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Variational Regularization for Image Registration: Theory and Algorithms

by

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Ph.D. Thesis in Computer Science

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Abstract

In applied science many problems emerge as inverse problems. It is also common that they are ill-posed, in the sense that small changes in the input data can lead to completely different solutions. This aspect calls for regularization in order to restore well-posedness. To that purpose, among the different techniques, variational methods have gained a primary place. They rely on the Tikhonov's idea which consists of minimizing an energy functional composed by the sum of a data fidelity term and a regularization term, weighted by a regularization parameter.

In this thesis we focus on the significant problem of image registration, which finds many applications in medical image analysis. This problem is well-known to be ill-posed and there exists a vast literature devoted to the study of different regularization techniques and algorithms. Nevertheless, image registration still lacks a proper mathematical foundation which cast the problem into a coherent theoretical framework and justify the regularization methods commonly used.

Our first contribution is to formally define image registration — mono-modal as well as multi-modal — as a nonlinear inverse problem and provide a detailed analysis of the well-posedness and convergence of the corresponding regularized problem for several notable regularizers. We devise a theoretical framework general enough to include the problem of interest, extending the classical theory of variational regularization in Banach spaces, which takes into account perturbations of the data as well as the operator and data fidelity measures more general than norms.

Our second contribution is about minimization algorithms for general Tikhonov functionals. We consider regularizers that allow sparseness or discontinuities in the solutions, like L^1 norms or total variation. The main difficulty with these regularizers is that, although convex, they are non smooth. Here, we study proximal gradient algorithms of forward-backward splitting type. In the convex case (linear problem) we provide an analysis of accelerated and inexact variants, proving conditions ensuring convergence. In the non convex case (nonlinear problem) we extend the convergence analysis of the basic algorithm to Banach spaces to include the registration problem. Finally, we propose a novel proximal Gauss-Newton method for least squares problems with non-smooth penalizers. This is actually a first attempt to deal with methods of higher order and, although the achieved results sound interesting per se, they still do not cover ill-posed nonlinear problems and deserve further investigation.

To my wife, Wanda, who follows my "hazardous" path of life.

...con i piedi fortemente poggiati sulle nuvole.
(...with feet firmly resting on the clouds.) (E. Flaiano)

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First and foremost I want to thank my advisor, Prof. Alessandro Verri, for his constant support and advice. Yet, he allowed me the room to do research my way, following my "mathematical sprite". My sincerest gratitude for this chance, it is not common in these days. In the end — I think — I was enough lucky (and determined) to accomplish most of my initial purposes. I do hope this work could be a "good" return for him. I am grateful also to Dr. Silvia Villa for introducing me to the research field of convex optimization. All the second part of the thesis is a joint work with her. We were a creative couple and working together has been a pleasure. I hope we can continue our collaboration. My gratitude also to Gabriele-"Chiuzzo" Chiusano, and Alessandro Rudi for the effort of carefully reading this manuscript: many gave up earlier. I finally want to thank all the people in *SlipGuru* group, an unconventional, unorthodox and evolving family of brilliant persons of disparate origins. In turn I have had useful and stimulating discussions with them. They are all valuable researchers and I am glad to have met them.

Saverio Salzo
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Chapter 1

Introduction

The need of image registration arises when there are two images that essentially show the same object, but it appears different in the two images due to changes in the object shape or in the imaging devise position. Thus, the images are not *aligned* or not *registered*, i.e. there is no direct spatial correspondence between them. *Image registration* is then the process of determining the spatial transformation that maps points from one image to homologous points in the second image. There is a large number of applications demanding registration. Areas range from remote sensing (constructing a global picture from different partial views), security (comparing current images with a data base), robotics (tracking of objects) and medical image analysis — see [Bro92] and [ZF03] for general reviews on the subject. In particular in radiological imaging, problems like computational anatomy, computer-aided diagnosis, fusion of different modalities, intervention and treatment planning, monitoring of diseases, motion correction, radiation therapy or treatment verification demand registration [HBHH01], [MV98], [MF93].

