV_α^k .

Definition 8.10. We denote by $P^k : L^{d/(d-1)}(\Omega, \text{Sym}^{l,d}) \rightarrow \text{Ker}(\mathcal{E}^k)$, a continuous projection onto the kernel of \mathcal{E}^k .

Recall, that $\text{Ker}(\mathcal{E}^k) = \text{Ker}(\text{TGV}_\alpha^k)$ is finite-dimensional and thus indeed such a projection P^k exists.

Lemma 8.11. For $k \in \mathbb{N}$, $l \in \mathbb{N}_0$, there is a constant $C > 0$, dependent on Ω, k, l , such that for $v \in \text{BD}(\Omega, \text{Sym}^{l,d})$ and $w \in \text{Ker}(\text{TGV}_\alpha^k) \subset L^1(\Omega, \text{Sym}^{l+1,d})$,

$$\|\mathcal{E}v\|_{\mathcal{M}} \leq C \left(\|\mathcal{E}v - w\|_{\mathcal{M}} + \|v\|_{L^1} \right). \quad (193)$$

Proof. We prove by contradiction, assuming there were sequences $(v_n)_{n \in \mathbb{N}}$ in $\text{BD}(\Omega, \text{Sym}^{l,d})$ and $(w_n)_{n \in \mathbb{N}}$ in $\text{Ker}(\text{TGV}_\alpha^k) \subset L^1(\Omega, \text{Sym}^{l+1,d})$, such that

$$\|\mathcal{E}v_n\|_{\mathcal{M}} = 1, \quad \text{and} \quad \frac{1}{n} \geq \|v_n\|_{L^1} + \|\mathcal{E}v_n - w_n\|_{\mathcal{M}}. \quad (194)$$

Then $\mathcal{E}v_n$ is bounded in \mathcal{M} and consequently also w_n is bounded in \mathcal{M} . However, $\text{Ker}(\mathcal{E}^k)$ is a finite-dimensional space, implying that $\lim_{n \rightarrow \infty} \|w_n - w\|_{\mathcal{M}} = 0$ subsequentially for some $w \in \text{Ker}(\mathcal{E}^k)$, and consequently also $\lim_{n \rightarrow \infty} \|\mathcal{E}v_n - w\|_{\mathcal{M}} = 0$. As $v_n \rightarrow 0$ in L^1 , closedness of \mathcal{E} implies $\mathcal{E}0 = w = 0$. Thus $\|\mathcal{E}v_n\|_{\mathcal{M}} \rightarrow 0$, contradicting the assumption (194). \square

With this, one can again obtain a Poincaré-type inequality and an estimate which leads to the topological equivalence of the spaces BGV^k and BD .

Theorem 8.12. There are constant $C_1, C_2 > 0$, solely dependent on k, l, Ω, α and the choice of P^k , such that for $u \in \text{BD}(\Omega, \text{Sym}^{l,d})$

$$\|\mathcal{E}u\|_{\mathcal{M}} \leq C_1 \left(\|u\|_{L^1} + \text{TGV}_\alpha^k(u) \right), \quad (195)$$

$$\|u - P^k u\|_{d/(d-1)} \leq C_2 \text{TGV}_\alpha^k(u), \quad (196)$$

where we understand $\frac{d}{d-1} = \infty$ in case $d = 1$.

Proof. We prove both statements via a single induction with respect to k , for fixed $l \geq 0$. We will work with $\alpha = (\alpha_0, \alpha_1, \dots)$, an infinite sequence, which is tacitly restricted to the first k indices $(\alpha_0, \dots, \alpha_{k-1})$ when used as parameter in TGV_α^k .

For $k = 1$, we note that $\text{TGV}_\alpha^1(u) = \alpha_0 \|\mathcal{E}u\|_{\mathcal{M}}$. Consequently (195) is immanent, and (196) is stated in Theorem 7.22 concerning similar statements for TD .

Hence we assume the statements to hold for $k \geq 1$ and $l \geq 0$. We start by proving (195) for $k+1$. By Lemma 8.11 and the triangle inequality, for arbitrary $w \in \text{BD}(\Omega, \text{Sym}^{l+1,d})$ we compute

$$\|\mathcal{E}u\|_{\mathcal{M}} \stackrel{(193)}{\leq} c\|\mathcal{E}u - P^{k+1}w\|_{\mathcal{M}} + \|u\|_{L^1} \leq \|\mathcal{E}u - w\|_{\mathcal{M}} + \|w - P^{k+1}w\|_{\mathcal{M}} + \|u\|_{L^1}. \quad (197)$$

Note that $w \in L^{d/(d-1)}$ by embedding Theorem 7.21, as well as $\|f\|_{\mathcal{M}} = \|f\|_{L^1}$ for $f \in L^1(\Omega, \text{Sym}^{l,d})$. Using these facts and the Poincaré inequality (196) for k , which hold due to induction assumption, one obtains

$$\|\mathcal{E}u\|_{\mathcal{M}} \leq c(\|\mathcal{E}u - w\|_{\mathcal{M}} + \|w - P^{k+1}w\|_{d/(d-1)} + \|u\|_{L^1}) \leq c(\|\mathcal{E}u - w\|_{\mathcal{M}} + \text{TGV}_{\alpha}^k(w) + \|u\|_{L^1}).$$

Finally, taking the minimum with respect to $w \in \text{BD}(\Omega, \text{Sym}^{l+1,d})$, and using the recursive representation of TGV_{α}^k stated in (190) yields

$$\|\mathcal{E}u\|_{\mathcal{M}} \leq C_1(\|u\|_{L^1} + \text{TGV}_{\alpha}^{k+1}(u)).$$

In order to show the Poincaré-type inequality, we do a proof by contradiction. We assume there is a sequence $u_n \subset \text{BD}(\Omega, \text{Sym}^{l,d})$, such that

$$\|u_n - P^{k+1}u_n\|_{d/(d-1)} = 1, \quad \text{and} \quad \frac{1}{n} \geq \text{TGV}_{\alpha}^{k+1}(u_n). \quad (198)$$

It is easy to see, that

$$\text{TGV}_{\alpha}^{k+1}(u_n) = \text{TGV}_{\alpha}^{k+1}(u_n - P^{k+1}u_n).$$

By (195) for $k+1$ (we just proved) one obtains for $v_n = u_n - P^{k+1}u_n$, that

$$\|\mathcal{E}(v_n)\|_{\mathcal{M}} \leq c\left(\text{TGV}_{\alpha}^{k+1}(u_n) + \|v_n\|_{L^1}\right) \leq K < \infty,$$

for some constant $K > 0$. Further, note that $\{v \in L^1(\Omega, \text{Sym}^{l,d}) \mid P^{k+1}v = 0\}$ is closed in L^1 due to the closedness of the operator \mathcal{E}^{k+1} . The compact embedding $\text{BD}(\Omega, \text{Sym}^{l,d}) \hookrightarrow L^1(\Omega, \text{Sym}^{l,d})$ and the fact that $P^{k+1}v_n = 0$ imply the existence of $v \in L^1(\Omega, \text{Sym}^{l,d})$ such that $\|v_n - v\|_{L^1} \rightarrow 0$ and $P^{k+1}v = 0$. However, by lower semi-continuity

$$\text{TGV}_{\alpha}^{k+1}(v) \leq \liminf_{n \rightarrow \infty} \text{TGV}_{\alpha}^{k+1}(v_n) = 0 \quad (199)$$

implying that $v \in \text{Ker}(\mathcal{E}^{k+1})$. Hence, $0 = P^{k+1}v = v$ and $v_n \rightarrow 0$ in $\text{BD}(\Omega, \text{Sym}^{l,d})$ resulting in $v_n \rightarrow 0$ in $L^{d/(d-1)}$, which however contradicts (198). \square

From those inequalities, the topological equivalence of BGV^k and BD is immanent.

Corollary 8.13. *There exist constants $c, C > 0$, again only dependent on l, k, Ω and α , such that for $u \in \text{BD}(\Omega, \text{Sym}^{l,d})$*

$$c\left(\|u\|_{L^1} + \text{TGV}_\alpha^k(u)\right) \leq \|u\|_{L^1} + \text{TD}(u) \leq C\left(\|u\|_{L^1} + \text{TGV}_\alpha^k(u)\right), \quad (200)$$

i.e. $\text{BGV}^k(\Omega, \text{Sym}^{l,d}) \cong \text{BD}(\Omega, \text{Sym}^{l,d})$ in the sense of Banach space isometry.

8.3. Total Generalised Variation of Vector-Valued Functions

Up to this point we considered functions $u(x) \in \text{Sym}^{k,d}$ and the corresponding Total Generalised Variation $\text{TGV}_\alpha^k(u)$. Next, we aim to generalise TGV to be also applicable to vector-valued functions, i.e. $u(x) \in (\text{Sym}^{k,d})^M = \text{Sym}^{k,d,M}$, in order to apply it as a joint regularisation functional for multiple inverse problems simultaneously.

Recall, that the variational definition of TGV given in Definition 8.1 was

$$\text{TGV}_\alpha^k(u) = \sup \left\{ \int_\Omega u \cdot \text{div}^k \phi \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d}) \right. \\ \left. \text{with } \|\text{div}^j \phi\|_\infty \leq \alpha_j \text{ for } j \in \{0, \dots, k-1\} \right\},$$

i.e. TGV_α^k is the supremum of products with the divergence of continuously differentiable functions ϕ subject to L^∞ conditions on $\text{div}^j \phi$. We wish to use an analogue definition for the vectorial TGV function, and therefore we have to extend the definition of the product, the norms and the operators to the functions $u = (u_1, \dots, u_M)$ with values in $\text{Sym}^{k,d,M}$.

Definition 8.14. *Let M, k, d, l and $\Omega \subset \mathbb{R}^d$ be as above. Then, in slight abuse of notation, we define the component-wise operations*

$$\begin{aligned} \mathcal{E} : \mathcal{C}_c^l(\Omega, \text{Sym}^{k,d,M}) &\rightarrow \mathcal{C}_c^{l-1}(\Omega, \text{Sym}^{k+1,d,M}) && \text{such that } [\mathcal{E}\phi]_i = \mathcal{E}(\phi_i), \\ \text{div} : \mathcal{C}_c^l(\Omega, \text{Sym}^{k+1,d,M}) &\rightarrow \mathcal{C}_c^{l-1}(\Omega, \text{Sym}^{k,d,M}) && \text{such that } [\text{div} \psi]_i = \text{div}(\psi_i), \end{aligned}$$

for $i \in \{1, \dots, M\}$, where $\psi \in \mathcal{C}_c^l(\Omega, \text{Sym}^{k+1,d,M})$, and $\phi \in \mathcal{C}_c^l(\Omega, \text{Sym}^{k,d,M})$. The operations $\text{div}^j = \text{div} \circ \text{div}^{j-1}$ and $\mathcal{E}^j = \mathcal{E} \circ \mathcal{E}^{j-1}$ are then again defined in an iterative manner and are equivalent to the component-wise iteration of the operations.

Next one needs to adapt the corresponding point-wise norms. Previously, we used the $|\cdot|$ norm as a norm on $\text{Sym}^{k,d}$, so a natural extension would be to use $\|\cdot\|_2$ where $\|\cdot\|_2$ is the standard euclidean norm on \mathbb{R}^M and $|u| = (|u_1|, |u_2|, \dots, |u_M|)$. However, in the following we allow for more general point-wise norms $|\cdot|_{A_i}: \text{Sym}^{l,d,M} \rightarrow \mathbb{R}$, and note that $\text{Sym}^{k,d,M}$ is finite-dimensional and thus all norms are topologically equivalent.

Definition 8.15. For a norm $|\cdot|_A$ on $\text{Sym}^{k,d,M}$, we define the norm

$$\|\cdot\|_{\infty,A}: C_0(\Omega, \text{Sym}^{k,d,M}) \rightarrow \mathbb{R}, \quad \text{such that} \quad \|u\|_{\infty,A} = \||u|_A\|_{\infty}, \quad (201)$$

i.e. the supremum of the point-wise evaluation of the $|\cdot|_A$ norm.

In order to generalise the product $u \cdot \text{div}^k \phi$ on the product space $\text{Sym}^{l,d,M}$, one can simply use the sum of the individual products, i.e. $u \cdot \text{div}^k \phi = \sum_{i=1}^M u_i \cdot \text{div}^k \phi_i$.

Definition 8.16. Let $\alpha = (\alpha_0, \dots, \alpha_{k-1}) \in (0, \infty)^k$ and let for $j \in \{0, \dots, k-1\}$ the function $|\cdot|_{A_j}$ be a norm on $\text{Sym}^{k+l-j,d,M}$. Then the corresponding Total Generalised Variation for $u \in L^1(\Omega, \text{Sym}^{l,d,M})$ is defined as

$$\text{TGV}_{\alpha}^k(u) = \sup \left\{ \sum_{i=1}^M \int_{\Omega} u_i \cdot \text{div}^k \phi_i \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d,M}) \right. \\ \left. \text{with } \|\text{div}^j \phi\|_{\infty, A_j} \leq \alpha_j \text{ for } j \in \{0, \dots, k-1\} \right\}. \quad (202)$$

In particular, we can again define

$$\text{BGV}^k(\Omega, \text{Sym}^{l,d,M}) = \{u \in L^1(\Omega, \text{Sym}^{l,d,M}) \mid \text{TGV}_{\alpha}^k(u) < \infty\}. \quad (203)$$

This is an analogue definition to the scalar TGV with more general norms. In particular, all basic properties we previously shown remain true for this vector-valued version of Total Generalised Variation.

Remark 8.17. We note that the specific choice of the set of norms affects the definition of TGV_{α}^k however we will in the following not explicitly state the dependence on the set of norms, but simply assume there is such in the background. All sets of norms induce an equivalent TGV functional, i.e. for sets of norms $(|\cdot|_{A_i})_{i=1}^k$ and $(|\cdot|_{\bar{A}_i})_{i=1}^k$ and the induced TGV_{α}^k and $\widetilde{\text{TGV}}_{\alpha}^k$ functionals there are constants $c_1, c_2 > 0$ such that

$$c_1 \text{TGV}_{\alpha}^k(u) \leq \widetilde{\text{TGV}}_{\alpha}^k(u) \leq c_2 \text{TGV}_{\alpha}^k(u). \quad (204)$$

This estimate follows from the standard norm-equivalence statement on finite-dimensional vector spaces. So, while the choice of norms will not completely change the properties of the corresponding TGV functional, choosing suitable norms allows to place the focus on certain properties or penalise some aspects more harshly than others.

Proposition 8.18. *For $p \geq 1$ the function $\text{TGV}_\alpha^k: L^p(\Omega, \text{Sym}^{k,d,M}) \rightarrow [0, \infty]$ is proper convex and lower semi-continuous.*

Proof. Completely analogous to the proof of Lemma 8.4. \square

Many of the properties of this TGV_α^k for vector-valued functions can be proven in a completely analogous manner, in particular Proposition 8.9 holds, i.e. $(\text{TGV}_\alpha^k)_{\alpha \in (0, \infty)^k}$ is a continuous family of regularisation functionals. However, to save some effort, one can show that TGV_α^k of vector-valued functions is topologically equivalent to the sum of the individual TGV functionals.

Proposition 8.19. *There are constants $c_1, c_2 > 0$ such that for all $u = (u_1, \dots, u_M) \in L(\Omega, \text{Sym}^{l,d,M})$, it holds that*

$$c_1 \sum_{i=1}^M \text{TGV}_\alpha^k(u_i) \leq \text{TGV}_\alpha^k(u) \leq c_2 \sum_{i=1}^M \text{TGV}_\alpha^k(u_i), \quad (205)$$

where $\text{TGV}_\alpha^k(u_i)$ denotes application of the scalar TGV, while $\text{TGV}_\alpha^k(u)$ corresponds to the TGV functional for vector-valued functions.

Proof. Due to the equivalence of TGV induced from different norms, we may assume without loss of generality that $|\cdot|_{A_i} = \|\cdot\|_\infty$ where $|\cdot|$ is the standard norm on $\text{Sym}^{k+l-i,d}$ and $\|\cdot\|_\infty$ is the standard supremum norm on \mathbb{R}^M .

However, since div is a component-wise operation, one computes in this setting

$$\begin{aligned} \text{TGV}_\alpha^k(u) &= \sup \left\{ \sum_{i=1}^M \int_{\Omega} u_i \cdot \text{div}^k \phi_i \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d,M}) \text{ with } \|\text{div}^j \phi\|_{\infty, A_j} \leq \alpha_j \right\} \\ &= \sup \left\{ \sum_{i=1}^M \int_{\Omega} u_i \cdot \text{div}^k \phi_i \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d,M}) \text{ with } \|\text{div}^j \phi_i\|_\infty \leq \alpha_j, \right. \\ &\quad \left. \text{for } i \in \{1, \dots, M\} \right\} \\ &= \sum_{i=1}^M \sup \left\{ \int_{\Omega} u_i \cdot \text{div}^k \phi_i \, dx \mid \phi_i \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d}) \text{ with } \|\text{div}^j \phi_i\|_\infty \leq \alpha_j \right\} \\ &= \sum_{i=1}^M \text{TGV}_\alpha^k(u_i), \end{aligned}$$

where we used that for this choice of norms, the condition $\|\operatorname{div}^j \phi\|_{\infty, A_j} \leq \alpha_j$ is equivalent to the conditions $\|\operatorname{div}^j \phi_i\|_{\infty} \leq \alpha_j$ for all $i \in \{1, \dots, M\}$. As these conditions are independent from one-another, one can split the supremum into several, and each is exactly the definition of TGV for the respective component. Again using the equivalence of $\operatorname{TGV}_{\alpha}^k$ induced by different sets of norms to switch back to the $\operatorname{TGV}_{\alpha}^k$ induced by the set of norms $(|\cdot|_{A_i})_{i=1}^M$, yields the desired estimate. \square

Remark 8.20. *Due to Proposition 8.19, all the topological properties of TGV for vector-valued functions are direct consequences of the ones for scalar functions. This particularly holds for all embedding theorems, Poincaré-type estimates and coercivity statements.*

Corollary 8.21. *The spaces $\operatorname{BGV}^k(\Omega, \operatorname{Sym}^{k,d,M}) \cong \operatorname{BD}(\Omega, \operatorname{Sym}^{k,d,M})$ in a topological sense, and in particular $\operatorname{BD}(\Omega, \operatorname{Sym}^{k,d,M})$ is a Banach space.*

The infimal convolution representation of $\operatorname{TGV}_{\alpha}^k$ holds analogously to the one stated in Theorem 8.6.

Theorem 8.22. *For $\operatorname{TGV}_{\alpha}^k$ induced by a set of norms $(|\cdot|_{A_i})_{i=0}^{k-1}$ the following representation holds:*

$$\operatorname{TGV}_{\alpha}^k(u) = \inf \left\{ \sum_{j=1}^k \|w_j - \mathcal{E}w_{j-1}\|_{\mathcal{M}, A_j^*} \right. \quad (206)$$

$$\left. \mid w_j \in \operatorname{BD}(\Omega, \operatorname{Sym}^{l+j,d,M}) \text{ for } j = 0, 1, \dots, k, w_0 = u, w_k = 0 \right\},$$

where $\|\cdot\|_{\mathcal{M}, A_i^*} = \| |\cdot|_{A_i^*} \|_{\mathcal{M}}$ with $(|\cdot|_{A_i^*})_{i=1}^k$ the adjoint norms to $(|\cdot|_{A_i})_i$, and $\|\cdot\|_{\mathcal{M}}$ is the standard norm on the real-valued measures.

Proposition 8.23. *Let $l = 0$ and consider $L^p(\Omega, \operatorname{Sym}^{l,d,M}) \cong L^p(\Omega, \mathbb{R}^M)$. Then,*

$$\operatorname{Ker}(\operatorname{TGV}_{\alpha}^k) = \left\{ u \in L^p(\Omega, \mathbb{R}^M) \mid u(x) \stackrel{\text{a.e.}}{=} \sum_{|\alpha| < k} a_{\alpha} x^{\alpha} \text{ with } x \in \Omega \text{ and } a_{\alpha} \in \mathbb{R}^M \right\}.$$

9. TGV Regularisation in a Linear Setting

In this chapter we summarise how application of TGV as regularisation can be applied in a linear setting, and in particular with the specific discrepancies previously discussed.

We consider independent problems as this is a common application of the multi-channel TGV functional, however analogue considerations in a non-independent setting can be made. Hence, we consider the following setting.

Problem 9.1. Let Ω be a bounded Lipschitz domain, let $X_i = L^{p_i}(\Omega, \mathbb{R})$ for some $p_i \in [1, \infty)$ and set $X = X_1 \times \cdots \times X_M$. Further, we assume that $(Y_i, \|\cdot\|_{Y_i})$ are normed spaces for $i \in \{1, \dots, M\}$, $Y = Y_1 \times \cdots \times Y_M$ and let $T_i: X_i \rightarrow Y_i$ be linear and weak-weak continuous and we use the notation $T = (T_1, \dots, T_M)$. We consider the problems to find $u = (u_1, \dots, u_M) \in X$ for $f^\dagger \in Y$ such that

$$T_1 u_1 = f_1^\dagger, \quad \dots \quad T_M u_M = f_M^\dagger. \quad (207)$$

Let $p_i \leq \bar{p} = \frac{d}{d-1}$ if $d > 1$ and $p_i < \infty$ if $d = 1$ and let $q_i \in [1, \infty)$. Further, let \mathcal{T}_X be the product topology of \mathcal{T}_{X_i} , which is the norm topology in L^{p_i} if $p_i < \bar{p}$, and otherwise the weak topology in $L^{\bar{p}}$. Further, we consider the topology $\mathcal{T}_Y = \mathcal{T}_{Y_1} \times \cdots \times \mathcal{T}_{Y_M}$ with $\mathcal{T}_{Y_i} = \mathcal{T}_{Y_i, W}$ and the topology \mathcal{T}_D , which is the product of the respective norm topologies. Then, we define

$$F_{\lambda, \alpha}: X \times Y \rightarrow \mathbb{R}, \quad F_{\lambda, \alpha}(u, f) = \sum_{i=1}^M \lambda_i \|T_i u_i - f_i\|_{Y_i}^{q_i} + \text{TGV}_\alpha^k(u), \quad (208)$$

where TGV_α^k denotes the TGV functional for vector-valued functions. As the corresponding Tikhonov problem we consider

$$u^\dagger \in \operatorname{argmin} F_{\lambda, \alpha}(u, f^\dagger), \quad F_{\lambda, \alpha}(u^\dagger, f^\dagger) < \infty. \quad (\text{TGV}_\alpha^k\text{-TIKH}_\lambda(f^\dagger))$$

One can also understand T_i as an operation \tilde{T}_i on the entirety of X by considering $\tilde{T}_i: X \rightarrow Y_i$ with $\tilde{T}_i u = T_i u_i$, and thus this is a special case of the theory of Part I. As previously stated, $(\text{TGV}_\alpha^k)_{\alpha \in (0, \infty)^k}$ is a continuous family of functions, and similarly to the TD situation, one can show coercivity in a linear setting.

Theorem 9.2. Let the situation in Problem 9.1 hold. Let the operator $T = (T_1, \dots, T_M)$ be such that $\operatorname{Ker}(T) \cap \operatorname{Ker}(\text{TGV}_\alpha^k) = \{0\}$. Then the function $F_{1,1}$ is uniformly coercive with respect to $\mathcal{T}_X = \mathcal{T}_{X_1} \times \cdots \times \mathcal{T}_{X_M}$ and \mathcal{T}_D .

Moreover, in this case the Problem $(\text{TGV}_\alpha^k\text{-TIKH}_\lambda(f^\dagger))$ is solvable, and the corresponding stability and convergence results are applicable.

Proof. We note that in this linear setting the function $v \equiv 0$ satisfies $v \in \operatorname{dom}(\text{TGV}_\alpha^k)$ and $\|T_i v_i - f_i\|_{Y_i} < \infty$, so the functional is indeed proper, and also Proposition 8.9 ensures the required continuity and modulus of continuity conditions on the family $(\text{TGV}_\alpha^k)_{\alpha \in (0, \infty)^k}$. All requirements concerning the discrepancy functions are satisfied by norm discrepancies. The only point to show is that $F_{1,1}$ is indeed uniformly coercive,

which we do by using BD embeddings in Theorem 7.21. Let sequences $(f^n)_n \subset Y$ be such that $f^n \rightarrow f^\dagger$ in the \mathcal{T}_D topology and $(u^n)_n \subset X$ be such that $F_{1,1}(u^n, f^n) < C$ for some $C > 0$.

From $C > \text{TGV}_\alpha^k(u) \geq c \sum_{i=1}^M \text{TGV}_\alpha^k(u_i)$, we can conclude that $\text{TGV}_\alpha^k(u_i) < C$ for all $i \in \{1, \dots, M\}$ and consequently $\|(id - P^k)u_i^n\|_{L^{p_i}} \leq \tilde{C}$ by the Poincaré-type inequality (196) where P^k is the corresponding projection onto the kernel of the scalar TGV. We note that $\text{Ker}(\text{TGV}_\alpha^k)$ is finite-dimensional and consequently $\|P^k u_i^n\|_{L^{p_i}} \rightarrow \infty$ would imply $\|T_i P^k u_i^n\| \rightarrow \infty$. Hence, in case $\|P^k u_i^n\|_{L^{p_i}}$ was unbounded, one would obtain

$$C > \|T_i u_i^n - f_i^n\| \geq \|T_i P^k u_i^n\| - \|T_i (id - P^k) u_i^n\| - \|f_i^n - f^\dagger\| - \|f^\dagger\| \rightarrow \infty$$

contradicting u^n being in the level sets. Hence u_i^n is bounded in BD, and the statements concerning compact embeddings in Theorem 7.21 in the case of $p_i < \frac{d}{d-1}$, and reflexivity in the case $p = \frac{d}{d-1}$ yield a convergent subsequence of u_i^n in \mathcal{T}_{X_i} , thus confirming coercivity. \square

Remark 9.3. *Note that the assumption that $\text{Ker}(\text{TGV}) \cap \text{Ker}(T) = \{0\}$ is a technical assumption, one can satisfy by changing the space $X = L^1(\Omega, \mathbb{R})$ to the factor space $X = L^1(\Omega, \mathbb{R}) / \text{Ker}(T)$ and the theory applies in a completely analogue manner.*

The following Theorem shows that a Tikhonov approach using norms and the Kullback-Leibler divergence as discrepancies and TGV for regularisation works.

Theorem 9.4. *Let $\{1, \dots, M\} = J_N \cup J_{KL} \cup J_{EN}$. For $i \in \{1, \dots, M\}$ let $q_i \in [1, \infty)$ and let the space and function (Y_i, \mathcal{T}_{Y_i}) and $D_i: Y_i \times Y_i \rightarrow [0, \infty]$ be as follows: For $i \in J_{KL}$ let there be a finite measure space (Ω_i, μ_i) and let $Y_i = L^1_{\mu_i}(\Omega_i)$ and $D_i(v_i, f_i) = D_{KL}(v_i, f_i)$. Let $(Y_i, \|\cdot\|_{Y_i})$ be a normed space and let $D_i(v_i, f_i) = \|v_i - f_i\|_{Y_i}^{q_i}$ for $i \in J_N$. Let a reflexive Banach space Z_i be continuously embedded in Y_i such that $D_i(v_i, f_i) = \|v_i - f_i\|_{Z_i}^{q_i}$ for $i \in J_{EN}$. Further, let (X, \mathcal{T}_X) be as in Problem 9.1, let $T_i: (X_i, \mathcal{T}_X) \rightarrow (Y, \mathcal{T}_{Y,W})$ be linear and continuous. Moreover, denote by \mathcal{T}_{D_i} the norm topologies for $i \in J_N \cup J_{KL}$ and the topology induced by the subnorm $\|\cdot\|_{Z_i}$ on Y_i for J_{EN} . Then the following 3 statements concerning coercivity, convergence and rates hold:*

1. *Consider the functional*

$$\begin{aligned} F_{\lambda,\alpha}: X \times Y \rightarrow [0, \infty], \quad F_{\lambda,\alpha}(u, f^\dagger) &= \text{TGV}_\alpha^k(u) + \sum_{i \in J_N} \lambda_i \|T_i u_i - f_i^\dagger\|_{Y_i}^{q_i} \\ &+ \sum_{i \in J_{EN}} \lambda_i \|T_i u_i - f_i^\dagger\|_{Z_i}^{q_i} + \sum_{i \in J_{KL}} \lambda_i D_{KL}(T_i u_i, f_i^\dagger). \end{aligned}$$

Then the functional $F_{1,1}$ is uniformly coercive in \mathcal{T}_X and \mathcal{T}_D , i.e. for all $C > 0$ the set $\bigcup_{n=1}^{\infty} \{u^n \mid F_{1,1}(u^n, f^n) < C\}$ is \mathcal{T}_X -precompact for any sequence $(f^n)_n$ with $f^n \xrightarrow{\mathcal{T}_D} f^\dagger$.

2. Let $I \subset \{1, \dots, M\}$ and let a parameter choice rule $\delta \mapsto \lambda^\delta \in \mathbb{R}^M$ be such that

$$\begin{cases} \lambda_i^\delta \rightarrow \lambda_i^\dagger \in (0, \infty) & \text{for } i \in I^c, \\ \lambda_i^\delta \delta_i \rightarrow 0, \lambda_i^\delta \rightarrow \infty = \lambda_i^\dagger & \text{for } i \in I, \end{cases} \quad (209)$$

is satisfied and let $\alpha^\delta \rightarrow \alpha^\dagger$. Let $(f^\delta)_\delta$ be a sequence in Y such that $f^\delta \rightarrow f^\dagger$ in \mathcal{T}_D and let \hat{u} be a $[\text{TGV}_{\alpha^\dagger}^k(\cdot) + \sum_{I^c} \lambda_i^\dagger D_i(T_i \cdot, f_i^\dagger)]$ -minimal I -partial solution to the inverse problem $Tu = f^\dagger$ with true data f^\dagger . Then the sequence of solutions u^δ to the Tikhonov problem corresponding to data f^δ with weights λ^δ and α^δ contains a \mathcal{T}_X -convergent subsequence and every \mathcal{T}_X -limit of a subsequence is a $[\text{TGV}_{\alpha^\dagger}^k(\cdot) + \sum_{I^c} \lambda_i^\dagger D_i(T_i \cdot, f_i^\dagger)]$ -minimal I -partial solution to $Tu = f^\dagger$.

3. Additionally to the previous points we set $q_i = 2$ for $i \in J_{KL}$ and for $i \in I$ choose λ_i^δ such that $c\delta_i^{-(1-\epsilon)} \leq \lambda_i^\delta \leq C\delta_i^{-(1-\epsilon)}$ if $q_i = 1$ and $c\delta_i^{\frac{1-q_i}{q_i}} \leq \lambda_i^\delta \leq C\delta_i^{\frac{1-q_i}{q_i}}$ otherwise and for $i \in I^c$ such that $|\lambda_i^\dagger - \lambda_i^\delta| = O(\delta_i^{\frac{1}{q_i}})$. Further, let u^\dagger be a $[\text{TGV}_{\alpha^\dagger}^k(\cdot) + \sum_{I^c} \lambda_i^\dagger D_i(T_i \cdot, f_i^\dagger)]$ -minimal I -partial solution to $Tu = f^\dagger$ and let for $i \in J_{KL}$ the condition $T_i u_i^\dagger, T_i u_i^\delta \in V_i = \{v_i \in L_{\mu_i}^1(\Omega_i) \mid \ln(\frac{v_i}{f_i^\dagger}) < C\}$ be satisfied. Then, there is a constant $c > 0$ such that for δ sufficiently small,

$$\begin{aligned} & \text{TGV}_{\alpha^\dagger}^k(u_i^\delta) + \sum_{i \in I^c} \lambda_i^\dagger D_i(T_i u_i^\delta, f_i^\dagger) \\ & \leq \text{TGV}_{\alpha^\dagger}^k(u^\dagger) + \sum_{i \in I^c} \lambda_i^\dagger D_i(T_i u_i^\dagger, f_i^\dagger) \\ & \quad + c \left(\left(\sum_{i \in I} \lambda_i^\delta \delta_i + \psi_i(\delta_i) \right) + \left(\sum_{i \in I^c} \psi_i(\delta_i) + |\lambda_i^\dagger - \lambda_i^\delta| \right) + \psi_{R_{\alpha^\dagger}}(d_{\mathcal{A}}(\alpha^\delta, \alpha^\dagger)) \right), \end{aligned}$$

i.e. the Tikhonov functional for the $i \in I^c$ is low for the iterates u^δ .

Let there be constants $\gamma_1, \gamma_2 \geq 0$ with $\gamma_1 < 1$ and $\epsilon_0 > 0$ such that the following source condition holds: There is $\xi \in \partial[R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)](u^\dagger)$ such that for u satisfying $R_{\alpha^\dagger, \lambda^\dagger, I}(u, f^\dagger) \leq R_{\alpha^\dagger, \lambda^\dagger, I}(u^\dagger, f^\dagger) + \epsilon_0$ and $\sum_{i \in I} D_i(T_i u, f_i^\dagger) \leq \epsilon_0$ also

$$-\langle \xi, u - u^\dagger \rangle_{X^* \times X} \leq \gamma_1 D_{R_{\alpha^\dagger, \lambda^\dagger, I}(\cdot, f^\dagger)}^\xi(u, u^\dagger) + \gamma_2 \sum_{i \in I} \phi_i(T_i u, T_i u^\dagger). \quad (\text{SC3})$$

Here, for $i \in I$, the function $\phi_i: Y_i \times Y_i \rightarrow [0, \infty]$ is such that for $v_i, f_i \in Y_i$

$$\phi_i(v_i, f_i^\dagger) = \begin{cases} \|v_i - f_i\|_{Y_i} & i \in I \cap J_N, \\ \|v_i - f_i\|_{Z_i} & i \in I \cap J_{EN}, \\ D_{KL}(v_i, f_i) & i \in I \cap J_{KL}. \end{cases}$$

Then, one can obtain the convergence rates

$$\begin{aligned} D_i(T_j(u_j^\delta, f_j^\delta)) &= O\left(\delta_j^{1-\epsilon} \left(\sum_{\{i \in I | q_i=1\}} \delta_i^\epsilon + \sum_{\{i | q_i > 1\}} \delta_i^{\frac{1}{q_i}} + \sum_{\{i \in I^c | q_i=1\}} \delta_i \right)\right) \quad \text{for } j \text{ s.t. } q_j = 1 \\ D_i(T_j u_j^\delta, f_j^\delta) &= O\left(\delta_j^{\frac{q_i-1}{q_i}} \left(\sum_{\{i \in I | q_i=1\}} \delta_i^\epsilon + \sum_{\{i | q_i > 1\}} \delta_i^{\frac{1}{q_i}} + \sum_{\{i \in I^c | q_i=1\}} \delta_i \right)\right) \quad \text{for } j \text{ s.t. } q_j > 1 \\ D_{\text{TGV}_\alpha^k(\cdot) + \sum_{i \in I^c} \lambda_i^\dagger D_i(T_i \cdot, f^\dagger)}^\xi(u^\delta, u^\dagger) &= O\left(\sum_{\{i \in I | q_i=1\}} \delta_i^\epsilon + \sum_{\{i | q_i > 1\}} \delta_i^{\frac{1}{q_i}} + \sum_{\{i \in I^c | q_i=1\}} \delta_i \right). \end{aligned}$$

Part IV.

Application to STEM CT Reconstruction

In this part we aim to apply the theory derived in the previous parts to the specific problem of reconstructing multi-spectral STEM [4] CT data.

While single transmission projection methods such as X-Ray are suitable for some purposes, they are often difficult to interpret as the information of a 3D density distribution is compressed into a 2D image making such methods unusable for certain applications. Hence the question arises, whether it is possible to obtain the 3D density distribution of an object from such 2D data, to which the obvious answer is no. A sequence of 2D projections taken from all different angles however might be sufficient.

This is the basic idea of Computed Tomography (CT) [3], taking X-ray projections from all directions, thus containing the information of the entire 3D density distribution.

A particular application field of CT approaches is the STEM (Scanning Transmission Electron Microscopy) [4] in material science. STEM is used for spectroscopy methods [51] such as EELS (Electron Energy Loss Spectroscopy) and EDS (Energy-Dispersive X-ray Spectroscopy) which can be applied for elemental analysis and chemical mappings of objects, i.e. determining the distribution of chemical elements inside a specimen. However, due to technical limitations the quality of such data is low and contains much noise, making proper regularisation relevant.

In particular, we present a Tikhonov regularisation scheme suitable for CT reconstruction problems, and show how this can be solved approximately. First the Radon transform, the process involved in such inverse problems is discussed, before a discretised framework and an optimisation method to solve the resulting problem are presented. Finally, for real data numerical results are discussed and their improvements over other methods are emphasised.

10. The Radon Transform

An inverse problem always consists of a process T , and data f one tries to invert, however, it is not yet clear how the specific operator T corresponding to the process of recording sinogram-data (CT data) works.

Thus, it is necessary to understand the process that transfers a 3D density distribution into the corresponding 2D projections, also known as the Radon transform. Furthermore, it is necessary to consider the analytic properties of this Radon transform, in order to ensure that the corresponding Tikhonov approach works out in a suitable manner.

10.1. Deriving the Radon Transform

The idea of Computed Tomography (CT) is to consider electron transmission projections (such as X-ray images) of an object from multiple angles around a fixed axis, and reconstruct the density distribution inside an object from those. Hence, we first need to understand how such transmission projections work and how densities u translate to measured data f , which requires mathematical and physical modelling of the process.

We assume here, that the electron transmission moves along a single straight line from the source to the detector (see Figure 3), that the object is 3-dimensional and contained inside $\Omega_R = B(0, 1) \times [0, Z]$, i.e. the cylinder with middle-point 0, radius 1 and height Z , and that the projections are taken from different angles rotating around the z axis. Note that the assumption of transmission along straight lines is a modelling assumption which is not physically accurate, and more sophisticated modelling is possible, e.g. cone-beam computed tomography assumes that the transmission moves from the source to the detector in a conical beam (see [31] and the references therein). However, for our considerations the model with straight lines is sufficient and will be the content of the following.

All such straight lines (which are constant in z -dimension) are described as follows.

Definition 10.1. For $s \in [-1, 1]$, $\phi \in [0, \pi)$ and $z \in [0, Z]$, we denote by

$$L(s, \phi, z) = \left\{ \mathbf{x}_L(t) = (0, 0, z)^T + s\omega(\phi) + t\omega^\perp(\phi) \in \mathbb{R}^3 \mid t \in [-1, 1] \text{ and} \right. \quad (210)$$

$$\left. \begin{aligned} \omega(\phi) &= (\cos(\phi), \sin(\phi), 0)^T, \\ \omega^\perp(\phi) &= (\sin(\phi), -\cos(\phi), 0)^T \end{aligned} \right\}$$

the line L through Ω_R with offset s , angle ϕ in the x - y plane and height z . Alternatively, the line $L(s, \phi, z)$ is defined as all $\mathbf{x} = (x, y, z) \in \Omega_R$ such that $\langle \mathbf{x}, \omega(\phi) \rangle = s$ and the third space-dimension of \mathbf{x} and L are the same.

For a constant angle $\phi \in [0, \pi]$ and offset s , the electron transmission projection is obtained when an electron moves through the object in a straight line, where the initial energy of said electron can be controlled, while a detector on the opposite end measures

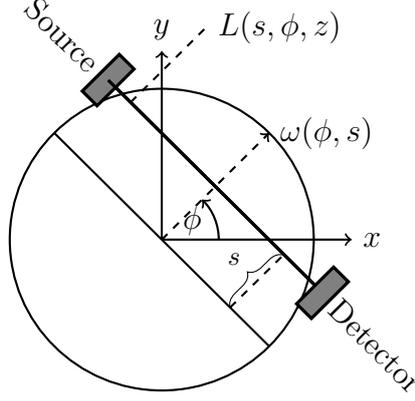


Figure 3: 2D cross-section illustrating a Line $L(s, \phi, z)$ for fixed z .

the intensity of the electron after having passed through the body, thus enabling us to consider the attenuation along this straight line. Further, let $u(\mathbf{x})$ denote the density of the object in $\mathbf{x} \in \Omega_R$. It is reasonable from a physical perspective to assume the infinitesimal loss of energy of the transmitting electron in a point \mathbf{x} to be proportional to the density $u(\mathbf{x})$ and the energy contained when passing through \mathbf{x} .

More precisely, for fixed $L = L(s, \phi, z)$, let $I_L(t)$ denote the intensity of an electron moving through an object along L at the position $\mathbf{x}_L(t)$. Then $I_L(-1) = I_0$ is the initial intensity one can control, and $I_L(1) = I_1$ is the terminal intensity one measures with a detector on the opposite side, and for $t \in (-1, 1)$ the loss of intensity in $\mathbf{x}_L(t)$ along the line L is modelled as

$$\frac{\partial I_L(t)}{\partial t} = -u(\mathbf{x}_L(t))I_L(t). \quad (211)$$

Solving this differential equation with initial intensity I_0 yields

$$I_L(t) = I_0 e^{-\int_{-1}^t u(\mathbf{x}_L(\tau)) d\tau}, \quad \text{and} \quad I_0 e^{-\int_{-1}^1 u(\mathbf{x}_L(\tau)) d\tau} = I_1. \quad (212)$$

Hence, it is easy to see that for sufficiently smooth functions u ,

$$\int_{-1}^1 u(\mathbf{x}_L(\tau)) d\tau = \ln \left(\frac{I_0(L)}{I_1(L)} \right), \quad (213)$$

where the right side is given via the (known) initial intensity, and the (measured) terminal intensity. So the right-hand side can be understood as the measured data f , while the left is solely dependent on the density u and can be understood as an operation $T_L u$. For a single line L , this could already be understood as an inverse problem $T_L u = f_L$

where f_L is the logarithm of the relative loss of intensity, while $T_L u$ accumulates the mass along the line L . On a larger scale, we can consider the operation modelling such processes along all possible lines, leading to the following definition.

Definition 10.2 (Radon Transform). *We define the sinogram space $\Omega_S = [-1, 1] \times [0, \pi] \times [0, Z]$, and consider the mapping*

$$\begin{aligned} \mathcal{R}: \mathcal{C}(\overline{\Omega_R}) &\rightarrow L^1(\Omega_S), \quad \text{such that} \quad \mathcal{R}u(s, \phi, z) = \int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} u(\mathbf{x}_{L(s, \phi, z)}(t)) dt \\ &= \int_{-1}^1 u(s\omega(\phi) + t\omega^\perp(\phi) + (0, 0, z)^T) dt, \end{aligned} \quad (214)$$

for $u \in \mathcal{C}(\overline{\Omega_R})$ which we tacitly extend with zero outside of Ω_R . We refer to this operation as the Radon transform.

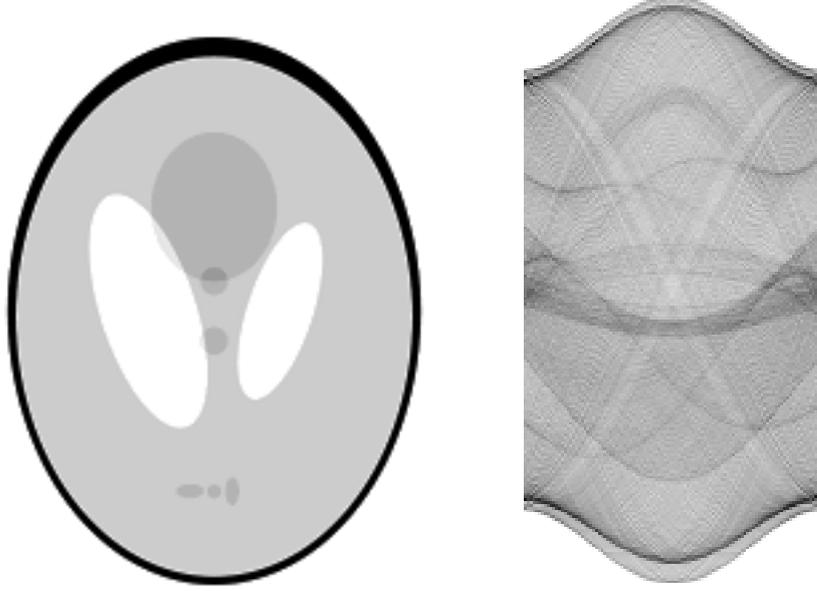
Remark 10.3. *Note that in this specific setting the Radon transform is well-defined as the line integral of continuous functions, and $\|\mathcal{R}u\|_{L^1} \leq c\|u\|_{L^\infty}$ ensures $\mathcal{R}u \in L^1(\Omega_S)$, however we will derive a more general functional-analytic setting in the next chapter, which makes it more suitable for applications of certain discrepancy and regularisation functionals.*

Also, we consider Ω_S which contains the projections from all angles $\phi \in [0, \pi]$, which can not be obtained in real data sets. Still we first discuss this setting for theoretical considerations, and will in later sections shift our attention to a discretised setting.

10.2. Analytical Properties

The Radon transform in Definition 10.2 is solely defined for continuous functions, which is too restrictive as one would expect jump discontinuities in a density distribution to occur. Thus, we try to widen the definition of the Radon transform to more general spaces, consider its continuity properties with respect to the occurring topologies, and discuss why indeed regularisation is required. Many of the following statements and more on tomography in general can for example be found in [34].

Proposition 10.4. *For each $p \in [1, \infty)$ there exists a linear and continuous extension $\mathcal{R}_p: (L^p(\Omega_R), \|\cdot\|_{L^p}) \rightarrow (L^p(\Omega_S), \|\cdot\|_{L^p})$ to \mathcal{R} as defined in (214) which we also refer to as Radon transform. We will in later parts not explicitly state the dependence on p when it is clear from the setting what p is, and refer to \mathcal{R}_p as \mathcal{R} .*



(a) Phantom density distribution for fixed z . (b) Sinogram for fixed z .

Figure 4: Phantom density distribution and the corresponding sinogram-data for fixed slice z .

Remark 10.5. *This setting might be surprising, since the definition of the Radon transform in (214) appears to require integration along lines, which are null-sets with respect to the Lebesgue measure, and one would thus expect those integrals to not be well-defined for all L^p functions. However, due to considering lines with all possible offsets s and heights z simultaneously, some might not be well-defined, but those are few in a suitable sense as the following proof shows.*

Proof of Proposition 10.4. Let $u \in \mathcal{C}(\overline{\Omega_R})$ and compute for $p \in [1, \infty)$ via Fubini's Theorem and Hölder's Inequality

$$\begin{aligned}
\|\mathcal{R}u\|_p^p &= \int_{\Omega_S} |\mathcal{R}u(s, \phi, z)|^p d(s, \phi, z) = \int_0^Z \int_0^\pi \int_{-1}^1 \left| \int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} u(\mathbf{x}_{L(s, \phi, z)}(t)) dt \right|^p ds d\phi dz \\
&\stackrel{\text{Hölder}}{\leq} \int_0^Z \int_0^\pi \int_{-1}^1 \left(\left(\int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} |u(\mathbf{x}_{L(s, \phi, z)}(t))|^p dt \right)^{\frac{1}{p}} \left(\int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} 1^{p^*} dt \right)^{\frac{1}{p^*}} \right)^p ds d\phi dz \\
&\leq 2^{p-1} \int_0^\pi \int_0^Z \int_{-1}^1 \left(\int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} |u(\mathbf{x}_{L(s, \phi, z)}(t))|^p dt \right) ds dz d\phi, \tag{215}
\end{aligned}$$

where the last inequality holds since we can estimate the integral containing 1^{p^*} with the value 2. Further, note that the domain covered by the variable $\mathbf{x}_L(t)$ for fixed ϕ and

$L = L(s, \phi, z)$ with t, s, z varying according to the integration boundaries is exactly Ω_R . Consequently, one can compute

$$\|\mathcal{R}_p u\|_p^p \leq 2^{p-1} \int_0^\pi \int_{\Omega_R} |u(\mathbf{x})|^p d\mathbf{x} d\phi = 2^{p-1} \pi \|u\|_p^p, \quad (216)$$

and thus the Radon transform is also continuous from $L^p \rightarrow L^p$. Since the continuous functions are dense in $L^p(\Omega_R)$, there is a unique continuous extension $\mathcal{R}_p: L^p(\Omega_R) \rightarrow L^p(\Omega_S)$. \square

Also, we note that for a set of angles \mathcal{A} different from $[0, \pi]$ and a different finite measure on it, e.g. finitely many angles equipped with the counting-measure, the same continuity results hold as ϕ did not play an important role in this proof. Thus, the continuity of the operator does not depend on the ϕ dimension in Ω_S as long as it is a finite measure space, and therefore later considering versions with finitely many angles will also be sensible.