From a mathematical standpoint image registration is treated as an optimization problem: one image is *warped* by means of suitable spatial transformations and compared with the other image, taken as reference; the *optimal* transformation is the one that makes the warped image as similar as possible to the reference image. The specification of the meaning of *suitable* and *similar* results in different scenarios and applications. This problem is known to be ill-posed (in the sense of Hadamard), that is small changes of the input images can lead to completely different registration results [CHR02, Mod04, FM08, CDH$^+$06]. Thereby, some kind of *regularization* is needed to restore well-posedness. In this context, among the different techniques, *variational regularization methods* constitute the most popular choice [FH04, HW01, DR04, Mod04, PS11]. They actually rely on the Tikhonov's regularization idea [TA77, Sch09] and consist of minimizing an energy functional — called *Tikhonov functional* — composed by the sum of a *matching term* (measuring the disparity between the images) and a *regularization term*, weighted by a regularization parameter.

This thesis is devoted to the mathematical and algorithmical aspects of the problem of image registration in the framework of variational regularization.

In the first part we deal with the mathematical foundations of image registration problem, giving a justification for a large class of variational regularization methods. We cast the problem into the theory of nonlinear inverse problems and provide an analysis of the well-posedness and convergence of the corresponding regularized problem. This reduces to study the above mentioned minimization problem under possible perturbations of the two images and with the regularization parameter tending to zero.

Although many articles recognize image registration as being an ill-posed inverse problem, the great majority pass directly to the algorithmic issues [Mod04, Mod09], and only a few pursue a stability or convergence analysis of the regularized problem. We found in fact two kinds of studies. On the one hand [FH04, FH02, HCF02] provide a partial answer exclusively to the stability issue — also, with a different meaning from ours, using a different approach and analyzing the restricted case of smooth regularizers. On the other hand [Dro05, DR04] treat convergence (the regularization parameter is let to tend to zero) but only without any perturbations of the images, thus missing the stability. For this reasons, the embedding of the image registration problem into the theory of nonlinear inverse problems is still not fully accomplished. Our work fills this gap.

The approach is based on an extension of the Tikhonov's regularization theory. In fact the complication of considering distance measures of statistical type as well as perturbations of both images to be registered makes the state-of-the-art variational regularization theory in Banach spaces [HFSHW07, Sch09] not directly applicable. There, almost invariabily, a data fit term based on some (power of) norm is considered. Only recentely more general *pseudo*-distances have appeared in [Fle10, FH10], but they are still not suitable for the image registration problem.

We shall consider two measures of the disparity between images: distances based on the L^q norm, for $q \geq 1$ and the mutual information, but our framework allows to treat other statistical measures as well with the same methods [HCF02]. These distances are then coupled with several significant regularizers: isotropic and anisotropic smoothing functionals, (linearized) elastic and hyperelastic functionals as well as the total variation.

We point out that one of the methods covered by our analysis is image registration based on total variation regularization. In the context of image registration, total variation has been considered in [HFSHW07, FSHW08], though it is used in an iterative regularization framework not directly linked with the Tikhonov regularization of the global problem. In [SPC09] an interesting method is proposed in the framework of Tikhonov regularization, but it is feasible only for the discrete problem. The appeal of regularizing with the total variation is that it leads to discontinuous correspondences which can indeed be suitable to handle certain type of problems, especially in medical image analysis where discontinuities do occur

[KFF07, RSTW09]. For the similar problem of optical flow estimation, regularizers based on the total variation has been widely and successfully employed [AK06, ADK00, WBBP06]. In case of registration, however, the main difficulty is that the corresponding Tikhonov functional is non-smooth and non-convex which makes its minimization a challenge.