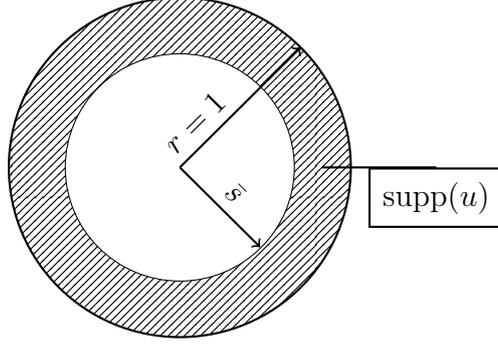
Proposition 10.6 (See [34] Thm 3.27, p 155 and its conclusions). *For all $p \in [1, \infty)$, the operation $\mathcal{R}_p: L^p(\Omega_R) \rightarrow L^p(\Omega_S)$ is injective.*

Next, we aim to show that the Radon transform is not continuously invertible and not surjective, thus indeed making regularisation necessary.

Proposition 10.7. *For any $p \in (1, \infty)$, the Radon transform $\mathcal{R}_p: L^p(\Omega_R) \rightarrow L^p(\Omega_S)$ is not continuously invertible with respect to the norm topologies. Furthermore, \mathcal{R}_p is not surjective for any $p \in [1, \infty)$.*

Proof. Let $u \in \mathcal{C}(\overline{\Omega_R})$ be such that $\text{supp}(u) = \{\mathbf{x} \in \Omega_R \mid u(x) \neq 0\} \subset (B(0, 1) \setminus B(0, \bar{s})) \times [0, Z]$ for fixed $\bar{s} \in (0, 1)$. Revisiting (215) but now using $v_{s, \phi, z}(t) = \mathcal{I}_{\text{supp}(u(\mathbf{x}_{L(s, \phi, z)}))}(t)$ with $\mathcal{I}_C(x) = 1$ if $x \in C$, and 0 otherwise for Hölder's inequality, and noting that the length of this support is uniformly bounded by a function $g(\bar{s})$ such that $g(\bar{s}) \rightarrow 0$ as $\bar{s} \rightarrow 1$ independently of ϕ or z , one computes

$$\|\mathcal{R}_p u\|_p^p \leq g(\bar{s})^{p-1} \int_0^\pi \int_0^Z \int_{-1}^1 \left(\int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} u(\mathbf{x}_L(t))^p dt \right) ds dz d\phi = \pi g(\bar{s})^{p-1} \|u\|_p^p. \quad (217)$$



Choosing $u_{\bar{s}}$ such that $\|u_{\bar{s}}\|_p = 1$ and $u_{\bar{s}}$ is supported only outside $B(0, \bar{s})$, e.g. $u_{\bar{s}}$ constant outside, we see that $\|\mathcal{R}_p u_{\bar{s}}\|_p \xrightarrow{\bar{s} \rightarrow 1} 0$, which since \mathcal{R}_p is injective implies that \mathcal{R}_p^{-1} cannot be continuous.

Note that this works since for $p > 1$ we can place less and less total mass closer and closer to the boundary of the cylinder while maintaining the norm to be equal to 1, ultimately leading to vanishing Radon transforms.

In particular, the Radon transform cannot be surjective or have closed range either for $p > 1$, since closed range would imply continuous invertibility by the Open Mapping Theorem.

For $p = 1$, we first show that for $u \in L^1(\Omega_R)$ the integral $\int_0^Z \int_{-1}^1 \mathcal{R}_p u(s, \phi, z) ds dz$ is constant for almost every ϕ . For an approximating sequence of continuous functions $(u^n)_n$, we see that for almost all $\phi \in [0, \pi)$,

$$\begin{aligned}
& \int_{\Omega_R} u(\mathbf{x}) d\mathbf{x} \xrightarrow{n \rightarrow \infty} \int_{\Omega_R} u^n(\mathbf{x}) d\mathbf{x} \\
&= \int_0^Z \int_{-1}^1 \int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} u^n((0, 0, z)^T + s\omega(\phi) + t\omega^\perp(\phi)) dt ds dz \\
&= \int_0^Z \int_{-1}^1 \mathcal{R}_p u^n(s, \phi, z) ds dz \xrightarrow{n \rightarrow \infty} \int_0^Z \int_{-1}^1 \mathcal{R}_p u(s, \phi, z) ds dz,
\end{aligned} \tag{218}$$

and consequently $\int_0^Z \int_{-1}^1 \mathcal{R}_p u(s, \phi, z) ds dz = \int_{\Omega_R} u d\mathbf{x}$ for almost every ϕ . Therefore, a function f which does not satisfy $\int_0^Z \int_{-1}^1 f(s, \phi, z) ds dz = c$ constant for almost every ϕ can not be in the range of \mathcal{R}_p and therefore \mathcal{R}_p can not be surjective. \square

Note that one would always expect the distribution of the density u to be non-negative almost everywhere, and also the data $f = \ln\left(\frac{I_0}{I_1}\right)$ to be non-negative as $I_0 \geq I_1$. With the goal of using the Kullback-Leibler divergence which requires $\mathcal{R}_p u$ to be non-negative, we next show that the non-negativity of u is transferred to non-negativity of $\mathcal{R}_p u$.

Proposition 10.8. *The linear continuous function $\mathcal{R}_p: L^p(\Omega_R) \rightarrow L^p(\Omega_S)$ for $p \in [1, \infty)$ maintains non-negativity, i.e. for $u \in L^p(\Omega_R)$ with $u \geq 0$ almost everywhere also $\mathcal{R}_p u \geq 0$ almost everywhere.*

Proof. For $u \in \mathcal{C}(\overline{\Omega_R})$ the statement follows immediately from the definition of the Radon transform, since the line-integrals of non-negative functions are non-negative. For $u \in L^p(\Omega_R)$, there is a sequence $(u^n)_n \subset \mathcal{C}(\overline{\Omega_R})$ such that $\|u^n - u\|_p \xrightarrow{n \rightarrow \infty} 0$, and we may assume without loss of generality that $u^n \geq 0$ since $\|(u^n)^+ - u\|_p \leq \|u^n - u\|_p \rightarrow 0$ with $a^+ = \max(a, 0)$. Hence $\mathcal{R}_p u^n \geq 0$ almost everywhere, and $\mathcal{R}_p u^n(s, \phi, z) \xrightarrow{n \rightarrow \infty} \mathcal{R}_p u(s, \phi, z)$ for almost all $(s, \phi, z) \in \Omega_S$ subsequentially, and consequently also $\mathcal{R}_p u \geq 0$ almost everywhere. \square

The linear and continuous Radon transform also possesses an adjoint operator, which allows more insight into \mathcal{R}_p and its properties.

Proposition 10.9. *The adjoint of the operator $\mathcal{R}_p: L^p(\Omega_R) \rightarrow L^p(\Omega_S)$ for $p \in [1, \infty)$ is the operation*

$$\mathcal{R}_p^*: L^{p^*}(\Omega_S) \rightarrow L^{p^*}(\Omega_R), \quad \text{with} \quad \mathcal{R}_p^* f(\mathbf{x}) = \int_0^\pi f(\mathbf{x} \cdot \omega(\phi), \phi, \mathbf{x}_z) d\phi \quad (219)$$

for f continuous and with $\mathbf{x} = (x, y, z) \in \Omega_R \subset \mathbb{R}^3$ and \mathbf{x}_z denotes the 3. component of \mathbf{x} .

Proof. Let $u \in \mathcal{C}(\overline{\Omega_R})$, $f \in \mathcal{C}(\overline{\Omega_S})$, and we compute

$$\begin{aligned} \langle \mathcal{R}_p u, f \rangle &= \int_{\Omega_S} \mathcal{R}_p u \cdot f(s, \phi, z) d(s, \phi, z) = \int_0^\pi \int_0^Z \int_{-1}^1 \mathcal{R}_p u \cdot f(s, \phi, z) ds d\phi dz \\ &= \int_0^\pi \int_0^Z \int_{-1}^1 f(s, \phi, z) \left(\int_{-1}^1 u((0, 0, z)^T + s\omega(\phi) + t\omega^\perp(\phi)) dt \right) ds d\phi dz \\ &= \int_{\Omega_R} u(\mathbf{x}) \int_0^\pi f(\mathbf{x} \cdot \omega(\phi), \phi, \mathbf{x}_z) d\phi d\mathbf{x} = \langle u, \mathcal{R}_p^* f \rangle, \end{aligned}$$

where we substituted $\mathbf{x} = s\omega(\phi) + t\omega^\perp(\phi) + (0, 0, z)^T$ for fixed ϕ . For $p > 1$ and $p^* < \infty$ the space $\mathcal{C}(\overline{\Omega_S})$ is dense in $L^{p^*}(\Omega_S)$, and one can extend this function uniquely to a function $\mathcal{R}_p^*: L^{p^*}(\Omega_S) \rightarrow L^{p^*}(\Omega_R)$, and since $\mathcal{C}(\overline{\Omega_R})$ is dense in $L^p(\Omega_R)$, \mathcal{R}_p^* is indeed the adjoint operation to \mathcal{R}_p .

For $p = 1$ and $p^* = \infty$, the continuous functions are not dense in $L^\infty(\Omega_S)$ and hence the same procedure does not work. However, it is easy to see that when understanding

\mathcal{R}_2 as a linear, not necessarily continuous function $\mathcal{R}_2: L^2(\Omega_R) \subset L^1(\Omega_R) \rightarrow L^1(\Omega_S)$, that

$$\mathcal{R}_1 \supset \mathcal{R}_2 \quad \text{and consequently} \quad \mathcal{R}_1^* \subset \mathcal{R}_2^*, \quad (220)$$

where these inclusion are the inclusions of linear operators, i.e. $\text{dom}(\mathcal{R}_1^*) \subset \text{dom}(\mathcal{R}_2^*)$ and $\mathcal{R}_2^* = \mathcal{R}_1^*$ on $\text{dom}(\mathcal{R}_1^*)$. Consequently, the adjoint Radon transform for $p = 1$ has the same form as the adjoint of \mathcal{R}_2 restricted to L^∞ and for smooth functions the integral representation holds. \square

10.3. Filtered Backprojection

When considering the Radon transform on $L^2(\Omega_R)$, one can take advantage of the Hilbert space structure of L^2 to understand how the inversion of \mathcal{R} works. More precisely, being on a Hilbert space allows to investigate the linear continuous operation \mathcal{R} with spectral theory, enabling us to find the inverse operation under additional assumptions.

To do so, we employ a multiplicative version of the spectral theorem that features unitary and partially unitary operations, and a multiplication operation, which in this case are related to the Fourier transform, see e.g. [20].

Definition 10.10. *We define the Fourier transform in d dimensions as*

$$\mathcal{F}: L^1(\mathbb{R}^d, \mathbb{C}) \rightarrow \mathcal{C}(\mathbb{R}^d, \mathbb{C}), \quad \text{with} \quad \mathcal{F}u(\xi) = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} u(x) e^{-i\xi \cdot x} dx \quad (221)$$

for $u \in L^1(\mathbb{R}^d, \mathbb{C})$, where i denotes the imaginary unit.

It is easy to see, that the Fourier transform is well-defined as $\mathcal{F}u$ is continuous due to dominated convergence and the operator is also linear and continuous. In particular, note that in this entire chapter we allow for complex-valued functions without further mention. The Fourier transform can be seen as a continuous version of Fourier series, splitting a signal into individual spectra or frequencies. Therefore the Fourier transform is commonly used in acoustics, where one tries to insulate individual signals from overlapping frequencies, which can be directly seen in the Fourier transformed version of the signal. Similarly, the operation \mathcal{R}^* is in a way overlapping many different "signals" in the form of integrating over all lines $L(s, \phi, z)$ which pass through a point \mathbf{x} and thus we will see the connection between the Fourier transformation and the Radon transform.

Proposition 10.11. *There is a unique linear and continuous extension from the Fourier transform on $L^2 \cap L^1(\mathbb{R}^d)$ to $\mathcal{F}: L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$. Moreover, this Fourier transform*

between L^2 spaces is unitary (bijective and isomorphic), and for continuous $v \in L^2(\mathbb{R}^d)$ the following inversion formula holds:

$$\mathcal{F}^*v(x) = \mathcal{F}^{-1}v(x) = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{is \cdot x} v(s) \, ds. \quad (222)$$

This proposition confirms that indeed the suitable spaces for the Fourier transform are the L^2 spaces.

Proof. See e.g. [27, Thm 1.95, p 279], and use density of continuous functions. \square

Definition 10.12. For sets $\hat{\Omega}_R = \mathbb{R}^2 \times [0, Z]$ and $\hat{\Omega}_S = \mathbb{R} \times [0, \pi] \times [0, Z]$, we define the Fourier transform with respect to the first, or the first two variables as the extension of the operations

$$\mathcal{F}_1v(\xi, \phi, z) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\xi \cdot s} v(s, \phi, z) \, ds, \quad \text{and} \quad \mathcal{F}_2u(\xi, z) = \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{-i\xi \cdot \mathbf{x}} u(\mathbf{x}, z) \, d\mathbf{x} \quad (223)$$

for $L^1 \cap L^2$ functions on the spaces $L^2(\hat{\Omega}_S)$ and $L^2(\hat{\Omega}_R)$ respectively, i.e. exactly the Fourier transformations of the function with respect to the first one or two arguments, while leaving the other arguments fixed. Again, these operations are linear, continuous and unitary operations on the corresponding L^2 spaces, and their inverse operations are given in analogue manner to (222).

The following is known as the Fourier Slice (see e.g. [34, Thm 3.27 p 155]), and shows that in a way the Fourier transform is adapted to the Radon transform.

Proposition 10.13. Let the operation $T: \text{dom}(T) \subset L^2(\hat{\Omega}_R) \rightarrow L^2(\hat{\Omega}_S)$, called the slice operator, with $\text{dom}(T) = \{v \in L^2(\hat{\Omega}_R) \mid (\mathbf{x}, z) \mapsto v(\mathbf{x}, z)/|\mathbf{x}|^{\frac{1}{2}} \text{ is in } L^2\}$ be defined such, that for u continuous and $\tilde{\omega}(\phi) = (\cos(\phi), \sin(\phi))^T$ the operation $Tu(s, \phi, z) = u(s\tilde{\omega}(\phi), z)$. Then $\mathcal{F}_2(L^2(\Omega_R)) \subset \text{dom}(T)$ and the Radon transform $\mathcal{R}: L^2(\Omega_R) \rightarrow L^2(\Omega_S)$ satisfies

$$\frac{1}{\sqrt{2\pi}} \mathcal{F}_1 \mathcal{R} = T \mathcal{F}_2 \quad \text{on } L^2(\Omega_R), \quad (224)$$

when tacitly extending functions from $L^2(\Omega_R)$ and $L^2(\Omega_S)$ with zero values to $L^2(\hat{\Omega}_R)$ and $L^2(\hat{\Omega}_S)$ respectively.

Proof. The operator T is well-defined as for $u \in \text{dom}(T)$,

$$\|Tu\|_2^2 = \int_{\hat{\Omega}_S} |u(s\tilde{\omega}(\phi), z)|^2 \, d(s, \phi, z) = \int_{\hat{\Omega}_R} |u(\mathbf{x}, z)|^2 \frac{1}{|\mathbf{x}|} \, d(\mathbf{x}, z) < \infty,$$

where we substituted $\mathbf{x} = s\tilde{\omega}(\phi)$.

Next, we consider $u \in \mathcal{C}(\overline{\Omega_R})$ and compute for almost all ϕ, z and ξ

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \mathcal{F}_1 \mathcal{R} u(\xi, \phi, z) &= \frac{1}{2\pi} \int_{-1}^1 e^{-i\xi \cdot s} \mathcal{R} u(s, \phi, z) ds \\ &= \frac{1}{2\pi} \int_{-1}^1 \int_{-1}^1 u(s\tilde{\omega}(\phi) + t\tilde{\omega}^\perp(\phi), z) dt e^{-i\xi s} ds \\ &= \frac{1}{2\pi} \int_{B(0,1)} e^{-i\xi \tilde{\omega} \cdot \mathbf{x}} u(\mathbf{x}, z) d\mathbf{x} = \mathcal{F}_2 u(\xi \cdot \tilde{\omega}(\phi), z) = T \mathcal{F}_2 u(s, \phi, z), \end{aligned}$$

where we substituted $\mathbf{x} = s\tilde{\omega}(\phi) + t\tilde{\omega}^\perp(\phi)$. Due to the density of continuous functions in L^2 , the equation remains valid for $u \in L^2(\Omega_R)$. In particular the computation shows that $u \in \text{dom}(T)$ and the both sides of the claimed equation are well-defined. \square

Theorem 10.14 (Filtered Backprojection, see [34]). *Let the multiplication operator $M: \text{dom}(M) \subset L^2(\hat{\Omega}_S) \rightarrow L^2(\hat{\Omega}_S)$ be such that $\text{dom}(M) = \{f \in L^2(\hat{\Omega}_S) \mid (s, \phi, z) \mapsto f(s, \phi, z)|s|^{\frac{1}{2}} \text{ is in } L^2 \cap L^1\}$ and $Mf(s, \phi, z) = f(s, \phi, z)|s|^{\frac{1}{2}}$. If $\mathcal{R} u = f$ for $u \in L^2(\Omega_R)$ and $f \in L^2(\Omega_S)$ such that $\mathcal{F}_2 u \in L^1(\hat{\Omega}_R)$ and $\mathcal{F}_1 f \in \text{dom}(M)$, then*

$$u = \frac{1}{2\pi} \mathcal{R}^* \mathcal{F}_1^{-1} M \mathcal{F}_1 f. \quad (225)$$

This formula is called the Filtered Backprojection, it is however only under suitable assumptions an inversion. In particular this process is not continuously dependent on f in L^2 .

Proof. We again use $\tilde{\omega}(\phi) = (\cos(\phi), \sin(\phi))^T$. Due to the Fourier Slice Theorem we know that $\mathcal{F}_1 f = \sqrt{2\pi} T \mathcal{F}_2 u$. Thus, one can compute, with the L^1 assumptions

$$\begin{aligned} u(\mathbf{x}, z) &= \mathcal{F}_2^{-1} \mathcal{F}_2 u(\mathbf{x}, z) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \mathcal{F}_2 u(\xi, z) e^{i\mathbf{x} \cdot \xi} d\xi \\ &= \frac{1}{2\pi} \int_0^\pi \int_{\mathbb{R}} |s| \mathcal{F}_2 u(s\tilde{\omega}(\phi), z) e^{is\mathbf{x} \cdot \tilde{\omega}(\phi)} ds d\phi \\ &= \frac{1}{2\pi} \int_0^\pi \int_{\mathbb{R}} \frac{1}{\sqrt{2\pi}} |s| \mathcal{F}_1 f(s, \phi, z) e^{is\mathbf{x} \cdot \tilde{\omega}(\phi)} ds d\phi = \frac{1}{2\pi} \mathcal{R}^* \mathcal{F}_1^{-1} M \mathcal{F}_1 f(\mathbf{x}, z). \end{aligned}$$

\square

Remark 10.15. *Although there are technical assumptions, the Filtered Backprojection can be used in applications, in particular in a discrete setting where these technical assumptions do not pose any problems. The Filtered Backprojection is thus often used*

as a first approach, however, the non-continuity in the continuous setting transfers into an ill-conditioned property in the discretised version, which amplifies noise.

11. Tikhonov Approach to Multi-Spectra STEM CT Reconstruction

Now that we understand the Radon transform, one can formulate the multi-data inverse problem of reconstructing STEM CT data. This means we possess M (analytical) sinogram data sets, each corresponding to the density distribution of one specific chemical element, e.g. aluminium, silicon, etc.. Note that from a mathematical viewpoint the sinograms and densities we aim to reconstruct do not differ from the ones we considered in previous sections, solely their interpretation as spectral densities is different. Usually, one of the sinograms corresponds to the HAADF (high-angle annular dark field, see e.g. [46]) signal, which represents the overall mass-density distribution, i.e. CT data as described in previous sections.

So theoretically one has a set of M independent inverse problems of inverting the Radon transform for data (f_1, \dots, f_M) to reconstruct M spectral density distributions (u_1, \dots, u_M) . However, to take advantage of the complementing information contained in the data sets, e.g. common edge location information, overall mass, etc, we apply joint regularisation to couple the problems, resulting in a multi-data inverse problem. This becomes imperative as due to technical limitations such as the high time consumption for obtaining analytical data sets or the limited amount of intensity being used due to potential beam damages, the analytical data is often strongly disturbed by noise, in particular Poisson distributed noise.

As stated before, inversion of the Radon transform requires regularisation, and in particular the joint regularisation should promote information exchange between the individual spectra. Thus, we briefly present a regularisation framework for such problems, however, for all practical purposes the question of how to solve the resulting problems is of equally great importance. Therefore, we devote the majority of this chapter to presenting a discretisation scheme and a numerical approach to solve the resulting problems.

11.1. Continuous Tikhonov Problem for STEM CT Reconstruction

With the Radon transform sufficiently discussed, we see that it is a suitable operator to model the forward operation of obtaining CT data from an object via electron transmission projection, and reconstructing the individual spectra of STEM CT data is solving

$$\mathcal{R} u_1 = f_1^\dagger, \quad \dots, \quad \mathcal{R} u_M = f_M^\dagger, \quad (\text{Mul-Spec-Rec})$$

where $u = (u_1, \dots, u_M)$ represents the (spectral) density distributions, \mathcal{R} is the Radon-transform on $L^1(\Omega_R)$ and $f^\dagger = (f_1^\dagger, \dots, f_M^\dagger)$ with $f_i^\dagger \in L^1(\Omega_S)$ is the sinogram data. This means that from a mathematical viewpoint the spectral STEM CT reconstruction is the inversion of the Radon transform with spectral sinogram data f_i^\dagger obtained through STEM methods such as EDS in order to obtain the spectral density distribution (density distribution of a specific element) u_i for $i = 1, \dots, M$.

As these problems typically suffer from Poisson noise, we use Kullback-Leibler discrepancies, and TGV_α^2 for vector-valued functions is used for regularisation as it is expected to promote exchange of information yielding common features and smooth solutions.

Problem 11.1. *So to regularise the Problem (Mul-Spec-Rec), we use the following Tikhonov approach:*

$$\begin{cases} u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda, \alpha}(u, f^\dagger) & \text{such that } F_{\lambda, \alpha}(u, f^\dagger) < \infty, \\ \text{with } F_{\lambda, \alpha}(u, f) = \text{TGV}_\alpha^2(u) + \chi_{\{\geq 0\}}(u) + \sum_{i=1}^M \lambda_i D_{KL}(\mathcal{R} u_i, f_i). \end{cases} \quad (\text{TIKH-STEM})$$

In the notation of Chapter 3, $X = L^1(\Omega_R)^M$, $Y_i = L^1(\Omega_S)$ for $i = 1, \dots, M$, τ_X is the strong topology on L^1 , τ_{Y_i} the L^1 weak topology and τ_{D_i} is the topology in Definition 5.6 (the weakest topology making D_{KL} continuous). Note that the characteristic function $\chi_{\{\geq 0\}}(u)$ attains the value 0 if $u \geq 0$ a.e., and infinity otherwise, thus forcing solutions to satisfy non-negativity, as would be expected from density distributions. In particular, the characteristic function is convex, lower semi-continuous and non-negative as $\{u \in L^1(\Omega_R) \mid u \geq 0 \text{ a.e.}\}$ is convex and closed. Thus the family of functions $(R_\alpha)_{\alpha \in (0, \infty)^2}$ with $R_\alpha(u) = \text{TGV}_\alpha^2(u) + \chi_{\{\geq 0\}}(u)$ is a continuous family since the family $(\text{TGV}_\alpha^2)_{\alpha \in (0, \infty)^2}$ is (see Proposition 8.9) and these properties are not affected by adding the characteristic function.

So the theory of Chapter 3 ensures the the problem (TIKH-STEM) is well-defined when proper, and convergence results hold in a suitable setting. But while the problem

is solvable, it is yet unclear how to find said solution, and the following chapters try to answer this question.

11.2. Discretisation Scheme

While the consideration in infinite-dimensional spaces was suitable to understand the analytical properties of the problems and give us a general model and understanding of the situation, in practice always only a finite amount of data is available, and more could not be measured and processed anyways.

Thus, we need to reduce the setting to a finite-dimensional one and therefore we need to obtain a finite-dimensional inverse problem and Tikhonov approach. However, this discretisation should be done in a manner that maintains the characteristic traits of the functions and operations being used, hence preserving the original problem best we can.

Consequently we try to solve

$$\operatorname{argmin}_{u \in U} \tilde{F}_{\lambda, \alpha}(u), \quad \text{with } \tilde{F}_{\lambda, \alpha}(u) = \sum_{i=1}^M \lambda_i \tilde{D}_{KL}(\tilde{\mathcal{R}}u_i, f_i) + \widetilde{\text{TGV}}_{\alpha}^2(u), \quad (\text{D-TIKH-STEM})$$

where $\tilde{D}_{KL}: \Upsilon_i \times \Upsilon_i \rightarrow \mathbb{R}^{\infty}$ denotes a discretised version of D_{KL} , analogously $\tilde{\mathcal{R}}$ and $\widetilde{\text{TGV}}_{\alpha}^2$ are discrete versions of their continuous counterparts, and $U, \Upsilon = \Upsilon_1 \times \dots \times \Upsilon_M$ are discrete versions of X and Y respectively. While there might not be a unique way to discretise the occurring functions, one would like to do it in a consistent manner so that it indeed relates to the original functions and settings.

Thus we consider the reconstruction space $U = \mathbb{R}^{M \times N_x \times N_x \times N_z} = U_1 \times \dots \times U_M$ with $U_c = \mathbb{R}^{N_x \times N_x \times N_z}$ for $c = 1, \dots, M$. For an instance $u \in U$ we use $u = (u_1, \dots, u_M)$ where $u_c \in U_c$ denotes the c -th channels for $c = 1, \dots, M$, and the values $u_c = (u_c^{x,y,z})_{x=0, y=0, z=0}^{N_x-1, N_x-1, N_z-1}$ represent the values attained in the c -th channel at the position x, y, z representing the three space-dimensions. The domain $\tilde{\Omega}_R = \{0, \dots, N_x - 1\} \times \{0, \dots, N_x - 1\} \times \{0, \dots, N_z - 1\}$ is a discretisation of a cuboid in Ω_R , and $u \in U$ can be understood as a M -dimensional vector-valued function on $\tilde{\Omega}_R$. The connection between the continuous domain Ω_R and the discretised domain $\tilde{\Omega}_R$ can be understood via the mapping depicted in (226), whose meaning is illustrated in Figure 5:

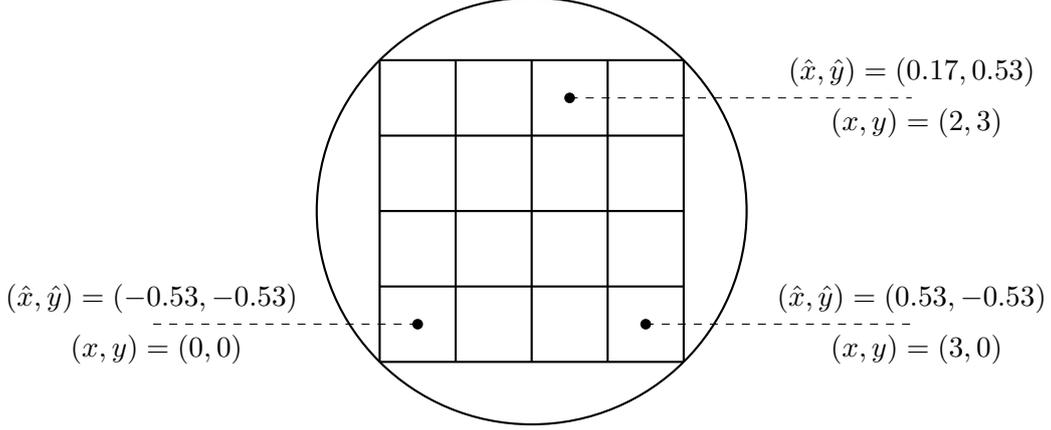


Figure 5: Cross-section illustration of the discretisation $\tilde{\Omega}_R$ in Ω_R for fixed z .

$$\begin{aligned} \hat{\cdot}: [-\frac{1}{2}, N_x - \frac{1}{2}] \times [-\frac{1}{2}, N_x - \frac{1}{2}] \times [-\frac{1}{2}, N_z - \frac{1}{2}] &\rightarrow \Omega_R \quad \text{with} & (226) \\ x \mapsto \hat{x} = -\frac{1}{\sqrt{2}} + (x + \frac{1}{2})\frac{\sqrt{2}}{N_x}, \quad y \mapsto \hat{y} = -\frac{1}{\sqrt{2}} + (y + \frac{1}{2})\frac{\sqrt{2}}{N_x}, \quad z \mapsto \hat{z} = (z + \frac{1}{2})\frac{\sqrt{2}}{N_z}, \end{aligned}$$

and we denote by $\check{\cdot}$ the inverse operation on a suitable domain.

The values in u can thus be understood as a vector of piece-wise constant functions in $L^1(\Omega_R)$ by interpreting the values as pixel values of adequately placed pixels in Ω_R . Here, N_x can be understood as the width and height (in form of pixels) of 2-dimensional images being stacked N_z times on top of one-another. Moreover, the vector space $V = (\mathbb{R}^3)^{M \times N_x \times N_x \times N_z}$ and the space $W = (\mathbb{R}^6)^{M \times N_x \times N_x \times N_z}$ have the same domain as U , but feature 3-dimensional vectors and 3×3 symmetric matrices, where $v \in V$ has the form $v = (v^1, v^2, v^3)$ with $v^i \in U$ and $w \in W$ with $w = (w^1, \dots, w^6)$ is such that w^1, w^2, w^3 represent the diagonal entries, and w^4, w^5, w^6 represent upper matrix entries of a symmetric matrix. These spaces will serve as the spaces containing the derivatives appearing in the discrete version of TGV as these can be understood as vector- and matrix-valued functions over the same domain. Note that although the Radon transform would require a cylinder, U contains functions defined over a cuboid, and we imagine functions $u \in U$ to be extended outside this cuboid with zero-values such that it is indeed defined in an enveloping cylinder.

The geometry of the cylinder is of course strongly related to the Radon transform, which leads us to the discretisation of the sinogram space, for which we consider the space $\Upsilon = \mathbb{R}^{M \times N_s \times N_a \times N_z}$ and $\Upsilon_c \in \mathbb{R}^{N_s \times N_a \times N_z}$ for $c = 1, \dots, M$ with $\Upsilon = \Upsilon_1 \times \dots \times \Upsilon_M$.

We use the notation $f = (f_1, \dots, f_M) \in \Upsilon$ such that $f_c \in \Upsilon_c$ for $c = 1, \dots, M$, where again the notation $f_c^{s,\phi,z}$ is used and the first axis represents the offsets, the second the corresponding angle, and the last the z space-dimension. Again, there is a connection between Ω_S and $\tilde{\Omega}_S = \{0, \dots, N_s - 1\} \times \mathcal{A} \times \{0, \dots, N_z - 1\}$ with set of angles \mathcal{A} , representing the domain for functions in Υ_i . We obtain a suitable interpretation of the discretisation, by considering the operation

$$\hat{\cdot}: \rightarrow [-\frac{1}{2}, N_s - \frac{1}{2}] \rightarrow [-1, 1] \quad s \mapsto \hat{s} = -1 + (s + \frac{1}{2})\frac{2}{N_s}, \quad (227)$$

and $z \mapsto \hat{z}$ as defined in (226). Thus $f \in \Upsilon$ can be interpreted as a vector-valued piece-wise constant function on Ω_S .

Accordingly, N_s denotes the number of pixel fitting in the diagonal of the corresponding square, or the radius of the enveloping cylinder and is roughly $\sqrt{2}N_x$. There are N_a angles from which projections are taken, and those angles are contained in a list \mathcal{A} . In slight abuse of notation, we will sometimes use $\phi \in \mathcal{A}$ as an index, and sometimes as the angle itself. Hence, for $f \in \Upsilon$, we use an analogous notation $f_c^{s,\phi,z}$ (with $\phi \in \mathcal{A}$ and not $\phi \in \{0, \dots, N_a - 1\}$) to denote the value of f corresponding to these instances s, ϕ, z and channel c . So again f can be understood as a vector-valued function on $\tilde{\Omega}_S$ (although the angles are not necessarily uniformly distributed in $[0, \pi)$) and represent pixel values in Ω_S . Note that here identical Υ_c for all c are used for the sake of simplicity, however, these spaces could be different, i.e. have different angles/resolutions, and one would need to adapt the following discretisations to the individual spaces which follows the same ideas.

The spaces U, Υ are equipped with norms $\|u\|^2 = \sum_{c=1}^M \sum_{x,y,z=0}^{N_x-1, N_x-1, N_z-1} |u_c^{x,y,z}|^2$ and $\|f\|^2 = \sum_{c=1}^M \sum_{x,y,z=0}^{N_s-1, N_a-1, N_z-1} |f_c^{s,\phi,z}|^2$ for $u \in U, f \in \Upsilon$ and with those U and Υ are Hilbert spaces, and the corresponding inner products are the sums of point-wise products.

Remark 11.2. *Note that this norm on Υ would only be a special case of the L^2 norm for piece-wise constant functions if the angles in \mathcal{A} were uniformly distributed in $[0, \pi)$, i.e. equi-distant placement in $[0, \pi)$, as otherwise some values might be representative of larger regions than others, thus making a weighting of the sum necessary. However, for our considerations we will not use such weights, i.e. assume uniformly distributed angles. One could also factor in this different weights into the norm and the measure used for the Kullback-Leibler divergence yielding slight changes to the following considerations.*

Remark 11.3. *Note that we consider the reconstruction on a cuboid $\tilde{\Omega}_R$ and not on*

a cylinder, which is for the sake of convenience and avoiding additional computational complications coming from more complex domains, while not creating any real drawbacks. In practice one looks at square images anyways, and one could assume no mass to be present outside a certain area by increasing the radius of the cylinder.

In the following we propose discretisations of relevant functions, which are designed in a manner which allows for parallel implementation, enabling quick execution of the corresponding operations while capturing the essence of the original functions. This in particular holds for the Radon transform and its adjoint, whose computation comes at great computational expense.

Discretisation: Kullback-Leibler divergence

Recall that $D_{KL}(v_i, f_i) = \int_{\Omega_S} \left(v_i - f_i - f_i \ln \left(\frac{v_i}{f_i} \right) \right) d(s, \phi, z)$ in the continuous setting. Since we assume all angles to carry the same weight as stated in Remark 11.2, and the nodes with respect to the other dimensions are equi-distantly distributed, we can discretise the integral to a simple sum over all entries, which is in particular unweighted as we use the Lebesgue-measure. Furthermore, to avoid unnecessary computational effort, for $v_i, f_i \in \Upsilon_i$ we can reduce the integrand $v_i - f_i - f_i \ln \left(\frac{v_i}{f_i} \right)$ of D_{KL} to the integrand $v_i - f_i \ln(v_i)$, as the difference of the two is constant with respect to v_i , and thus this change does not alter the minimisation problem's solutions.

Consequently we obtain the following discrete version of D_{KL} for $v_i, f_i \in \Upsilon_i$:

$$\tilde{D}_{KL}(v_i, f_i) = \begin{cases} \sum_{s, \phi, z} v_i^{s, \phi, z} - f_i^{s, \phi, z} \ln(v_i^{s, \phi, z}), & \text{if } v_i, f_i \geq 0 \text{ and } v_i^{s, \phi, z} = 0 \Rightarrow f_i^{s, \phi, z} = 0, \\ \infty, & \text{else.} \end{cases} \quad (228)$$

Note that this function is indeed a discretised version of D_{KL} , and one could adapt this functional to incorporate more general measures concerning the angles and the other dimensions.

Discretisation: Total Generalised Variation

To discretise TGV_α^2 , we use the infimal convolution representation as stated in (183) and discretise it. For $k = 2$, this representation reduces to $\text{TGV}_\alpha^2(u) = \inf_v \alpha_1 \|v - \nabla u\|_{\mathcal{M}, A_1^*} + \alpha_0 \|\mathcal{E}v\|_{\mathcal{M}, A_0^*}$ for suitable v with $\|\cdot\|_{\mathcal{M}, A_i^*} = \|\|\cdot\|_{A_i^*}\|_{\mathcal{M}}$ with $\|\cdot\|_{A_i^*}$ a norm on $\text{Sym}^{2-i, d}$, and consequently we need to generalise the occurring norms and differential operators.

First we note, that the definitions of the point-wise norms $|\cdot|_{A_i}$ on $\text{Sym}^{2-i,d}$ still make sense in the respective spaces V and W as point-wise norms, when understanding the values of $v \in V$ and $w \in W$ as multilinear functions. Classical choices are Frobenius type norms but more sophisticated choices are possible, e.g. the nuclear norm, see [29]. Also, the occurring functions $v \in V$, $w \in W$ satisfy $|v|_{A_1} \in L^1$ and $|w|_{A_0} \in L^1$ when understood as piece-wise constant functions since they are bounded, and thus one can reformulate $\| |v|_{A_1^*} \|_{\mathcal{M}} = \| |v|_{A_1^*} \|_{L^1}$ which in this discrete setting reduces to $\| |v|_{A_1^*} \|_{l^1} = \sum_{x,y,z=0}^{N_x-1, N_x-1, N_z-1} |v_c^{x,y,z}|_{A_1^*}$ and analogously for w .

To define the differential operations on U and V , we use a standard finite differences approach. Thus we define for $u \in U$

$$\begin{aligned} \tilde{\nabla}: U &\rightarrow V, & \tilde{\nabla}u &= (\delta_x^+ u, \delta_y^+ u, \delta_z^+ u) \text{ with} & (229) \\ \delta_x^+, \delta_y^+, \delta_z^+: U &\rightarrow U, & (\delta_x^+ u)_c^{x,y,z} &= \begin{cases} u_c^{x+1,y,z} - u_c^{x,y,z} & \text{if } x \in \{0, \dots, N_x - 2\}, \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

and analogously for δ_y^+ and δ_z^+ . Furthermore, we define the discretised symmetric Jacobian for $v = (v^1, v^2, v^3)$ via

$$\begin{aligned} \tilde{\mathcal{E}}: V &\rightarrow W, & \tilde{\mathcal{E}}v &= \left(\delta_x^- v^1, \delta_y^- v^2, \delta_z^- v^3, \frac{\delta_x^- v^2 + \delta_y^- v^1}{2}, \frac{\delta_x^- v^3 + \delta_z^- v^1}{2}, \frac{\delta_y^- v^3 + \delta_z^- v^2}{2} \right) & (230) \\ \delta_x^-: U &\rightarrow U, & \text{such that } (\delta_x^- u)_c^{x,y,z} &= \begin{cases} u_c^{x,y,z} - u_c^{x-1,y,z} & \text{if } x > 0, \\ 0 & \text{else,} \end{cases} \end{aligned}$$

and analogously δ_y^- , δ_z^- . We will also require the adjoint to these operations and thus introduce a discrete divergence such that $-\widetilde{\text{div}} = \tilde{\nabla}^*$ and $-\widetilde{\text{div}} = \tilde{\mathcal{E}}^*$ in their respective spaces. In order to do so, we define operations

$$\hat{\delta}_x^+: U \rightarrow U \quad \text{with} \quad (\hat{\delta}_x^+ u)_c^{x,y,z} = \begin{cases} u_c^{x,y,z} - u_c^{x-1,y,z} & \text{if } x = 1, \dots, N_x - 2, \\ u_c^{0,y,z} & \text{if } x = 0, \\ -u_c^{N_x-2,y,z} & \text{if } x = N_x - 1, \end{cases} \quad (231)$$

and

$$\hat{\delta}_x^- : U \rightarrow U \quad \text{with} \quad (\hat{\delta}_x^- u)_c^{x,y,z} = \begin{cases} u_c^{x+1,y,z} - u_c^{x,y,z} & \text{if } x = 1, \dots, N_x - 2, \\ u_c^{1,y,z} & \text{if } x = 0, \\ -u_c^{N_x-1,y,z} & \text{if } x = N_x - 1, \end{cases} \quad (232)$$

and analogously for other axes. Then, for $v \in V$ and $w \in W$, we obtain the adjoint operations

$$\begin{aligned} \tilde{\nabla}^* v &= -\tilde{\text{div}} v, & \tilde{\mathcal{E}}^* w &= -\tilde{\text{div}} w = -((\tilde{\text{div}} w)^1, (\tilde{\text{div}} w)^2, (\tilde{\text{div}} w)^3), \\ \tilde{\text{div}} v &= \hat{\delta}_x^+ v^1 + \hat{\delta}_y^+ v^2 + \hat{\delta}_z^+ v^3, & (\tilde{\text{div}} w)^1 &= \hat{\delta}_x^- w^1 + \hat{\delta}_y^- w^4 + \hat{\delta}_z^- w^5, \\ (\tilde{\text{div}} w)^2 &= \hat{\delta}_x^- w^4 + \hat{\delta}_y^- w^2 + \hat{\delta}_z^- w^6, & (\tilde{\text{div}} w)^3 &= \hat{\delta}_x^- w^5 + \hat{\delta}_y^- w^6 + \hat{\delta}_z^- w^3. \end{aligned} \quad (233)$$

So we finally define

$$\widetilde{\text{TGV}}_\alpha^2(u) = \inf_{v \in V} \alpha_1 \|v - \tilde{\nabla} u|_{A_1^*}\|_{L^1} + \alpha_0 \| |\tilde{\mathcal{E}} v|_{A_0^*} \|_{L^1}. \quad (234)$$

Discretisation: Adjoint Radon transform

For the algorithmic solution of the problem, we will also require a discretisation of the adjoint of the operator featured in the inverse problem, and since the interpretation of this is easier to understand and motivates the discretisation used on the Radon transform, we start with the adjoint.

Recall that for a function f on the sinogram space, the adjoint Radon transform has the form $\mathcal{R}^* f(\mathbf{x}) = \int_{\Omega_s} f(\mathbf{x} \cdot \omega(\phi), \phi, z) d\phi$ where $\mathbf{x} = (x, y, z)$. Since all angles carry the same weight, we can reduce the integral to a summation over all angles in \mathcal{A} . Thus, the only issue is the evaluation of f at s with $\hat{s} = (\hat{\mathbf{x}} \cdot \omega(\phi))$ which will not be an integer in general and thus does not allow evaluation for $f \in \Upsilon_c$. Therefore, we wish to interpolate between adjacent integer values in the s axis, and in order to do so we introduce the following notation.

For fixed $\phi \in \mathcal{A}$ and $\mathbf{x} \in \tilde{\Omega}_R$ we say \mathbf{x} is between $s \in \{0, \dots, N_s - 1\}$ and $s + 1$ if $\hat{s} \leq \hat{\mathbf{x}} \cdot \omega(\phi) < \widehat{s + 1}$, and also say $L(s, \phi, z)$ and $L(s + 1, \phi, z)$ are the adjacent lines of \mathbf{x} . Conversely, we call all \mathbf{x} as above which are between s and $s + 1$ or between $s - 1$ and s adjacent to $L(s, \phi, z)$ (see Figure 6).

With these notations, for fixed ϕ we define the mapping $s_\phi(\mathbf{x})$ to denote the smaller adjacent offset. Moreover, $p_\phi(\mathbf{x}) = \hat{\mathbf{x}} \cdot \omega(\phi) - \hat{s}_\phi(\mathbf{x})$ denotes the distance between $\hat{s} = \hat{\mathbf{x}} \cdot \omega$

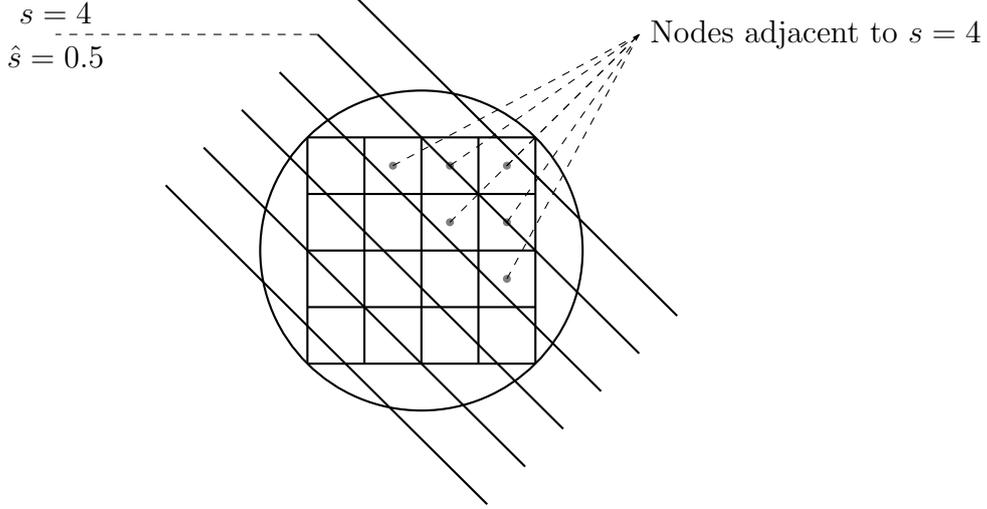


Figure 6: Illustration of the adjacency relation between s and \mathbf{x} for fixed ϕ .

and $\hat{s}_\phi(\mathbf{x})$, and $1 - p_\phi(\mathbf{x})$ is the distance from \hat{s} to $\widehat{s_\phi(\mathbf{x}) + 1}$. So interpolation implies $f_i(\hat{\mathbf{x}} \cdot \omega(\phi), \phi, \hat{z}) \approx p_\phi(\mathbf{x}) f_i(\widehat{s_\phi(\mathbf{x}) + 1}, \phi, \hat{z}) + (1 - p_\phi(\mathbf{x})) f_i(\hat{s}_\phi(\mathbf{x}), \phi, \hat{z})$.

Putting these considerations together, for $f_i \in \Upsilon_i$ and $\mathbf{x} = (x, y, z) \in \tilde{\Omega}_R$ we define

$$\begin{aligned} \tilde{\mathcal{R}}^* : \Upsilon_i &\rightarrow U_i \quad \text{with} \quad \tilde{\mathcal{R}}^* f_i(\mathbf{x}) = \sum_{\phi \in \mathcal{A}} \underbrace{p_\phi(\mathbf{x}) f_i(\widehat{s_\phi(\mathbf{x}) + 1}, \phi, \hat{z}) + (1 - p_\phi(\mathbf{x})) f_i(\hat{s}_\phi(\mathbf{x}), \phi, \hat{z})}_{\approx f(\hat{\mathbf{x}} \cdot \omega(\phi), \phi, \hat{z})} \\ &= \sum_{\phi \in \mathcal{A}} p_\phi(\mathbf{x}) f_i^{s_\phi(\mathbf{x})+1, \phi, z} + (1 - p_\phi(\mathbf{x})) f_i^{s_\phi(\mathbf{x}), \phi, z}. \end{aligned} \quad (235)$$

Discretisation: Radon transform

Finally, we consider the discretisation of the Radon transform, and note that there is no completely obvious way to discretise it. As the adjoint operator features an interpolation in the s dimension, one would expect a distribution of mass in \mathbf{x} onto adjacent lines in the s dimension to occur in the discretised Radon transform.

Consequently, one would imagine that for fixed s, ϕ, z a contribution to the line integral along $L = L(s, \phi, z)$ is made by all \mathbf{x} adjacent to L , and the corresponding weights to be relative to the respective distances, which computes as $|\hat{s} - \hat{\mathbf{x}} \cdot \omega(\phi)|$.

However, unlike in the case of the adjoint operator, now for fixed s, ϕ, z there is potentially a large number of adjacent integer nodes \mathbf{x} , and thus we require an efficient scheme to find adjacent nodes.