The second part of the thesis is devoted to the study of algorithms for minimizing the Tikhonov functional for general *non-smooth variational methods* for convex as well as nonconvex problems. The last two decades witnessed an exceptional development of these methods. In particular non-smooth regularization techniques for convex problems impacted many fields of research — apart image processing, it is worth to mention *learning theory*. Chapter 5 is devoted to these kind of methods and there a taste of some applications to image processing as well as learning theory will be given. The non-convex case (as it is the problem of image registration) is much less mature. Indeed, minimizing a general non-convex and non-smooth functional is a difficult task and very few algorithms can possibly cope with it [BK09, RT10]. However in both cases, we carry on a study of proximal gradient methods of *forward-backward* splitting type, which employs the so called *proximity operator* to set up the iterative procedure. They are first-order methods and in fact generalization of the projected gradient algorithm. We shall study convergence properties separately for the two scenarios, depending on whether the data term is convex or not. In the convex case we analyze accelerated versions in the presence of computational errors which always occur for certain regularizers as the total variation. We prove rate of convergence in dependence on the error's decay. In the non convex case we show that the basic (non-accelerated) algorithm still keeps some (weaker) convergence properties even in infinite dimensional setting and show its applicability to the image registration problem.

The last contribution is a first attempt to deal with algorithms of higher order. Motivation comes from the so called *warping technique*, which is a standard strategy in optical flow/image registration literature to overcome nonlinearities in the model. It in fact relies on the Gauss-Newton method and recently it has been applied also within a non-smooth regularization framework in the context of optical flow [PUZ$^+$07]. However the method in this generality is far from being theoretically justified. We propose a new proximal Gauss-Newton method for least squares problems with non-smooth penalizers which interlaces the classical Gauss-Newton step with a proximal step. We are able to prove convergence to local minima, giving also estimates of the basin of convergence, but under the same hypothesis of the classical Gauss-Newton method, which in fact are suitable only for well-posed problems. Thus, the results at this stage cannot cover the problem of non-parametric image registration and further study is needed — Section 1.2 will provide details about this issue and a discussion. However, the method might be pertinent for regularizing nonlinear *parametric* models. Indeed methods with a finite number of parameters often meet the required regularity and the algorithm can be useful to force the parameters to obey some constraint (see section 6.5 of [Mod09] for further information on regularizing parametric image registration).

Summarizing our contribution

- An extension of the theory of Tikhonov's regularization for nonlinear inverse problems in abstract spaces is provided which account for general distances for the data fit term as well as general regularizers and perturbations of both the operator and data.
- The problem of image registration is formalized as a genuine nonlinear inverse problem (specifying function spaces, topologies and operators) and put into a rational theoretical framework. *Well-posedness* and *convergence* properties of several significant variational regularization methods are established for the mono-modal as well as multi-modal case and considering perturbations of both the images to be registered.
- An accelerated proximal gradient methods for minimizing functions composed by the sum of a convex smooth data term and a convex possibly non smooth penalty term is considered. We carry on a convergence analysis of the algorithm under inexact computation of the proximity operator. Novel and significant results on the convergence rate for the function values are established. The results have been collected in two articles [SV12a, SV11].
- Convergence of a proximal gradient algorithm is analyzed for non-convex problems and Banach space setting. The algorithm is show to be applicable to the problem of image registration based on total variation.
- A new proximal Gauss-Newton method is proposed to find local minimizers of penalized nonlinear least squares problems, under generalized Lipschitz assumptions. Convergence results of local type are obtained, as well as an estimate of the radius of the convergence ball. These results have been published in [SV12b].

Outline of the thesis

The following section gives first a qualitative description of image registration looking at the many applications in different fields. Next, the problem is described in a more formal way and some crucial theoretical issues, addressed in this thesis, are highlighted. Section 1.2 gives details about the problem of optical flow estimation emphasizing similarities and differences with the problem of image registration. Chapter 2 collects some mathematical facts and tools that will be used during the progress of the thesis.

The rest of thesis is divided in two parts. The first one comprises Chapter 3 and 4, and addresses the theoretical and modeling issues related to variational image registration. The second part, in three chapters, analyzes algorithms tailored to the minimization of the Tikhonv functional in three scenarios.

In Chapter 3 a generalized Tikhonov regularization theory is presented. It address both the regularization of genuine minimization problems and the regularization of inverse problems. In Chapter 4, taking into account the abstract theory, a complete theoretical analysis of the problem of image registration is discussed.