For fixed s, ϕ and z with $\omega(\phi) = (\omega_x, \omega_y, 0) = (\cos(\phi), \sin(\phi), 0)$ and $L = L(s, \phi, z)$, eligible $\mathbf{x} = (x, y, z) \in \tilde{\Omega}_R$ are all that satisfy $\widehat{s-1} \leq \omega_x \hat{x} + \omega_y \hat{y} < \widehat{s+1}$. We fix

$y \in \{0, \dots, N_x - 1\}$ and by reformulating this equation one sees that suitable x are between x_{low} and x_{high} (dependent on s, ϕ, y) which are computed as follows:

$$\begin{aligned} \tilde{x}_{\text{low}} &= (\omega_x^{-1}(\widehat{s-1} - \omega_y \hat{y}))^\sim, & \tilde{x}_{\text{high}} &= (\omega_x^{-1}(\widehat{s+1} - \omega_y \hat{y}))^\sim & \text{if } \omega_x > 0, \\ \tilde{x}_{\text{low}} &= (\omega_x^{-1}(\widehat{s+1} - \omega_y \hat{y}))^\sim, & \tilde{x}_{\text{high}} &= (\omega_x^{-1}(\widehat{s-1} - \omega_y \hat{y}))^\sim & \text{if } \omega_x < 0, \\ \tilde{x}_{\text{low}} &= 0 & \tilde{x}_{\text{high}} &= N_x - 1 & \text{if } \omega_x = 0, \end{aligned} \quad (236)$$

and $x_{\text{low}} = \max(\text{ceil}(\tilde{x}_{\text{low}}), 0)$ and $x_{\text{high}} = \min(\text{floor}(\tilde{x}_{\text{high}}), N_x - 1)$ which describes the boundary of all x values such that $\mathbf{x} = (x, y, z)$ is adjacent to $L(s, \phi, z)$ and obviously only nodes in $[0, \dots, N_x - 1]$ are relevant. The corresponding distance between \mathbf{x} and L is again given by $|\hat{s} - \omega_x \hat{x} - \omega_y \hat{y}|$, so for each y , one can find all x such that (x, y, z) are sufficiently close to L and we understand the line integral along the line L as a weighted sum of the function values in these points. Hence, we define

$$\begin{aligned} \tilde{\mathcal{R}}: U_i \rightarrow \Upsilon_i, \text{ s.t. } \tilde{\mathcal{R}}u(s, \phi, z) &= \sum_{y=0}^{N_x-1} \sum_{\substack{x \in \mathbb{N} \\ x \in [x_{\text{low}}, x_{\text{high}}]}} (1 - |\hat{s} - \omega(\phi)_x \hat{x} - \omega(\phi)_y \hat{y}|) u_i(\hat{x}, \hat{y}, \hat{z}) \\ &= \sum_{y=0}^{N_x-1} \sum_{\substack{x \in \mathbb{N} \\ x \in [x_{\text{low}}, x_{\text{high}}]}} (1 - |\hat{s} - \omega(\phi)_x \hat{x} - \omega(\phi)_y \hat{y}|) u_i^{x,y,z} \end{aligned} \quad (237)$$

for $u_i \in U_i$, where $\sum_{x_{\text{low}}}^{x_{\text{high}}} = 0$ if $x_{\text{low}} > x_{\text{high}}$.

We note that these discretised versions $\tilde{\mathcal{R}}, \tilde{\mathcal{R}}^*$ of \mathcal{R} and \mathcal{R}^* are indeed adjoint. To show this we prove

$$\langle \tilde{\mathcal{R}}u, v \rangle = \langle u, \tilde{\mathcal{R}}^* v \rangle \quad (238)$$

for delta functions $u = \mathcal{I}_{\bar{x}, \bar{y}, \bar{z}_1} \in U_i$ and $v = \mathcal{I}_{\bar{s}, \bar{\phi}, \bar{z}_2} \in \Upsilon_i$ with $\bar{x}, \bar{y} \in \{0, \dots, N_x - 1\}$, $\bar{z}_1, \bar{z}_2 \in \{0, \dots, N_z - 1\}$ $\bar{s} \in \{0, N_s - 1\}$ and $\bar{\phi} \in \mathcal{A}$, those functions are 1 in case the argument is $(\bar{x}, \bar{y}, \bar{z}_1)$, $(\bar{s}, \bar{\phi}, \bar{z}_2)$ respectively and zero otherwise. Therefore we solely need to compute $\tilde{\mathcal{R}}u(\bar{s}, \bar{\phi}, \bar{z}_2)$ and $\tilde{\mathcal{R}}^* v(\bar{x}, \bar{y}, \bar{z}_1)$ and observe that they are equal.

In order for the value $\tilde{\mathcal{R}}u(\bar{s}, \bar{\phi}, \bar{z}_2)$ to be non-zero, $\bar{x}, \bar{y}, \bar{z}$ must appear in the sum in (237), so $\bar{x} \in [x_{\text{low}}, x_{\text{high}}]$ which depend on $\bar{y}, \bar{s}, \bar{\phi}$ must be satisfied. Recall that \bar{x} satisfies this condition if and only if $\bar{\mathbf{x}} = (\bar{x}, \bar{y}, \bar{z}_1)$ is adjacent to $L(\bar{s}, \bar{\phi}, \bar{z}_2)$, and in this case the coefficient $(1 - |\hat{s} - \omega(\bar{\phi})_x \hat{x} - \omega(\bar{\phi})_y \hat{y}|)$ denotes "one minus the distance from $\hat{\mathbf{x}}$ to $L(\bar{s}, \bar{\phi}, \bar{z}_2)$ ". So $\tilde{\mathcal{R}}u(\bar{s}, \bar{\phi}, \bar{z}_2) = 0$ if $\bar{\mathbf{x}}$ is not adjacent to $L(\bar{s}, \bar{\phi}, \bar{z}_2)$, and one minus the distance otherwise.

Conversely, if we compute $\tilde{\mathcal{R}}^* v(\bar{\mathbf{x}})$ with the definition in (235), the sum is empty if

$s_{\bar{\phi}}(\bar{\mathbf{x}}) \notin \{\bar{s}, \bar{s} - 1\}$ and in this case $\tilde{\mathcal{R}}^* v(\bar{\mathbf{x}}) = 0$. Otherwise, $L(\bar{s}, \bar{\phi}, \bar{z}_2)$ is adjacent to $\bar{\mathbf{x}}$, and in this case the coefficients are $1 - p_{\bar{\phi}}(\bar{\mathbf{x}})$ or $p_{\bar{\phi}}(\bar{\mathbf{x}})$ which denote the distance to $s_{\bar{\phi}}(\bar{\mathbf{x}}) + 1, \hat{s}_{\bar{\phi}}(\bar{\mathbf{x}})$ respectively. So $\tilde{\mathcal{R}}^* v(\bar{\mathbf{x}})$ is "one minus the distance from $L(\bar{s}, \bar{\phi}, \bar{z}_2)$ to $\hat{\mathbf{x}}$ " if they are adjacent, and zero otherwise. Hence

$$\langle u, \tilde{\mathcal{R}}^* v \rangle = \tilde{\mathcal{R}}^* v(\bar{\mathbf{x}}) = \tilde{\mathcal{R}} u(\bar{s}, \bar{\phi}, \bar{z}_2) = \langle \tilde{\mathcal{R}} u, v \rangle, \quad (239)$$

and thus the operators are indeed adjoint.

Remark 11.4. *We note that the relevant analytic properties such as continuity and coercivity statements of the occurring functions transfer into this discrete setting. We leave the proof to the interested reader.*

11.3. Primal-Dual Optimisation Algorithm

After having defined the problem (D-TIKH-STEM) in a suitable discrete setting, one needs to actually solve it in practical applications. However, TGV is not differentiable in the classical sense making many of the common choices for optimisation methods such as gradient descent or Newton [10, 7, 33] not applicable. Therefore, we apply the primal-dual algorithm presented in [17], which is used to solve convex minimisation problems with linear and continuous operators in it. More precisely, we consider the (primal) problem

$$\min_{x \in H_1} F(x) + G(Ax) \quad (240)$$

on Hilbert spaces H_1 and H_2 , with proper, lower semi-continuous, convex functions $F: H_1 \rightarrow \mathbb{R}^\infty$ and $G: H_2 \rightarrow \mathbb{R}^\infty$ and linear and continuous operation $A: H_1 \rightarrow H_2$.

Via the statement of Proposition 1.45, one can reformulate (240) to the saddle-point problem

$$\min_{x \in H_1} \sup_{\xi \in H_2} \mathcal{L}(x, \xi), \quad \text{with} \quad \mathcal{L}(x, \xi) = \langle \xi, Ax \rangle + F(x) - G^*(\xi). \quad (\text{Gen-Sad})$$

Note that cases $\infty - \infty$ are not relevant due to the properness, and thus ξ such that $G^*(\xi) = \infty$ will not be relevant to the supremum. We assume throughout the chapter that a pair $(x^*, \xi^*) \in H_1 \times H_2$ exists that solves (Gen-Sad).

Before we can state the solution algorithm, we require a definition and proposition in order to understand the operations in the algorithm and ensure they are well-defined. For a more detailed discussion of these, we refer to [41] as well as the references therein.

Definition 11.5. Let H be a Hilbert space and let $F: H \rightarrow \mathbb{R}^\infty$ be proper, convex and lower semi-continuous. Then, for $\sigma > 0$, the mapping

$$\text{prox}_\sigma^F: H \rightarrow H, \quad \text{prox}_\sigma^F(x_0) = \underset{x \in X}{\operatorname{argmin}} \frac{\|x - x_0\|^2}{2} + \sigma F(x) = (I + \sigma \partial F)^{-1}(x_0) \quad (241)$$

is called the proximal mapping (or proximation, resolvent) of F .

The following proposition confirms that the proximal mapping is indeed well-defined as a mapping, and not a set-valued mapping.

Proposition 11.6. For a Hilbert space H and $F: H \rightarrow \mathbb{R}^\infty$ proper, convex and lower semi-continuous, for each $x_0 \in H$ there is a unique $x \in H$ such that $x \in \text{prox}_\sigma^F(x_0)$, and consequently prox_σ^F can indeed be understood as a mapping from H to H .

For the saddle-point problem (Gen-Sad), [17] proposes Algorithm 1.

Algorithm 1 Primal-Dual Algorithm

INPUT: Operators A, A^* between Hilbert spaces H_1 and H_2 , reals $\sigma, \tau > 0$ such that $\sigma\tau\|A\|^2 < 1$ and proximal mappings $\text{prox}_\sigma^F, \text{prox}_\tau^{G^*}$.

- 1: Initialise $x^0 = 0 \in H_1, \xi^0 = 0 \in H_2$ and $\bar{x} = 0 \in H_1$.
 - 2: **for all** $n = 0, 1, \dots$ **do**
 - 3:
$$\begin{cases} \xi^{n+1} = \text{prox}_\sigma^{G^*}(\xi^n + \sigma A\bar{x}) \\ x^{n+1} = \text{prox}_\tau^F(x^n - \tau A^*\xi^{n+1}) \\ \bar{x} = 2x^{n+1} - x^n \end{cases}$$
-

Output: Sequence of pairs $(x^n, \xi^n)_n$ which converge to a solution of (Gen-Sad).

Remark 11.7. Note that in practical applications one does not compute the loop in Algorithm 1 for infinitely many n , but uses a stopping criteria. Aside from stopping after a predetermined number of iterations, one can use a posteriori convergence criteria such as the primal-dual gap criteria [17].

The following theorem stated in [17] ensures the convergence of the iterates.

Theorem 11.8. If the dimensions of H_1 and H_2 are finite and there exists a solution to (Gen-Sad), then the iterates $(x^n, \xi^n)_n$ converge to a saddle-point $(\hat{x}, \hat{\xi})$.

Consequently the algorithm is indeed correct and when terminating after finitely many steps, one obtains an approximate solution. Note that similar convergence results can be found for infinite-dimensional spaces, however we will not require them as we will apply Algorithm 1 to (D-TIKH-STEM).

11.4. STEM CT Reconstruction Algorithm

In order to apply Algorithm 1 to (D-TIKH-STEM), we need to first reformulate it as a saddle-point problem, and compute the required proximal mappings.

We denote with H_1, H_2 the spaces $H_1 = U \times V$ and $H_2 = (\Upsilon \times V \times W)$, denote by $F: H_1 \rightarrow \mathbb{R}^\infty$ and $G: H_2 \rightarrow \mathbb{R}^\infty$ the functions

$$F((u, v)) = \chi_{\{\cdot \geq 0\}}(u), \quad G((y, p, w)) = \sum_{i=1}^M \lambda_i \tilde{D}_{KL}(y_i, f_i) + \alpha_1 \|p\|_{l^1, A_1^*} + \alpha_0 \|w\|_{l^1, A_0^*}, \quad (242)$$

and by $A: H_1 \rightarrow H_2$ and $A^*: H_2 \rightarrow H_1$ the (adjoint) mappings

$$\begin{aligned} A(u, v) &= \left((\tilde{\mathcal{R}}u_1, \dots, \tilde{\mathcal{R}}u_M), \tilde{\nabla}u - v, \tilde{\mathcal{E}}v \right), \\ A^*(\xi, p, w) &= \left((\tilde{\mathcal{R}}^* \xi_1, \dots, \tilde{\mathcal{R}}^* \xi_M) - \widetilde{\text{div}} p, -\widetilde{\text{div}} w - p \right). \end{aligned} \quad (243)$$

Those will serve as functions as in (Gen-Sad) for this concrete problem. With these definitions, we compute

$$\begin{aligned} \min_{u \in U} \tilde{F}_{\lambda, \alpha}(u) &= \min_{u \in U} \sum_{i=1}^M \lambda_i \tilde{D}_{KL}(\tilde{\mathcal{R}}u_i, f_i) + \chi_{\{\cdot \geq 0\}}(u) + \widetilde{\text{TGV}}_\alpha^2(u) = \\ &= \min_{(u, v) \in H_1} \sum_{i=1}^M \lambda_i \tilde{D}_{KL}(\tilde{\mathcal{R}}u_i, f_i) + \chi_{\{\cdot \geq 0\}}(u) + \alpha_1 \|\tilde{\nabla}u - v\|_{l^1, A_1^*} + \alpha_0 \|\tilde{\mathcal{E}}v\|_{l^1, A_0^*} \\ &= \min_{(u, v) \in H_1} \sup_{(\xi, p, w) \in H_2} \chi_{\{\cdot \geq 0\}}(u) + \langle (u, v), A^*(\xi, p, w) \rangle - G^*(\xi, p, w). \end{aligned} \quad (244)$$

So in order to apply the Algorithm 1 to the saddle-point problem

$$\begin{cases} \min_{(u, v) \in H_1} \sup_{(\xi, p, w) \in H_2} \mathcal{L}((u, v), (\xi, p, w)), \\ \text{with } \mathcal{L}((u, v), (\xi, p, w)) = \langle (u, v), A^*(\xi, p, w) \rangle + F(u, v) - G^*(\xi, p, w), \end{cases} \quad (\text{Saddle-Tikh})$$

we need to compute the norm of $\|A\|$ and the proximal mappings corresponding to F and G^* .

For the computation of the norm of $\|A\|$ one can apply the Power-Iteration [8] used to find the greatest singular value, which due to the Hilbert space norm is equal to the norm of the operator.

To compute $\text{prox}_\sigma^{\chi_{\{\cdot \geq 0\}}}(u_0) = \text{argmin}_{u \in U} \frac{\|u - u_0\|^2}{2} + \sigma \chi_{\{\cdot \geq 0\}}(u)$, it is easy to see that this

minimum is attained only by the projection of u_0 onto $\{u \in U \mid u \geq 0\}$, i.e.

$$\text{prox}_\sigma^{\chi_{\{\cdot \geq 0\}}}(u_0) = \text{proj}_{\{u \geq 0\}}(u_0) = u_0^+, \quad (245)$$

with $a^+ = \max(a, 0)$ point-wise. Determination of $\text{prox}_\tau^{G^*}$ involves more computation due to its greater complexity. First, we see due to the independence of the terms in G that

$$\begin{aligned} G^*(\xi, p, w) &= \sup_{(y, \nu, \omega) \in H_2} \langle \xi, y \rangle + \langle \nu, p \rangle + \langle \omega, w \rangle \\ &\quad - \left(\left[\sum_{i=1}^M \lambda_i \tilde{D}_{KL}(y_i, f_i) \right] + \alpha_1 \|\nu\|_{l^1, A_1^*} + \alpha_0 \|\omega\|_{l^1, A_0^*} \right) \\ &= \left[\sum_{i=1}^M \sup_{y_i \in Y_i} \left(\langle \xi_i, y_i \rangle - \lambda_i \tilde{D}_{KL}(y_i, f_i) \right) \right] + \sup_{\nu \in V} \left(\langle \nu, p \rangle - \alpha_1 \|\nu\|_{l^1, A_1^*} \right) \\ &\quad + \sup_{\omega \in W} \left(\langle \omega, w \rangle - \alpha_0 \|\omega\|_{l^1, A_0^*} \right) \\ &= \left[\sum_{i=1}^M (\lambda_i \tilde{D}_{KL}(\cdot, f_i))^*(\xi_i) \right] + (\alpha_1 \|\cdot\|_{l^1, A_1^*})^*(p) + (\alpha_0 \|\cdot\|_{l^1, A_0^*})^*(w) \end{aligned}$$

and we can thus compute the convex conjugate functions independently for the occurring functions. Since the convex conjugate functions only depend on one variable each, it is easy to see that also

$$\text{prox}_\tau^{G^*}(\xi, p, w) = \begin{pmatrix} \text{prox}_\tau^{(\lambda_1 \tilde{D}_{KL}(\cdot, f_1))^*}(\xi_1), \\ \vdots \\ \text{prox}_\tau^{(\lambda_M \tilde{D}_{KL}(\cdot, f_M))^*}(\xi_M), \\ \text{prox}_\tau^{(\alpha_1 \|\cdot\|_{l^1, A_1^*})^*}(p), \\ \text{prox}_\tau^{(\alpha_0 \|\cdot\|_{l^1, A_0^*})^*}(w) \end{pmatrix} \quad (246)$$

and thus we can also compute the prox operations individually.

Starting with the norm operations, computation shows

$$(\|\cdot\|_B)^* = \chi_{\{\|\cdot\|_{B^*} \leq 1\}} \quad \text{and consequently for } i = 0, 1 \quad (\alpha_i \|\cdot\|_{l^1, A_i^*})^* = \chi_{\{\|\cdot\|_{l^\infty, A_i} \leq \alpha_i\}}. \quad (247)$$

Analogously to F , the proximal mapping then reduces to a projection in the Hilbert

space topology, which exists for convex closed sets, and thus

$$\text{prox}_\tau^{(\alpha_i \|\cdot\|_{l^1, A_i^*})^*}(z) = \text{proj}_{\{\|\cdot\|_{l^\infty, A_i} \leq \alpha_i\}}(z). \quad (248)$$

So it remains to find the convex conjugate and proximal mappings of the Kullback-Leibler divergence with given data $f_i \in \Upsilon_i$ and $f_i \geq 0$. We obtain $(\lambda \tilde{D}_{KL}(\cdot, f_i))^*(\xi_i) = \sup_{y_i \in \Upsilon_i} \langle \xi_i, y_i \rangle - \lambda \tilde{D}_{KL}(y_i, f_i)$ for $\xi_i, f_i \in \Upsilon_i$ with $f_i \geq 0$ by computing the point-wise suprema for $g(y_i) = \xi_i y_i - \lambda(y_i - f_i \ln(y_i))$. In points with $f_i > 0$, the supremum cannot be attained by $y_i = 0$, hence, by differentiation we obtain the optimality condition $0 = \xi_i - \lambda \mathbf{1} + \lambda \frac{f_i}{y_i}$, where the operations are understood point-wise. In case $f_i = 0$, $g(y_i) = (\xi_i - \lambda)y_i$, whose supremum is infinity if $\xi_i > \lambda$ and zero otherwise. These computations result for $\xi_i \leq \lambda$ with equality only where $f_i = 0$ in

$$(\lambda \tilde{D}_{KL}(\cdot, f_i))^*(\xi_i) = \lambda \langle f_i, \ln \left(\frac{\lambda f_i}{\lambda - \xi_i} \right) - \mathbf{1} \rangle, \quad \partial[(\lambda \tilde{D}_{KL}(\cdot, f_i))^*](\xi_i) = \left\{ \lambda f_i \left(\frac{1}{\xi_i - \lambda} \right) \right\}, \quad (249)$$

and for other ξ_i result in the value $(\lambda \tilde{D}_{KL}(\cdot, f_i))^*(\xi_i) = \infty$ and the subdifferential being empty. So we can compute for $\zeta_i, \xi_i \in \Upsilon_i$ the proximal mapping

$$\begin{aligned} \text{prox}_\tau^{(\lambda \tilde{D}_{KL}(\cdot, f_i))^*}(\zeta_i) = \xi_i &\Leftrightarrow \zeta_i \in (\mathbf{I} + \tau \partial[(\lambda \tilde{D}_{KL}(\cdot, f_i))^*])(\xi_i) \\ &\Leftrightarrow \zeta_i = \xi_i + \tau \lambda f_i \left(\frac{1}{\xi_i - \lambda} \right) \quad \text{and } \xi_i \leq \lambda \text{ a.e.} \\ &\Leftrightarrow \xi_i = \zeta_i - \frac{(\zeta_i - \lambda) \pm \sqrt{(\zeta_i - \lambda)^2 + 4f_i \tau \lambda}}{2} \quad \text{and } \xi_i \leq \lambda \text{ a.e.} \end{aligned}$$

which, when considering the condition $\xi_i \leq \lambda$ reduces to

$$\text{prox}_\tau^{(\lambda \tilde{D}_{KL}(\cdot, f_i))^*}(\zeta_i) = \zeta_i - \frac{(\zeta_i - \lambda) + \sqrt{(\zeta_i - \lambda)^2 + 4f_i \tau \lambda}}{2}. \quad (250)$$

Recall that the primal-dual algorithm required the existence of a saddle-point in order to work. The following proposition ensures this condition is indeed satisfied.

Proposition 11.9. *Let $f \in \Upsilon$ with $f \geq 0$, and $f = 0$ in $\text{Rg}(\tilde{\mathcal{R}})^\perp$. Then Problem (Saddle-Tikh) possesses a saddle-point. Moreover, any u^* such that $((u^*, v^*), (\xi^*, p^*, w^*))$ is a saddle-point for some ξ^*, v^*, p^*, w^* is also a solution to (D-TIKH-STEM).*

Proof. Note that $(u, v) \mapsto \mathcal{L}((u, v), (\xi, p, w))$ is convex and lower semi-continuous, and $(\xi, p, w) \mapsto \mathcal{L}((u, v), (\xi, p, w))$ is concave and upper semi-continuous. Also, we consider the problem solely for $\tilde{H}_2 = \text{Rg}(\tilde{\mathcal{R}})^M \times V \times W \subset H_2$, as this allows to show required

coercivity statements. Also, a saddle-point on $H_1 \times \tilde{H}_2$ is also a saddle-point on $H_1 \times H_2$ as the function value $\mathcal{L}((u, v), (\xi, p, w)) = \mathcal{L}((u, v), (\xi + \zeta, p, w))$ for $\zeta \in (\text{Rg}(\mathcal{R})^M)^\perp$. Due to [18, VI Prop 2.4, p. 176], it is sufficient for the existence of a saddle-point to show that

$$\lim_{\|(u,v)\| \rightarrow \infty} \sup_{\substack{(u,v) \in H_1 \\ (\xi,p,w) \in \tilde{H}_2}} \mathcal{L}((u, v), (\xi, p, w)) = \infty, \quad (251)$$

and the coercivity statement that for some fixed $(u, v) \in H_1$

$$\lim_{\|(\xi,p,w)\| \rightarrow \infty} \inf_{(\xi,p,w) \in \tilde{H}_2} \mathcal{L}((u, v), (\xi, p, w)) = -\infty. \quad (252)$$

To show (251), we note that

$$\sup_{(\xi,p,w) \in \tilde{H}_2} \mathcal{L}((u, v), (\xi, p, w)) = \sum_{i=1}^M \lambda_i D_{KL}(Ru_i, f_i) + \alpha_1 \|\tilde{\nabla}u - v\|_{l^1, A_1^*} + \alpha_1 \|\tilde{\mathcal{E}}v\|_{l^1, A_0^*} \quad (253)$$

by Proposition 1.45 and therefore

$$\tilde{F}_{\lambda,\alpha}(u) \stackrel{(244)}{=} \inf_{\tilde{v} \in V} \sup_{(\xi,p,w) \in \tilde{H}_2} \mathcal{L}((u, \tilde{v}), (\xi, p, w)) \leq \sup_{(\xi,p,w) \in \tilde{H}_2} \mathcal{L}((u, v), (\xi, p, w)).$$

So the coercivity of $\tilde{F}_{\lambda,\alpha}$, which holds similarly to the coercivity of $F_{\lambda,\alpha}$ in the continuous setting, shows coercivity for u independent of v . So it is left to show that for bounded u , the function is coercive in v independent of bounded u , which follows immediately from the alternative formulation (253).

To show (252), we fix $(u, v) \in H_1$ with $\tilde{\mathcal{R}}u_i \geq 1$ on $\text{Rg}(\tilde{\mathcal{R}})$. The proof for the existence of such u is left to the interested reader. Recall

$$\mathcal{L}((u, v), (\xi, p, w)) = \langle (u, v), A^*(\xi, p, w) \rangle + F(u, v) - G^*(\xi, p, w)$$

where $F(u, v) = \chi_{\{\cdot \geq 0\}}(u)$ and $G^*(\xi, p, w)$ features characteristic functions limiting the norm of p, w and the convex conjugate of $\lambda \tilde{D}_{KL}$ derived in (249). The mentioned characteristic functions limit the norms of p, w and it remains to show uniform coercivity with respect to ξ for bounded p, w .

To show coercivity for ξ , we consider the function

$$g_i: (-\infty, \lambda_i] \times [1, \infty) \times [0, \infty) \rightarrow [-\infty, \infty) \quad \text{with} \quad g_i(a, b, c) = ba - \lambda_i c \ln \left(\frac{\lambda_i c}{\lambda_i - a} \right), \quad (254)$$

where we understand $0 \cdot \ln(0) = 0$. This function represents point-wise evaluations in the sum defining the parts of \mathcal{L} which depend on ξ .

This function satisfies $g_i(a, b, c) \rightarrow -\infty$ for $a \rightarrow -\infty$ uniformly for all $b \in [1, C]$ and $c \in [0, C]$ for some constant $C > 0$. Indeed, for a sufficiently small, $-\lambda_i c \ln\left(\frac{\lambda_i c}{\lambda_i - a}\right) < d|a|^{\frac{1}{2}}$ for some constant $d > 0$ independent of c , and consequently the linear term ba dominates the logarithmic term, confirming the claimed coercivity statement. Moreover, the function $g_i(\cdot, \cdot, \cdot)$ is bounded on $(-\infty, \lambda_i) \times [1, C] \times [0, C]$, as $g_i(a, b, c) \rightarrow -\infty$ for $a \rightarrow \lambda_i$ unless $c = 0$, in which case it converges to $b\lambda_i$, and the function is continuous and coercive. In particular, note that for bounded b, c , the boundedness and coercivity estimates hold uniformly.

With this in mind, note that $\|\xi\|$ large implies that ξ contains an entry in some i^*, s^*, ϕ^*, z^* such that $-(\xi)_{i^*}^{s^*, \phi^*, z^*} = O(\|\xi\|)$, and that the terms depending on p, w in \mathcal{L} are bounded. We estimate

$$\mathcal{L}((u, v), (\xi, p, w)) \leq \underbrace{\sum_{i=1}^M \sum_{s=0, z=0, \phi \in \mathcal{A}}^{N_s-1, N_z-1} g_i(\xi_i^{s, \phi, z}, \tilde{\mathcal{R}}u_i^{s, \phi, z}, f_i^{s, \phi, z})}_{\langle \tilde{\mathcal{R}}u_i, \xi_i \rangle - (D_{KL}(\cdot, f_i))^*(\xi_i)} + K, \quad (255)$$

for some constant $K > 0$. Further, $g(\xi_i^{s, \phi, z}, Ru_i^{s, \phi, z}, f_i^{s, \phi, z})$ is uniformly bounded from above with respect to the first component for all s, ϕ, z , and for some i^*, s^*, ϕ^*, z^* , the value $-g_{i^*}(\xi_{i^*}^{s^*, \phi^*, z^*}, Ru_{i^*}^{s^*, \phi^*, z^*}, f_{i^*}^{s^*, \phi^*, z^*}) = O(\|\xi\|)$, yielding the required coercivity statement for \mathcal{L} .

Consequently [18, VI Prop 2.4, p. 176] ensures that a saddle-point $((u^*, v^*), (\xi^*, p^*, w^*))$ to (Saddle-Tikh) exists. Also, due to [18, III Prop 3.1, p. 57], u^* is indeed a solution to the primal problem (D-TIKH-STEM). \square

Thus, all required proximal mappings are computed and assumptions are satisfied, and hence we can adapt Algorithm 1 to the specific structure of the STEM reconstruction yielding Algorithm 2.

Due to Theorem 11.8, Algorithm 2 is indeed correct, i.e. the sequence $(u^n)_n$ converges to a solution of (D-TIKH-STEM). Thus this algorithm is an adequate method to solve (D-TIKH-STEM), and consequently it is a reconstruction algorithm for multi-spectral STEM CT data.

Algorithm 2 Discrete Radon Reconstruction

INPUT: Operators A, A^* between Hilbert spaces H_1 and H_2 as in (243), and sinogram data $f \in \Upsilon$,

- 1: $\|A\| = \text{Power-iteration}(A, A^*)$
 - 2: Initialise $u^0 = 0 \in U$, $v^0 = 0 \in V$, $\xi^0 = 0 \in \Upsilon$, $\bar{u} = 0 \in U$, $\bar{v} = 0 \in V$, $p = 0 \in V$, $w = 0 \in W$ and $s \in \Upsilon$, choose $\tau, \sigma > 0$ such that $\sigma\tau\|A\|^2 < 1$.
 - 3: **for all** $n = 0, 1, \dots$ **do**
 - Dual update for $i = 1, \dots, M$:

$$\begin{cases} z_i = \xi_i^n + \sigma \tilde{\mathcal{R}} \bar{u}_i \\ \xi_i^{n+1} = z_i - \frac{(z_i - \lambda_i) + \sqrt{(z_i - \lambda_i)^2 + 4\tau \lambda_i f_i}}{2} \end{cases}$$

$$p^{n+1} = \text{proj}_{\{\|v\|_{l^\infty, A_1} \leq \alpha_1\}}(p^n + \sigma(\tilde{\nabla} \bar{u} - \bar{v}))$$

$$w^{n+1} = \text{proj}_{\{\|w\|_{l^\infty, A_0} \leq \alpha_0\}}(w^n + \sigma \tilde{\mathcal{E}} \bar{v})$$
 - 4: Primal update for $i = 1, \dots, M$:

$$\begin{cases} u_i^{n+1} = \text{proj}_{\{u \geq 0\}}(u^n - \tau(\tilde{\mathcal{R}}^* \xi_i^{n+1} - \widetilde{\text{div}} p_i^{n+1})) \\ v^{n+1} = (v^n + \tau(p^{n+1} + \widetilde{\text{div}} w^{n+1})) \end{cases}$$
 - Extragradient update:

$$\bar{u} = 2u^{n+1} - u^n$$

$$\bar{v} = 2v^{n+1} - v^n$$
-

Output: Sequence $(u^n)_n$ which converge to a solution of (D-TIKH-STEM).

12. Discussion of Numerical Results

With the Reconstruction Algorithm 2, we are able to compute reconstructions of sinogram data. The purpose of this chapter is to discuss numerical results, explain occurring effects and observe improvements made by the proposed algorithm compared to other methods.

To create these results, we use an implementation of Algorithm 2 in Python 2 with operations as defined in Chapter 11.2. These operations used for the iteration rules are implemented via PyOpenCL, a version of OpenCL (see [28] and references therein) adapted to Python, which allows a parallel implementation on the GPU (graphics processing unit). This allows an efficient implementation as the needed operations are suitable for such implementations. We note that the majority of computational effort is required for evaluation of the Radon transform and its adjoint, and differential operations. The differential operations are sparse and thus can be implemented in a swift manner. This leaves the Radon transform and its adjoint, which are not sparse as each row in the matrix representing $\tilde{\mathcal{R}}$ corresponding to (s, ϕ, z) contains non-zero entries in all columns corresponding to adjacent nodes, and the number of those nodes grows at the same rate as the resolution N_s . Still, the number of adjacent nodes does not grow very fast compared to the overall growth of data, making a parallel implementation suitable. In particular for the Radon transform and its adjoint there is a significant increase in speed from the cpu- to the gpu-implementation.

We first show that preprocessing might be required to obtain suitable reconstructions, using exemplary artificial data sets to illustrate certain undesired effects and their causes. Then the effects of using TGV and the Kullback-Leibler divergence compared to TV and L^2 subnorms are shown, and the effects of excessive and insufficient regularisation are depicted. After this, we look at real practical data sets obtained through Scanning Transmission Electron Microscopy (TEM and STEM) [4] and the reconstruction computed in a single-data and multi-data setting. In the chapter concerning single-data reconstruction, we compare the result with reconstructions obtained through standard methods, and depict results illustrating the capabilities of Algorithm 2. In the final chapter, multi-data reconstructions are considered. There, a particular focus lies on the improvements made through coupling compared to uncoupled reconstructions.

12.1. Preprocessing

For the Tikhonov approach to yield reliable results for the noisy data, it is imperative for data to fit the assumptions made in the model leading to the Tikhonov regularisation and in particular to the discrepancy used. Unfortunately, often the measured data does not fit these assumptions. Possible causes are that data passes through a sequence of processes before being available for the actual solution of the Tikhonov problem or that some theoretical assumptions are not satisfied by reality or the measurement process. This however might lead to the data not satisfying these initial assumptions, sometimes in very basic ways, which might not allow for the approach to realise its full potential.

Therefore, in the following we present some of such deficiencies in the data, and show how they impact the reconstruction and how to correct these deficiencies. This might be helpful to detect and identify issues in concrete data on which one works. Note that the scale of the depicted deficiencies here is purposely exaggerated to illustrate the effects on reconstruction, but similar weaker effects can be seen in practical applications.

Original setting

We consider the data set depicted in 7(a) which was obtained through STEM measurements and represents the density distribution in a specimen. The data contain projections from $N_a = 139$ angles and has resolution $N_s = 998$ and thus has dimension 139×998 and only one slice, i.e. $N_z = 1$, where the angles are represented by the vertical axis. Moreover, the values in the data are scaled to be between 0 and 1, where 0 represent no density being present.

We consider here two different approaches, both applying TGV_α^2 regularisation, but one using Kullback-Leibler divergences while the other uses the subnorm $\|\cdot\|_{L^2}^2$. We refer to those as Kullback-Leibler reconstruction and L^2 reconstruction respectively. The parameter choices leading to the later depicted reconstructions are obtained through manual selection of suitable results.

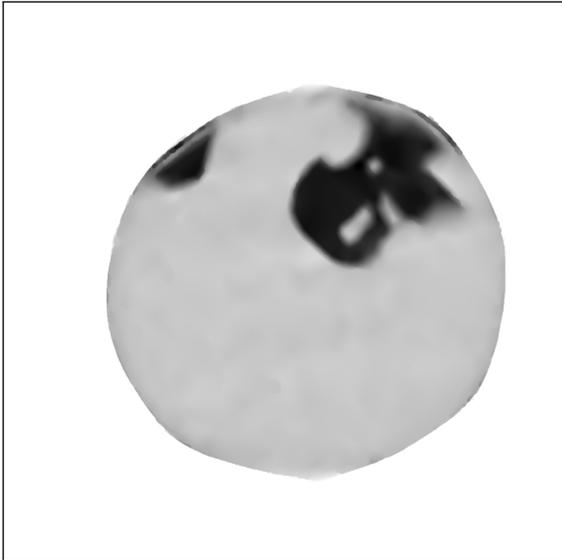
Fluctuating brightness

In electron tomography data, one might observe intensity fluctuations between different tilt angles. There are two main sources creating these effects due to physical effects and technical limitations. One being partial shadowing of the detector, the other is residual diffraction contrast.

Partial detector shadowing happens due to technical limitations in obtaining data, as



(a) Original sinogram



(b) Kullback-Leibler reconstruction of the original sinogram using $\alpha = (4, 1)$ and $\lambda = 0.001$



(c) L^2 reconstruction of the original sinogram using $\alpha = (4, 1)$ and $\lambda = 1$

Figure 7: Original sinogram data and corresponding reconstructions for Section 12.1.

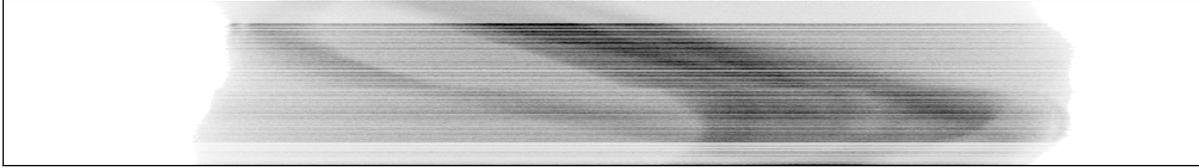
electrons hit parts of the installation of the detector under certain angles, reducing the intensity of measured electrons.

Diffraction contrast is a natural phenomenon occurring in the measured data, and although diffraction contrast contributions to the measurements are small when using STEM techniques [23], some contribution of diffraction contrast can still be present, which leads to brightness fluctuations depending on tilt angles.

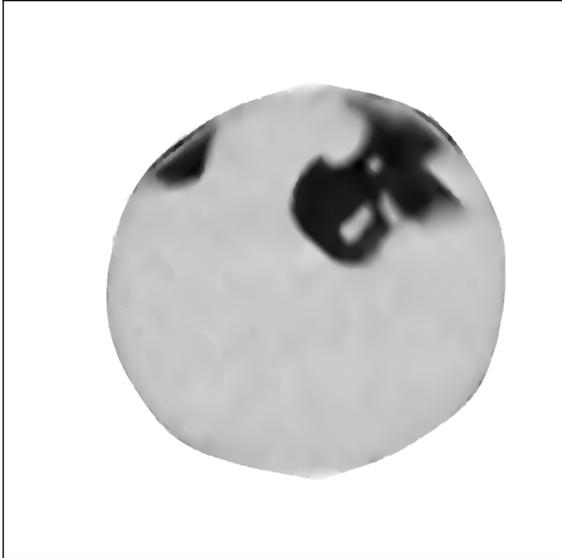
Such brightness fluctuations are depicted in Figure 8(a), where we modified the brightness of the projection for each angle (row in the image) by a random value which is normal distributed with expected value 1 and standard deviation 0.2. Moreover, we reduced the intensity of the first and last 20 projections by 50% to simulate partial detector shadowing. In the L^2 reconstruction This can lead to artifacts appearing inside and outside the observed object as shown in Figure 8(c). This happens because the algorithm tries to position mass in a way that affects the projections with little intensity less than the others, leading to the substantial amount of mass being placed on the sides. Note that for the Kullback-Leibler reconstruction this does not occur (see Figure 8(b)), as placing mass outside the object (where $f = 0$) would lead to a linear penalty, however, when raising the baseline (value representing no mass) slightly, the same effect as for L^2 reconstruction occurs, see Figure 8(d). To reduce these effects, one can rescale all projections to be non-negative and to have a common mean. Additionally, projections with very strong diffraction contrast, and hence containing unsatisfactory information, should be removed completely. In particular, we note that bad information might cause more problems than possessing no information at all for a specific angle, and the number of such projections is usually small compared to the total number of projections.

Non-zero baseline & Gaussian noise:

Often, the data get rescaled in the line of procession before reconstruction starts, however, for the Radon transform it is imperative that the baseline (the value representing no density) has the value 0. Also, such data suffers from thermic (Gaussian) noise due to the electronics of the detector. Though generally much lower than the Poisson noise, Gaussian noise is particularly relevant in points with no density (where consequently no Poisson noise occurs), which is not consistent with the noise model. As depicted in Figure 9(a), we added normal distributed values with expectation 0.1 and standard deviation 0.03 to the sinogram, i.e. change the baseline to 0.1 and add Gaussian noise, to simulate this situation. Therefore, the reconstruction scheme must insert additional mass to make up for the non-zero baseline and noise outside the object, resulting in



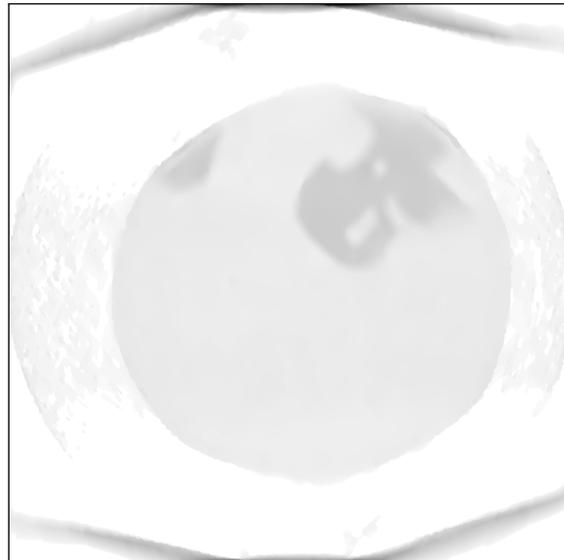
(a) Sinogram with brightness fluctuations



(b) Kullback-Leibler reconstruction of the sinogram with brightness fluctuations using $\alpha = (4, 1)$ and $\lambda = 0.001$



(c) L^2 reconstruction of the sinogram with brightness fluctuations using $\alpha = (4, 1)$ and $\lambda = 1$



(d) Kullback-Leibler reconstruction of the sinogram with brightness fluctuations and non-zero baseline using $\alpha = (4, 1)$ and $\lambda = 1$

Figure 8: Brightness fluctuations and its effects on reconstructions.

noise and halo artifacts appearing as depicted in Figures 9(b) and 9(c). In particular, this effect appears in similar gravity for both Tikhonov approaches. The reason for the occurrence of such artifacts is that halo functions are similar to preimages of constant functions, and so the algorithm works faithfully, but the solution is different from what one would expect or is looking for. Indeed, Figure 9(d) illustrates the solution of a sinogram with constant values, and shows that the halo is indeed an (approximate) solution to constant sinograms. To achieve an zero baseline, and simultaneously remove noise in points without density, hard thresholding can be applied.

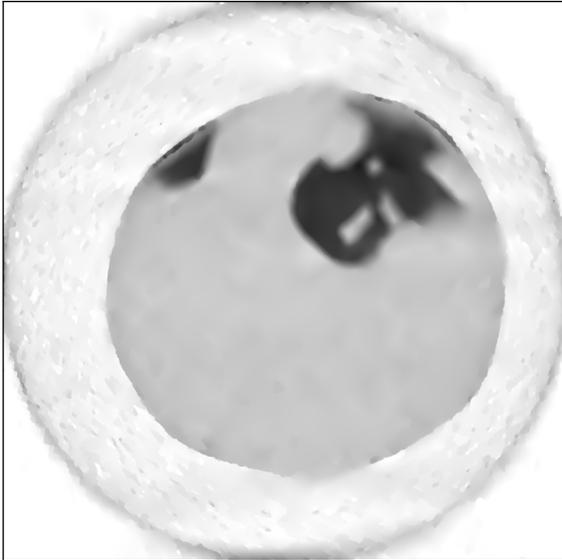
Misalignment:

Misalignment of the tilt series can be an issue in electron tomography. One must be wary, that the alignment of the projection is correct, meaning that each projection is centered with respect to a common tilt axis. An example for a severely misaligned sinogram is shown in Figure 10(a), where we modified the sinogram data by shifting the projections randomly for each angle by a normal distributed value. A non-correct alignment leads to blurring of the image, and artifacts outside the object as one can see in Figures 10(b) and 10(c). In particular the blurring appears in both reconstructions, but again the artifacts outside the object only appear in the L^2 reconstruction while in the Kullback-Leibler reconstruction the boundary accumulates unnatural mass formations. For proper alignment one can use center of mass and common-line alignment methods, see e.g. [43, 21].

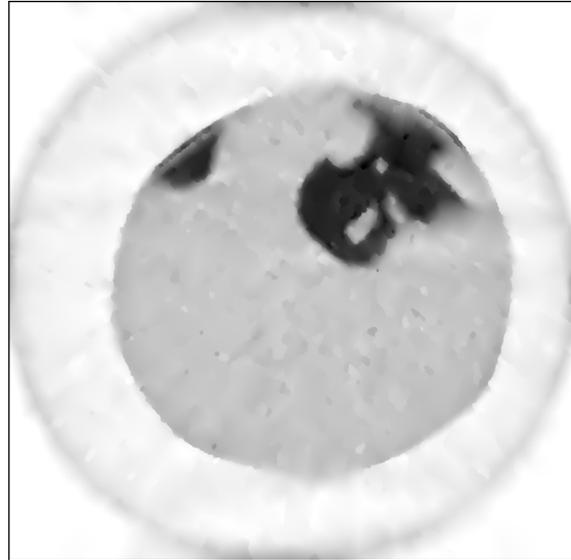
We note that although each of these artifacts appearing without preprocessing might not be very significant, when all the described problems occur at once, they further amplify one another.



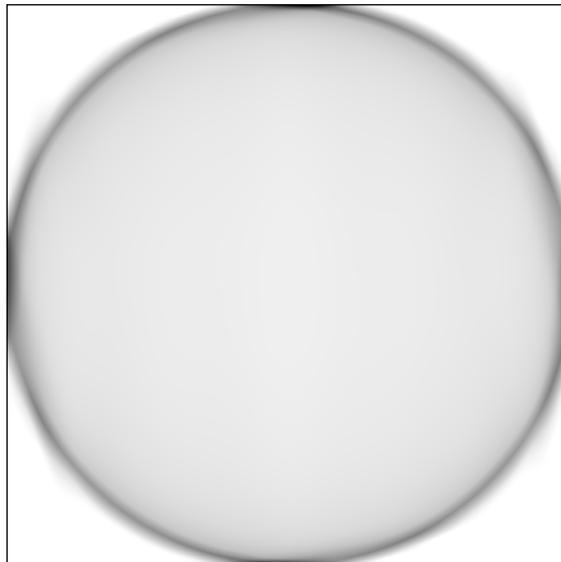
(a) Sinogram with modified baseline and added Gaussian noise



(b) Kullback-Leibler reconstruction of the sinogram with shifted baseline using $\alpha = (4, 1)$ and $\lambda = 0.001$



(c) L^2 reconstruction of the sinogram with shifted baseline using $\alpha = (4, 1)$ and $\lambda = 1$

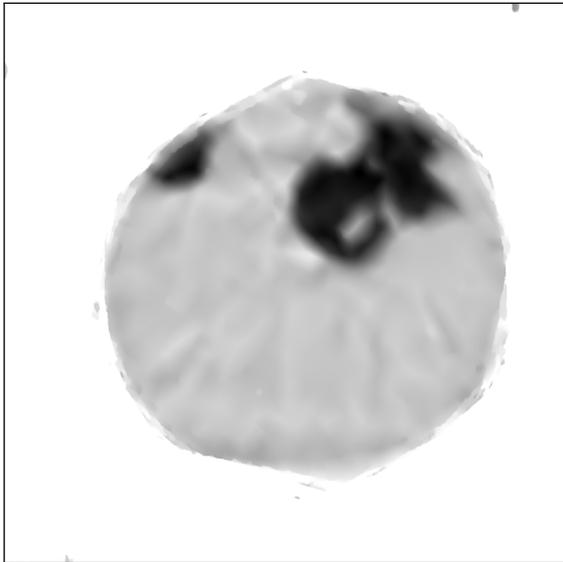


(d) Reconstruction of data representing a constant sinogram, i.e. $f \equiv 1$

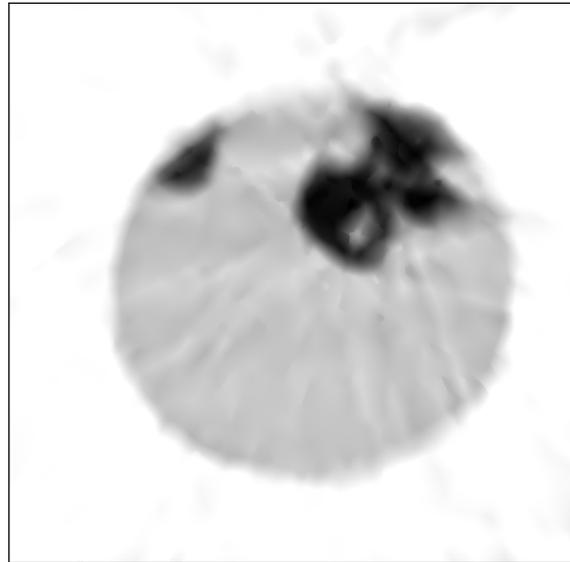
Figure 9: Sinogram with modified baseline and added Gaussian noise, and the corresponding effects on reconstruction.