Chapter 5 is devoted to the analysis of a class of accelerated and inexact proximal gradient methods in Hilbert spaces. In Chapter 6 the behavior of the basic forward-backward splitting algorithm is studied for non-convex functionals on Banach spaces. The new proximal Gauss-Newton algorithm for least squares problems with a non-smooth penalty term is analyzed in Chapter 7.

1.1 Image registration

In this section we describe the problem of image registration, classify different methods and give several examples of applications.

1.1.1 The problem

Image registration means finding a *suitable* spatial transformation such that a transformed image becomes *similar* to another one. Typically this problem occurs if the images are taken from different perspectives, times or imaging device. Registration is treated as an optimization problem: one image is *warped* by means of given spatial transformations and compared with the other image (that instead remains fix); the *optimal* transformation is the one that makes the warped image as similar as possible to the reference image.

The basic input data to the registration process are two images (with overlapping field): that one leaved fix is defined as the *reference* (or *fixed*) image and the other as the *template* (or *moving*, *test*) image. Depending on the nature of images and on the applications, the proper method for aligning the images can vary considerably. Nevertheless, from a general point of view, all registration methods share few logical components.

Usually one has some priors on the type of the transformation that can bring the two images into alignment. Thus, a *class of transformations* need to be specified among all the possible transformations between the image domains — it forms the *search space* of the optimization problem where the optimum is supposed to belong to. Furthermore, following the definition above, being able to evaluate the *similarity* between two images is required. In the most general setting, this is accomplished by first representing images in a proper *feature space* and then measuring the *distance* between their representers in that space. Introducing a feature space serves to based the similarity criterion just on a part of information conveyed by the images: features are usually geometric structures like fiducial points, curves, surfaces, etc. As an extreme case, the space of images itself can be taken as a feature space: this corresponds to the choice of using all the content of the images for evaluating their distance. Summarizing, looking at image registration as an optimization problem, it is easy to recognize that each registration method can be viewed as different combinations of choices for the following three components:

1. a class of spatial transformations (search space);
2. a feature space;
3. a distance on the feature space (for evaluating the closeness of two images).

Depending on the choices above, registration methods are being classified accordingly.

As regards the class of transformations, there is, first of all, a classification depending, roughly speaking, on how big the class is. If that space have finite dimension, it becomes parametrizable and forms a family of transformations with a finite number of parameters: in that case one speaks of *parametric methods*. Whereas, if the space have infinite dimension, the method is called *non-parametric* [Mod04, Mod09]. Among parametric methods, we have *rigid* registration if we chose the class of rigid mouvements of the space; *affine* registration if the class of linear affine transformations (they add scale changes and skew deformations to the rigid mouvements) is chosen; and finally *perspective registration* if the transformation class is that of *perspective transformations* or *plane homographies* — they recover exactly the transformation relating two different views of a scene taken from the *same centre* or two views of a *planar scene* from different centres. Note that all those models are considered *linear* in the sense that they all transform straight line into straight line — although a perspective transformation is not linear if viewed as a transformation between cartesian coordinates. In the case of more general transformations, the term *non-linear* or *non-rigid* registration is used. Normally, non-linear methods lies on constraining the smoothness of the transformation or other measures of its behaviour. For this kind of methods, strong relationships exist with the field of continuum mechanics and methods as well as vocabulary are inherited from that field of research. Table 1.1 illustrates the different names given to the registration methods according to the choice of the transformation space.

Concerning the choice of the feature space, the method is said to be *geometry-based* if corresponding geometrical structures (features) are identified and extracted from the two images and only the distance between those corresponding structures is checked. On the other side, if the whole images are used as features, i.e. for evaluating the distance between the images, then the method is called *intensity-based* or *intensity-driven*. Note that the nature of the images also affects the choice of the distance. Indeed they can be obtained by the same sensor or by different sensors. In the first case one speaks of *mono-modal* registration, in the second case of *multi-modal* registration. In the mono-modal case, there

parametric linear	**parametric non-linear**	**non-parametric non-linear**
Rigid	Free-Form Deformation	Elestic registration
Affine	Thin Plate Spline	Hyperelastic registration
Perspective		Fluid registration
		Diffusion registration
		Diffeomorphic registration

Table 1.1: Transformation Space choice

Geometric-based	**Intensity-based**
Landmark-based	Sum of Squared Differences
Surface-Based	Mutual Information
	Cross Correlation

Table 1.2: Metric choice

is a linear relationship between the intensities of homologous points of the images and metrics that check the similarity of the images by comparing corresponding intensity values (such as the sum of squared differences) make sense. In the multi-modal case, however, the relationship often is not so simple and those metrics are no longer valid — think of a still picture taken by an ordinary camera compared with an infrared image. The classification related to the choice of the features/metric is summarized in Table 1.2.