(a) Sinogram data with severe misalignment



(b) Kullback-Leibler reconstruction of the sinogram with shifted alignment using $\alpha = (4, 1)$ and $\lambda = 0.001$



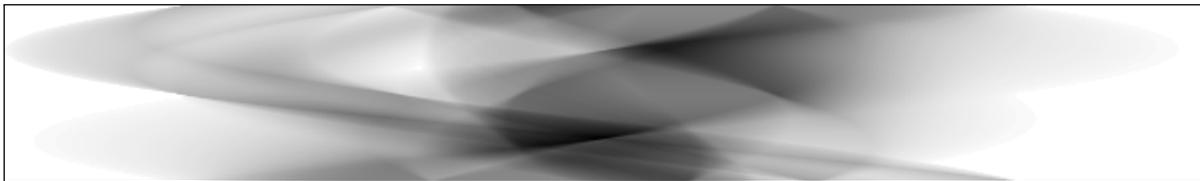
(c) L^2 reconstruction of the sinogram with shifted alignment using $\alpha = (4, 1)$ and $\lambda = 1$

Figure 10: Sinogram with shifted alignments and the corresponding reconstructions.

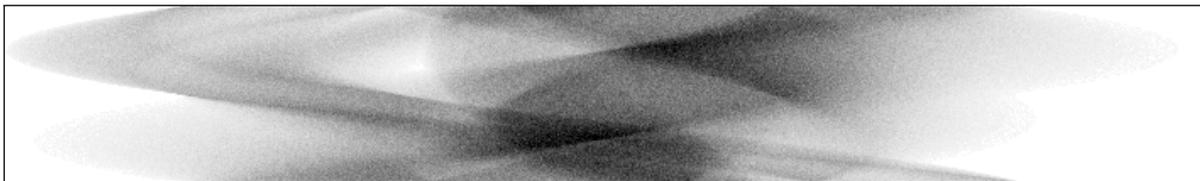
12.2. Synthetic Experiments

We use an artificial example to highlight the effects of different discrepancy and regularisation functions in the Tikhonov scheme, as this artificial setting allows us more insight in how the algorithm reacts to certain situations and modifications in data. In particular, the advantages of TGV_α^2 and Kullback-Leibler divergence D_{KL} over TV (Total Variation, a commonly used regularisation functional in imaging, which for scalar-valued functions is identical to TD) and subnorms $\|\cdot\|_{L^2}^2$ become apparent in these observations. Therefore, we consider the following two sinograms in $2D$ where the second is a version of the first which is disturbed with Poisson noise as depicted in Figure 11.

The data has format 105×708 , i.e. resolution $N_s = 708$ and $N_a = 105$ projections are considered, and $N_z = 1$, i.e. only a single slice is considered.



(a) Sinogram of original distribution



(b) Sinogram with Poisson noise

Figure 11: Sinogram data for Section 12.2.

Note that the noise is stronger in parts of the sinogram containing much mass, while those without mass remain unaffected.

The density distribution from which the original sinogram was computed, is depicted in Figure 12(a) and contains several different aspects of functions occurring in it. From the top there is a linear increase downwards with respect to the y axis, while the ramp coming from the left is a quadratic function with respect to the x axis. Those two ramps continuously lead into a block in the middle of the image with a constant value and a hard transition to the surrounding areas which hold no density. On one vertex of this square block, a quadratic function describing the square distance to said vertex overlays the constant block in a circular way. In the bottom-right corner two boxes are placed whose values describe the square distance to two respective middle-points,

however, now not in a circular but in a square shape, and the two functions are inverse of another, leading to a hard transition with opposite trends on their shared boundary. So to summarise, the density features constant, linear and quadratic parts, partially with continuous and partially with hard transitions.

As can be seen in Figure 12(b), the application of Filtered Backprojection reconstruction of the original sinogram is not perfect, which is due to the Radon transform with finitely many angles not being injective. But the effect is far stronger for the noisy data, where the Filtered Backprojection reconstruction is not usable and strongly amplifies noise, even in points containing no mass, see Figure 12(c).

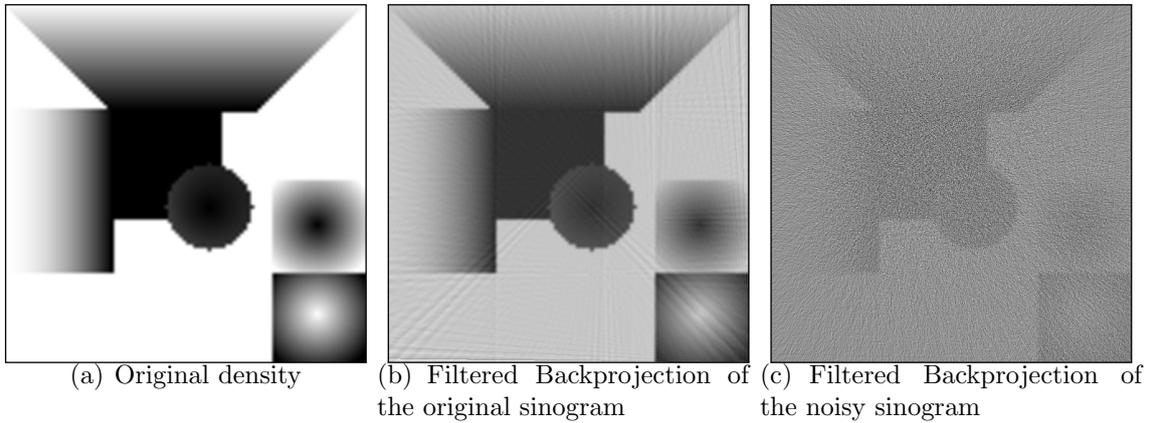


Figure 12: Original Density distribution and Filtered Backprojection reconstructions for Chapter 12.2.

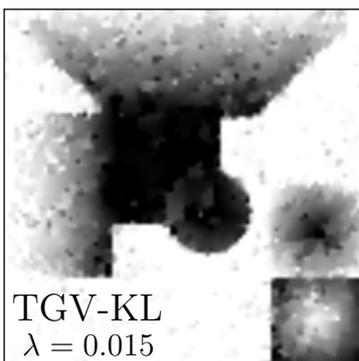
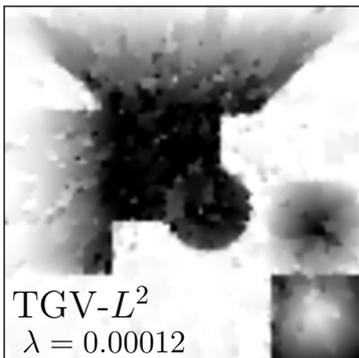
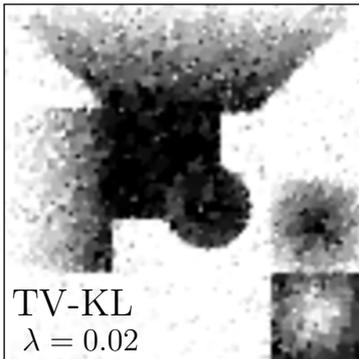
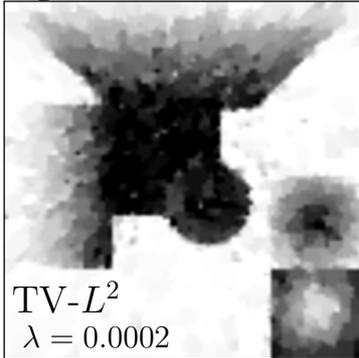
So obviously this Filtered Backprojection method is not suitable when strong noise is occurring in the data, and thus we consider reconstructions made using Tikhonov regularisation with TGV or TV for the regularisation functional as well as D_{KL} or $\|\cdot\|_{L^2}^2$ (short KL or L^2) as discrepancies. Applying those reconstruction methods to the sinogram with noise leads to the results depicted in Figure 13. Here we show 3 different parameter choices for each approach in order to illustrate what the effect of excessive, insufficient or appropriate regularisation on the reconstruction is. Note that the used parameter choices were determined manually by examining results of some reconstructions.

In the first and second line of Figure 13 one sees the approaches using Total Variation, where it becomes apparent that TV promotes piece-wise constant areas in the solutions leading to staircase artifacts. Hence, in the constant regions with hard transitions the reconstruction is very good, however in the linear and quadratic regions the solutions are non-smooth and look unnatural. TGV^2 appears to reconstruct the non-constant areas

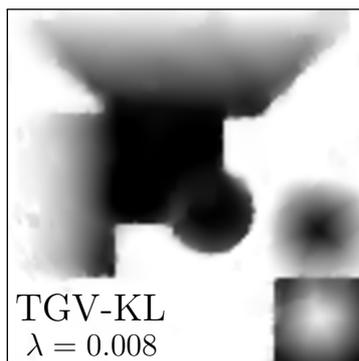
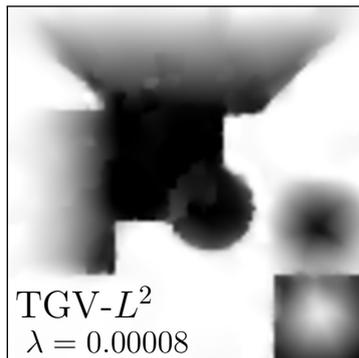
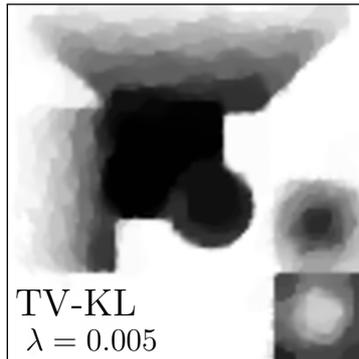
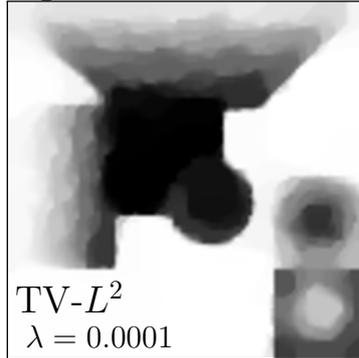
well and also allows for jumps and discontinuities, although sometimes the transitions are a bit blurry. As TGV^2 promotes piece-wise linear functions, it comes as no surprise that on the linear and quadratic sections TGV^2 is superior to TV and yields smoother results.

There seems to be no big difference in the results between using L^2 and KL. As we are aware of the original image, one can quantify the errors made by the reconstructions, which shows a slight advantage of KL over L^2 (as would be expected), however the difference is not significant and both yield suitable reconstructions.

Insufficient
regularisation:



Appropriate
regularisation:



Excessive
regularisation:

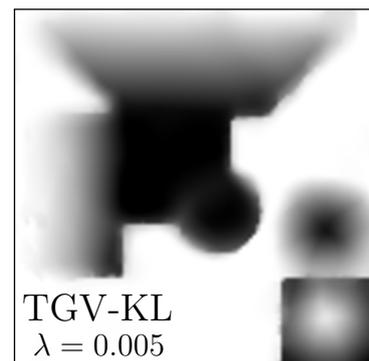
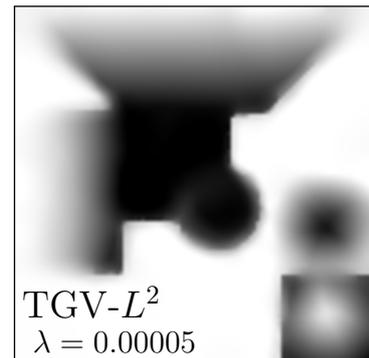
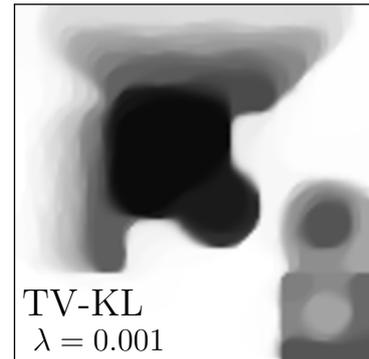
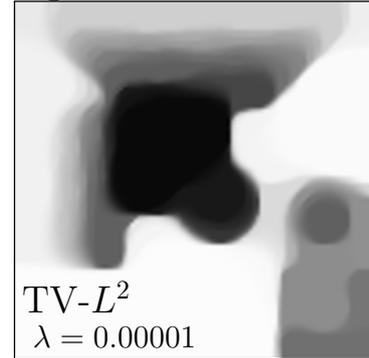


Figure 13: Reconstruction of noisy data with varying methods and regularisation parameter. The first row shows a TV- L^2 approach, the second a TV-KL, the third a TGV- L^2 and the last a TGV-KL approach with different degrees of regularisation, first column for insufficient, second for adequate and last for excessive regularisation. 158

12.3. Reconstruction of Single-Data HAADF Signals

As an application we consider the reconstruction of a single density distribution for data obtained by Transmission Electron Microscopy (TEM). Here, HAADF (high-angle annular dark field, see e.g. [46]) detectors are used to obtain mass-projections and thus one retrieves sinogram information from which one tries to reconstruct the mass-density distribution.

Mathematically speaking, this is the inverse problem of reconstructing a single density distribution by inversion of the Radon transform on a single sinogram.

Such sinogram data is depicted in Figure 14, these however are not all projections, and just serve as illustration. For the practical computation done in this chapter, we consider HAADF sinogram data consisting of $N_a = 155$ projections, with resolution $N_s = 1248$, and $N_z = 34$ slices are considered. We also note that preprocessing steps were applied to this data set.

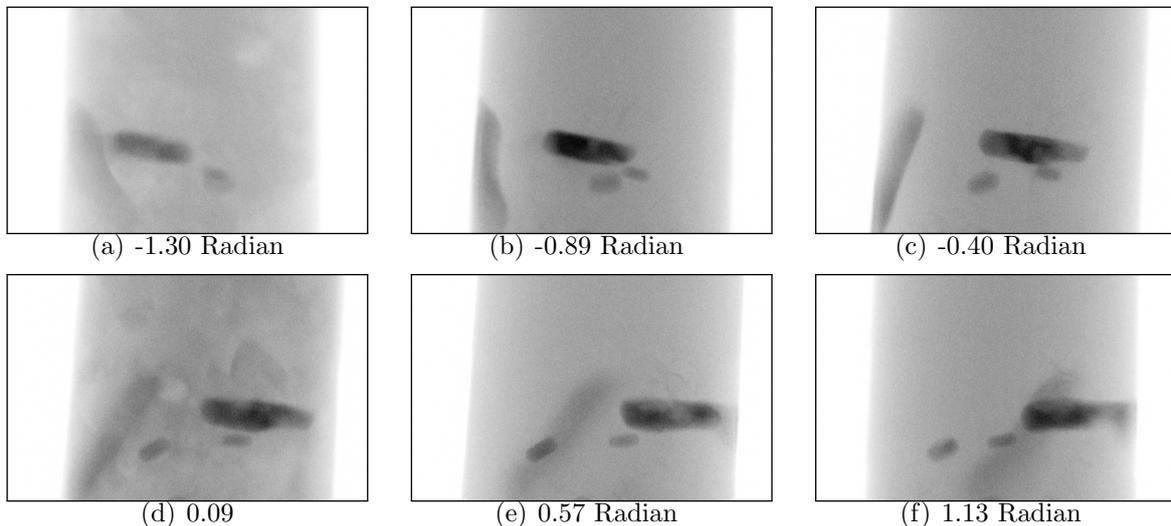


Figure 14: HAADF projections of a specimen from different angles.

Note that the data supposedly contains Poisson and Gaussian distributed noise, however, the noise is much weaker than it was in Section 12.2. Thus, we again consider Filtered Backprojection, as well as other standard algorithms for reconstruction, namely Filtered Backprojection (FBP), Simultaneous Iterative Reconstruction Technique (SIRT) [24], Simultaneous Algebraic Reconstruction Technique (SART) [1] and the Conjugate Gradient Least Square method (CGLS) [45] and the results are depicted in Figure 15.

These results were computed using the ASTRA toolbox [39, 49] for one specific slice of the data, and although one gets a general idea of what the object looks like, the results still contain noise.

Therefore, we applied Algorithm 2 to solve a TGV-KL approach as in (TIKH-STEM) and again a suitable parameter choice is obtained through manual optimisation. Further, we consider the effects of preprocessing on the results, where we use the preprocessing methods as proposed in Section 12.1. The difference between a reconstruction with and without preprocessing is depicted in Figure 16 and the corresponding heat-maps illustrate that while the reconstruction inside the object is proper even without preprocessing, quite some noise accumulates outside the object unlike in the preprocessed version. While for the human eye this noise outside the object might not pose any real problem, for possible postprocessing this could be an issue, e.g. segmentation algorithms could view this noise as an additional object.

We further note that the Radon transform is basically a two-dimensional operation we consider for different heights z and so the reconstruction of different slices are computed independently by many algorithms. The proposed Tikhonov TGV approach however links the different slices through penalising the gradient in z direction. The noise in a certain slice might lead to artifacts, however as the noise is random, the noise of the adjacent slices most likely leads to other artifacts. Thus, TGV penalises these artifacts, although these artifacts would be reasonable when just considering the two-dimensional reconstruction. Such effects can be observed in Figure 16(c), where we see that while the reconstruction of the object is done well, some artifacts appear in the grey mass.

Also, in Figure 17 a sequence of reconstructions of different slices are shown to further illustrate the effect of Algorithm 2 on preprocessed data. One sees that the algorithm succeeds in gaining smooth reconstructions, allowing for hard and soft transitions, and still retrieves details like the small entrapments which can be seen in the second row of Figure 17. Furthermore, the algorithm creates a stark contrast between the object and its surrounding without mass, which is due to the linear penalty imposed by the Kullback-Leibler divergence on points in the sinogram with signalvalue 0.

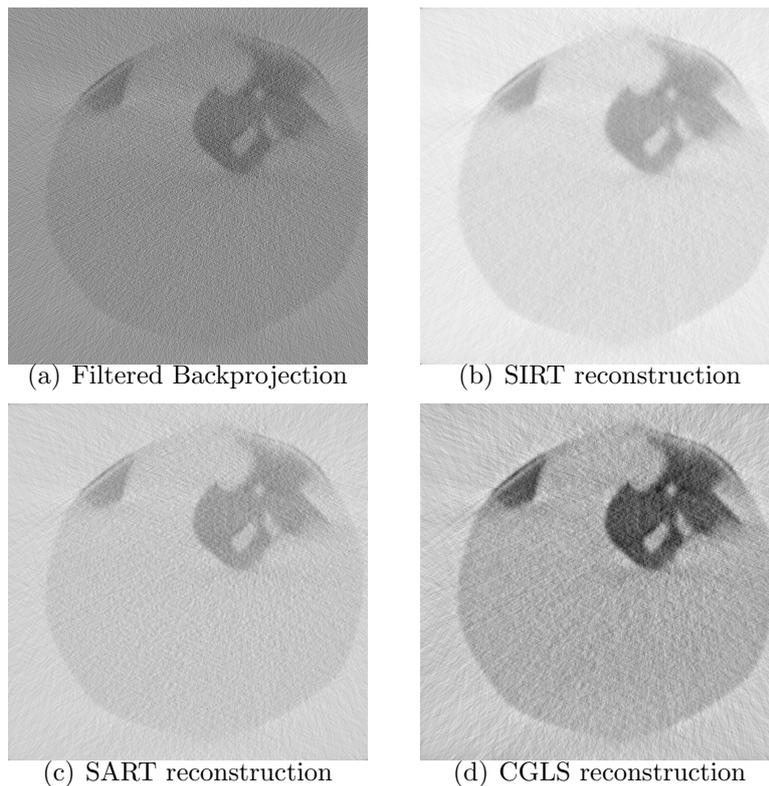


Figure 15: Reconstructions created by commonly used reconstruction algorithms for one specific slice in the data set in Section 12.3.

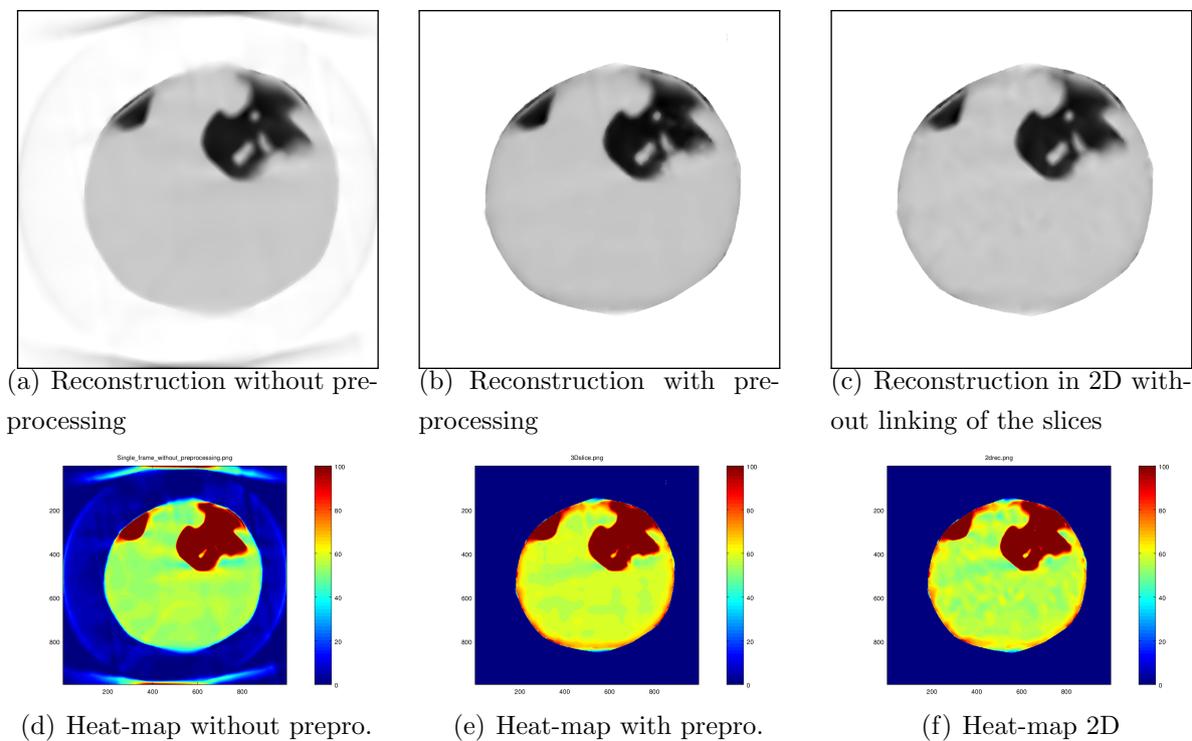


Figure 16: Reconstructions with TGV and KL using $\alpha = (4, 1)$ and $\lambda = 0.00025$

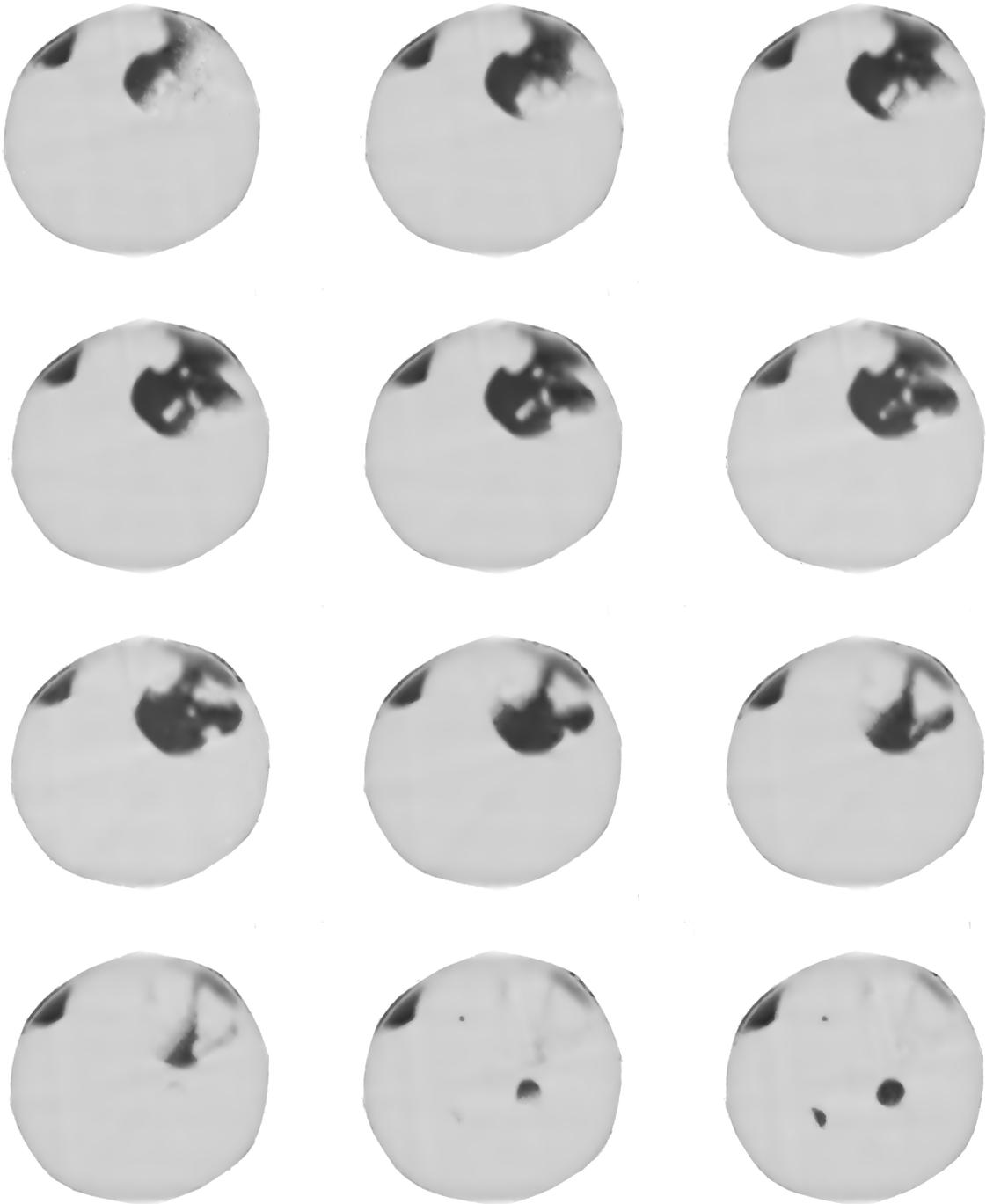


Figure 17: Series of slices (read along rows) from reconstructions with TGV and KL using $\alpha = (4, 1)$ and $\lambda = 0.00025$.

12.4. STEM Multi-Spectral Reconstructions

Finally, we apply the Reconstruction Algorithm 2 to STEM data obtained via EDS representing several spectra. We work with a data set containing a HAADF signal as well as analytical data for aluminium, silicium and ytterbium, see Figure 18. The data has resolution $N_s = 296$ with $N_a = 39$ projections and $N_z = 276$ slices.

From a mathematical standpoint this data is not different from the HAADF data previously obtained, only that the physical interpretation is different as it does not represent mass-density but the density for certain elements used to do elemental analysis and create a chemical mapping.

Unfortunately, due the higher technical effort in obtaining data, these sinogram data have lower quality and contain stronger noise, as can be seen in Figure 18. This leads to potential complications, as one requires strong regularisation to remove the noise, which on the other hand might lead to blurry transitions and non-sharp features. Thus, we consider two different TGV approaches and the choice of parameter is again done manually. One approach reconstructs the spectra independently, i.e. the norms $|\cdot|_{A_1^*}$ and $|\cdot|_{A_0^*}$ in the definition of TGV^2 are the l^1 norms over all entries, while the other uses Frobenius norms for both instances, leading to a coupling of the problems promoting common edges. The corresponding reconstruction results are presented in Figure 19 and 20 where the four channels (HAADF, aluminium, silicium, ytterbium) are placed from left to right.

The uncorrelated approach yields satisfying results inside the objects, yet becomes blurry, particularly on the boundaries but also elsewhere. Moreover, due to the blurring, small features such as the small entrapment in ytterbium spectrum are lost. It is easy to see, that the density distribution of ytterbium is the same as the highest density parts in the HAADF reconstruction. Consequently the reconstruction of the low quality ytterbium data could greatly benefit from edge information in the HAADF reconstruction. Therefore, in the coupled reconstruction, the ytterbium reconstruction improves significantly by drawing on this information. For example the entrapments in the ytterbium density becomes more visible and the transition gets sharper in the coupled reconstruction, while in the uncoupled reconstruction these entrapments were rather blurry. This shows that the information from the HAADF data with higher quality can improve the low quality ytterbium reconstruction.

Also, one sees that the edges in the aluminium and silicium signals are complementing each other in the coupled reconstruction, which makes sense from a physical point of view as they have almost the same density. In the uncorrelated reconstruction however,

these shared edges in the aluminium reconstruction are less defined. So also information exchange between two low quality signals can be observed to the benefit of both reconstructions.

Furthermore, note that there is information exchange between HAADF and aluminium, as the hole in the top left of the aluminium reconstruction corresponds to a higher mass in the HAADF reconstruction, and coupling makes the features of said hole sharper. Also, the outer boundary of the aluminium density seems to be not very smooth and rather frayed in the uncoupled reconstruction, while the outer boundary of the HAADF reconstruction is smooth. Coupling results in this boundary of the sinogram becoming smoother by adjusting to the HAADF's boundary.

So to summarise, while the uncorrelated reconstruction already creates suitable results, the approach with joint regularisation succeeds in creating sharp edges, preserving small details more efficiently and allowing for information exchange, both between high and low quality signals, or between two signals of similar quality.

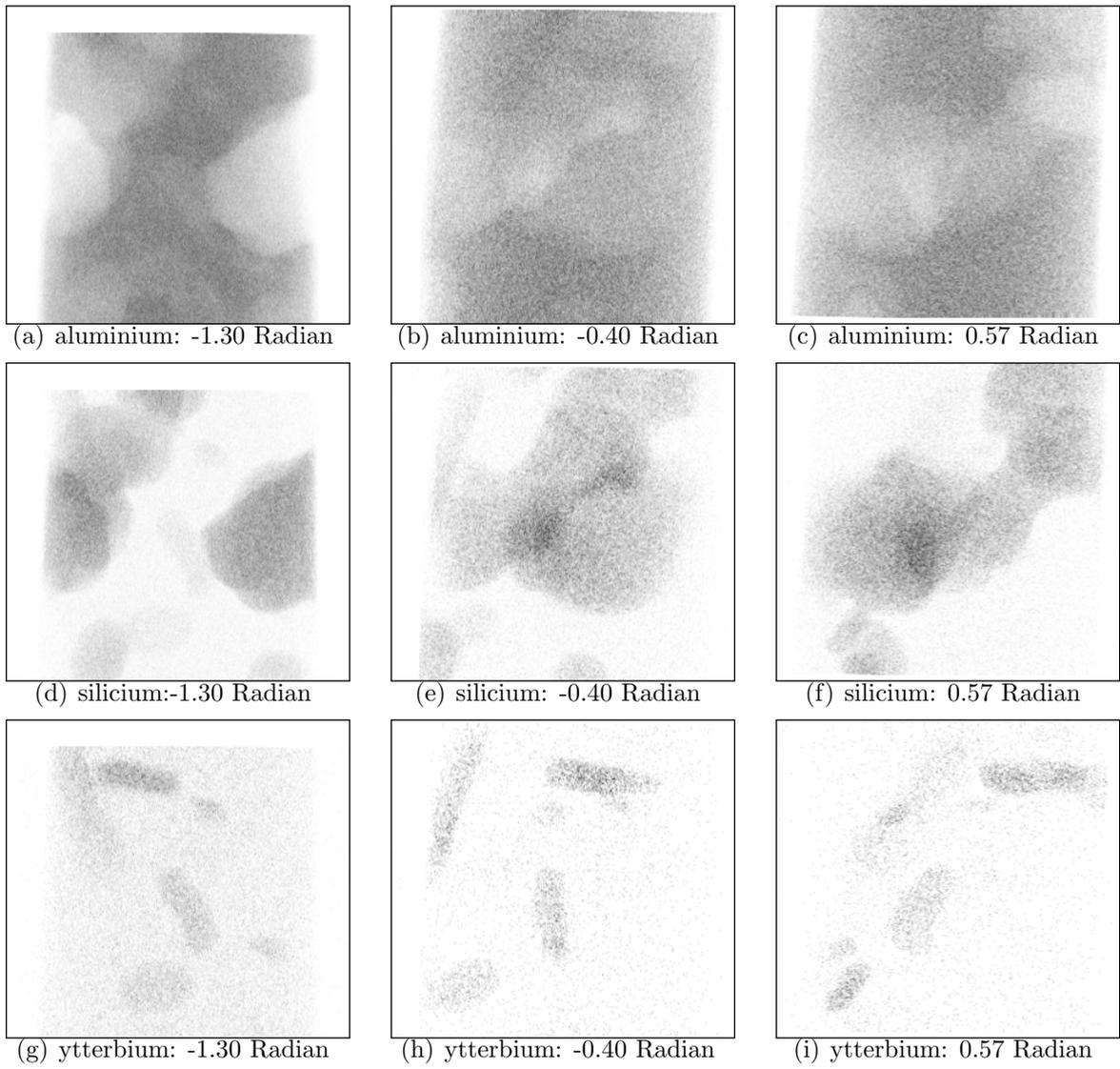


Figure 18: Spectral projections of a specimen from different angles.

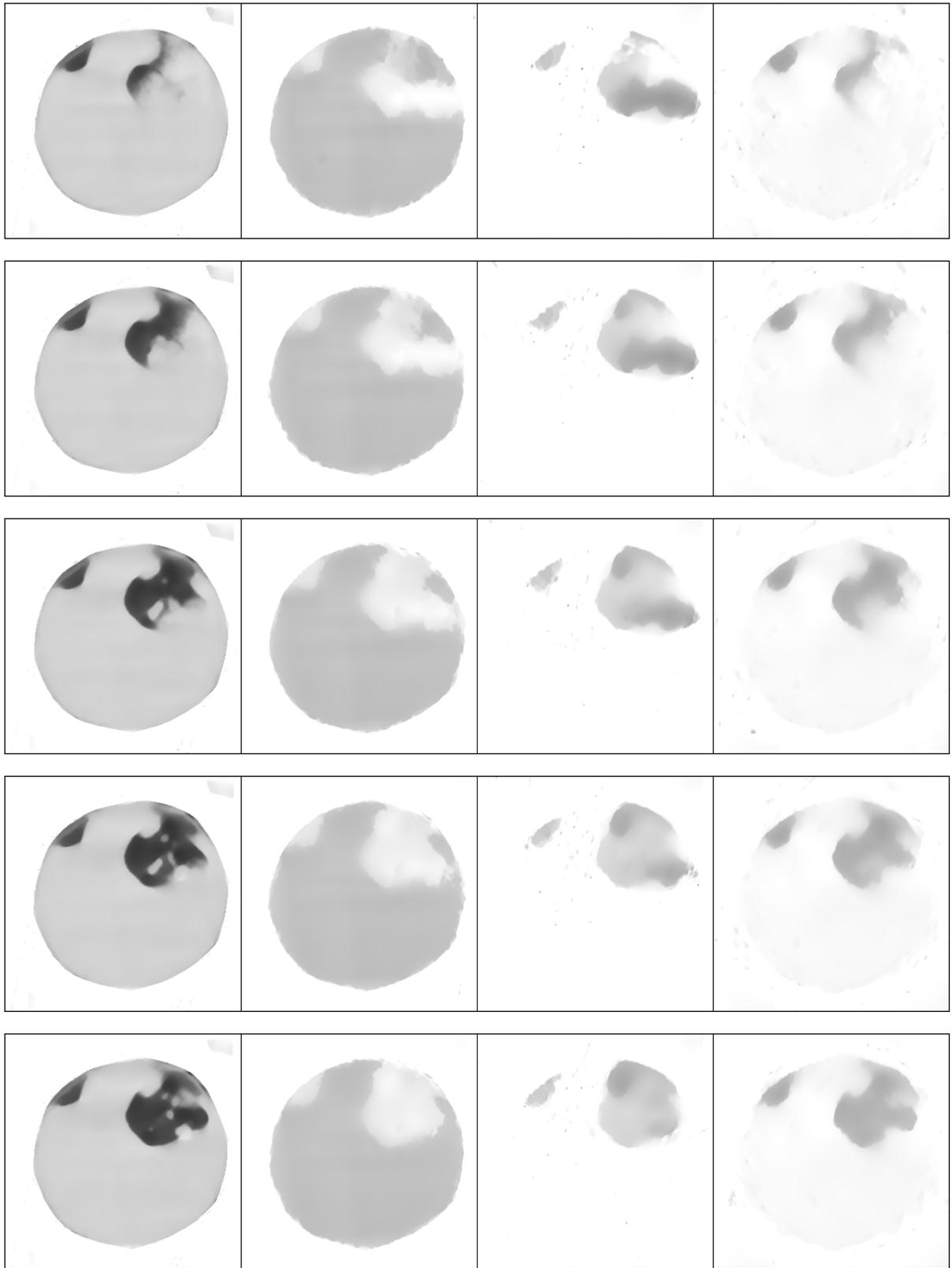


Figure 19: Uncoupled TGV-KL reconstruction of data in Section 12.4 with $\alpha = (4, 1)$ and $\lambda = (0.05, 0.005, 0.002, 0.0015)$, showing from left to right HAADF, aluminium, silicium and ytterbium.

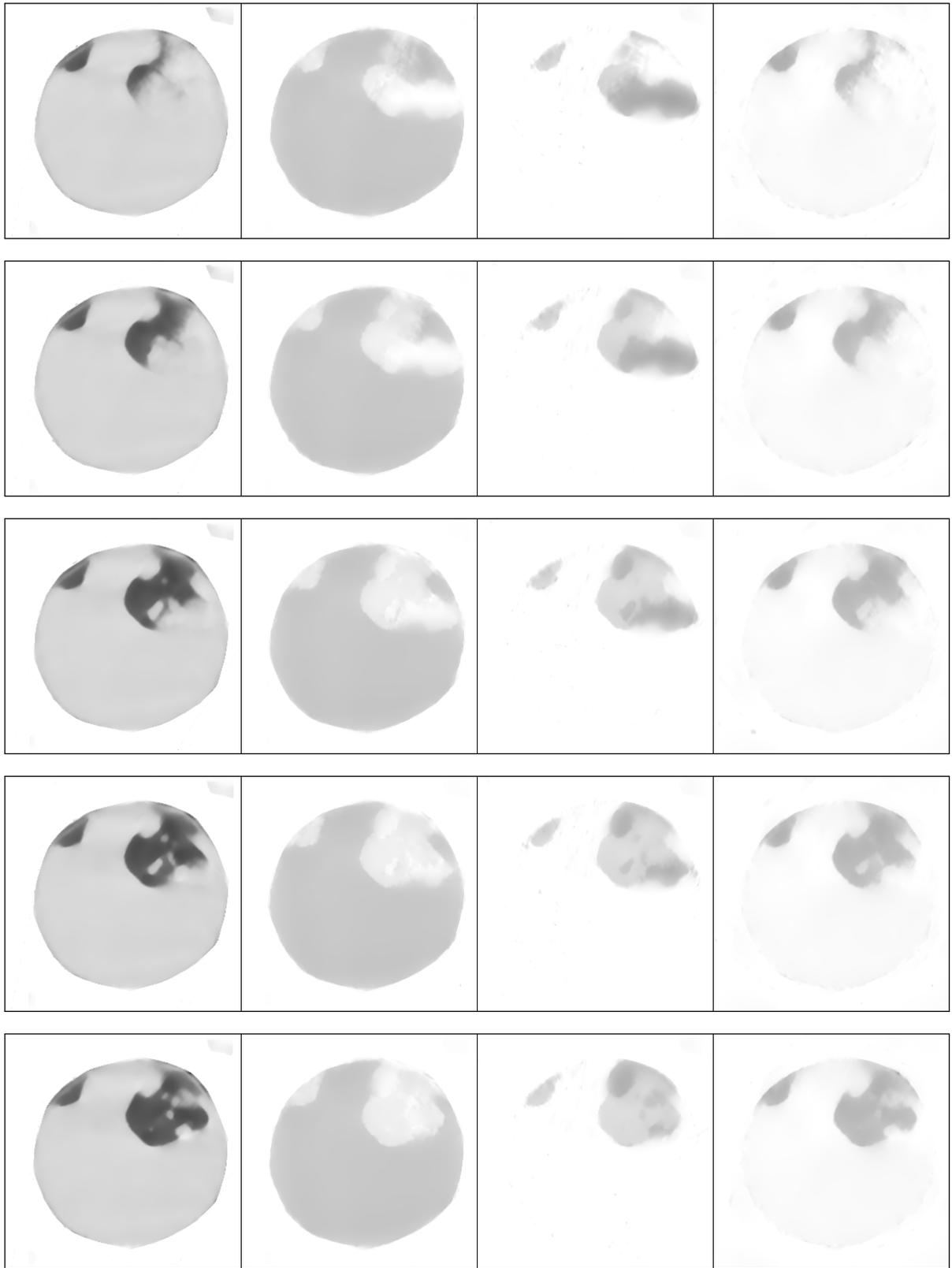


Figure 20: Joint TGV-KL reconstruction of data in Section 12.4 using Frobenius norms with $\lambda = (0.05, 0.002, 0.001, 0.0008)$ and $\alpha = (4, 1)$, showing from left to right HAADF, aluminium, silicium and ytterbium.

Summary

We want to quickly recapitulate the most relevant results and methods presented in this thesis. The overall topics discussed were analytical and numerical aspects of multi-data Tikhonov approaches as well as their application to STEM CT reconstruction.

The first part focused on the analytical properties of multi-data Tikhonov approaches, which are schemes to solve multi-data inverse problems

$$T_1 u = f_1, \quad \dots \quad T_M u = f_M \quad (256)$$

with M subproblems featuring forward operators T_i and data f_i . These approaches use discrepancy functions D_i for $i = 1, \dots, M$ and a family of regularisation functionals $(R_\alpha)_{\alpha \in \mathcal{A}}$ and parameters $\lambda \in \mathbb{R}^M$ and $\alpha \in \mathcal{A}$, and consist in solving

$$u^\dagger \in \operatorname{argmin}_{u \in X} F_{\lambda, \alpha}(u, f) \quad \text{with} \quad F_{\lambda, \alpha}(u, f) = R_\alpha(u) + \sum_{i=1}^M \lambda_i D_i(T_i u, f_i). \quad (257)$$

In order to guarantee that this problem is indeed well-defined and satisfies expected properties, we introduced the concepts of basic, continuous and strongly continuous discrepancy functions as well as continuous and strongly continuous families of regularisation functionals. With these and standard coercivity assumptions, one can show that this approach is well-defined in the sense that an solution exists in case $F_{\lambda, \alpha}$ is proper.

Further, convergence results for vanishing noise similar to the ones for classical Tikhonov problems are discussed. In this context, not only convergence to solutions, but also to partial solutions can be considered as such are possible due to the multi-data structure.

When denoting by $R_{\alpha, \lambda, I}(u, f) = R_\alpha(u) + \sum_{I^c} \lambda_i D_i(T_i u, f_i)$ the extended regularisation functional, the focus lies on $R_{\alpha, \lambda, I}$ -minimal I -partial solutions, and convergence to those under additional parameter choice rules is considered. These $R_{\alpha, \lambda, I}$ -minimal I -partial solutions also allow interpretation as solutions to a Tikhonov problem for the unsolved problems $T_{I^c} u = f_{I^c}$, using $T_I u = f_I$ as prior. This is true, as $R_{\alpha, \lambda, I}(u, f)$ represents a Tikhonov functional for the subproblems in I^c , and the prior condition enforces being I -partial solution. So the Tikhonov approach can be seen as an approximation scheme for solving said Tikhonov problems with prior.

Indeed, for vanishing noise we show that subsequential convergence to such an $R_{\alpha, \lambda, I}$ -minimal I -partial solution (if existent) can be obtained, when using continuous discrepancies and families of regularisation functionals and applying a suitable parameter choice

strategy. Moreover, under additional source conditions and modulus of continuity estimates (strongly continuous discrepancies and regularisation functionals), one can also derive convergence rates for the residuals and the Bregman distance of $R_{\alpha,\lambda,I}$. From these, one can find parameter choice strategies to obtain optimal rates, and in particular the rates are affected by the noise levels of all subproblems. Therefore, one might improve the convergence rate for one subproblem by changing the parameter choices, but risks slowing down the others' convergence.

With these general results, we aimed to apply specific discrepancies and families of regularisation to it, in order to show that the required assumptions are indeed reasonable and are fulfilled by a number of concrete functions.

For discrepancies on a vector space we first considered norm and subnorms, i.e.

$$D_i(v_i, f_i) = \|v_i - f_i\|_i^{p_i} \quad (258)$$

with vector space norms or subnorms. For such, under natural assumptions and topologies we obtained that these are indeed continuous discrepancies, which are $t^{\frac{1}{p_i}}$ -strongly continuous, and so they pose a suitable choice for discrepancies and satisfy all requirements without any restrictions.

More challenging is the discussion of the Kullback-Leibler divergence as a discrepancy functional, i.e. the discrepancy $D_i = D_{KL}$ on $L^1_\mu(\Omega)$ with

$$D_i(v_i, f_i) = D_{KL}(v_i, f_i) = \int_\Omega v_i - f_i - f_i \ln\left(\frac{v_i}{f_i}\right) d\mu. \quad (259)$$

This discrepancy is suitable to tackle Poisson distributed noise due to its connection to the corresponding likelihood function. Unlike norms, the Kullback-Leibler divergence is not adapted to the linear operations, thus requiring more analytical discussion. Still, under acceptable assumptions and choices of topology, we showed that the Kullback-Leibler divergence is a continuous discrepancy in every v_0 and f_i^\dagger . However, strong continuity in f_i^\dagger is only obtained on the set

$$V_i = \left\{ v_i \in L^1_\mu(\Omega) \mid \ln\left(\frac{v_i}{f_i^\dagger}\right) \in L^\infty_\mu(\{v_i \neq 0, f_i^\dagger \neq 0\}) \right\}, \quad (260)$$

where one obtains local $\frac{1}{2}$ -Hölder continuity.

As an example for regularisation functionals, TGV (Total Generalised Variation) is

considered, where for $\alpha \in (0, \infty)^k$,

$$\text{TGV}_\alpha^k(u) = \sup \left\{ \int_\Omega u \cdot \text{div}^k \phi \, dx \mid \phi \in \mathcal{C}_c^k(\Omega, \text{Sym}^{k+l,d}) \right. \quad (261)$$

$$\left. \text{with } \|\text{div}^j \phi\|_\infty \leq \alpha_j \text{ for } j \in \{0, \dots, k-1\} \right\}.$$

This is a regularisation functional frequently used in imaging that penalises derivatives in order to promote smooth solutions, however does it in a way that allows for discontinuities. After introducing these functionals, their analytical properties are discussed, and in particular, it is shown that the family $(\text{TGV}_\alpha^k)_{\alpha \in (0, \infty)^k}$ is indeed a strongly continuous family of functions, and thus applicable as a family of regularisation functionals. Moreover, we discuss a version of TGV for vector-valued functions, allowing the coupling of inverse problems with the exchange of edge location information in order to promote common features in Tikhonov reconstructions.

Furthermore, the properties of TGV in a linear setting are discussed, i.e. T_i linear and $D_i = \|\cdot\|_i^{p_i}$, showing that the TGV regularisation also leads to a coercive Tikhonov functional, thus creating a suitable Tikhonov approach.

As application of the discussed choices of discrepancy and regularisation functionals, we consider the multi-data inverse problem of reconstruction of STEM CT data. These problems feature multiple independent inverse problems

$$\mathcal{R} u_1 = f_1, \quad \dots \quad \mathcal{R} u_M = f_M \quad (262)$$

of reconstructing density distributions u_1, \dots, u_M from corresponding sinogram data f_1, \dots, f_M with \mathcal{R} the Radon transform. These densities represent the densities of specific chemical elements, thus one tries to obtain a chemical mapping of an object. A Tikhonov approach using the Kullback-Leibler divergence and TGV for vector-valued functions is employed to solve the inverse problem, in the hope of tackling Poisson noise efficiently and promoting information exchange and smooth solutions.

Therefore, the Radon transform, the forward operation for such problem, is discussed. It is shown that it satisfies analytical requirements for a Tikhonov approach and that regularisation is indeed necessary as the inverse problems are not well-posed.

In order to solve the resulting Tikhonov approach, a discretised problem is introduced, and a primal-dual algorithm is employed to solve said discrete problem. In particular, the discrete problem is derived in a way that allows a parallel implementation on the GPU, resulting in an efficient reconstruction algorithm.

Finally, numerical results are discussed, highlighting the effects, advantages and shortcomings of such a Tikhonov approach, and illustrating that indeed satisfactory results can be obtained, which are superior to other reconstruction methods. The algorithm produces smooth reconstruction while allowing for sharp features and in particular succeeds in eliminating noise without blurring the reconstructions and applies suitable exchange of information yielding sharp edges.

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EIDESSTATTLICHE ERKLÄRUNG

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I declare that I have authored this thesis independently, that I have not used other than the declared sources/resources, and that I have explicitly indicated all material which has been quoted either literally or by content from the sources used.

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