1.1.2 Fields of application

There are mainly three research areas where the image registration problem occurs.

- Computer Vision
- Medical Image Analysis
- Remote Sensing

Each one of those research areas, has developed registration methods for solving their own specific problems, but actually there is a lot of commonality among them. The applications of image registration can be broadly classified into four groups, each one with a different main goal. Obviously, a real life problem can fall simultaneously into more then one group, meaning that the problem shares the specific characteristics of several classes at the same time.

Multiview image analysis

The problem is to align images taken from *different viewpoints*. The aim is to gain a larger 2D view or a 3D representation of the scanned scene. Example of applications are: *mosaicing* in Remote Sensing; *photo stitching* and *shape from stereo* in Computer Vision; *total body imaging* in medical applications.

Figure 1.1: Alcatraz Island, seen in an example of a panorama created by image stitching

In this problem the scene is fixed and the camera moves around the scene to take different views (note that the scene is supposed to not change during the acquisitions). Linear-parametric methods are employed, most often perspective registration is performed and both geometry-based or intensity-driven similarity metrics can be used.

Algorithms for aligning images and stitching them into seamless photo-mosaics [Sze06] are among the oldest and most widely used in computer vision. Frame-rate image alignment is used in every camcorder that has an "image stabilization" feature. Image stitching algorithms create the high-resolution photo-mosaics used to produce today's digital maps and satellite photos. They also came together with every digital camera being sold nowadays and can be used to create ultra wide-angle panoramas — *PhotoStitch* by Canon is one example.

Also 3D reconstruction from 2D views algorithms have by now reached complete development and they are beginning to become available as commercial software. For instance *Photo Tourism* is a system for browsing large collections of photographs in 3D, developed by Microsoft Research. Their approach takes as input large collections of images from either personal photo collections or internet photo sharing sites, and automatically computes each photo's viewpoint and a sparse 3D model of the scene. The photo explorer interface enables the viewer to interactively move about the 3D space by seamlessly transitioning between photographs, based on user control. Microsoft Live Labs (`http://livelabs.com/`) has turned these research ideas into a streaming multi-resolution Web-based service called *Photosynth*.

Multitemporal image analysis

Images of the same scene are acquired at *different time* intervals that might range from fractions of seconds to several months or even years. The aim is to find and evaluate changes in the scene which appeared between the consecutive image acquisitions. The setting here is that the sensor (camera) is fix, but the scene is evolving. In computer vision, *motion analysis* and *motion tracking* are both instances of this kind of problem and they are characterized by short time changes. Normally a whole sequence of images constitutes the input data of the problem and the main goal is to retrieve the *motion* of the object, i.e. the trajectory that it follows. Actually, only the apparent motion of brightness patterns observed can be measured — the so called *optical flow*. This is one of the earlier and still not completely solved problem of computer vision [HS81], [VP89].

In medical applications the setting is slightly different. Indeed, most often one is interested in medium or long time changes between the acquisitions. The problem is usually reffered as *intrasubject* registration, where anatomical parts of a given subject, that might change their appearance or shape due to certain diseases, are being monitored on regular basis and usually by a fixed imaging device. In this case, the comparison among the images is performed pair-wise and the assumption of small deformations as well as of smooth deformations can fail: tumor growth or lesions occurrences make the deformation field (describing the spatial correspondence) discontinuous and more complex. Although this is the main framework for doing multitemporal analysis with medical images, recently, with the increasing acquisition speed of digital imaging devices, motion analysis is becoming to be performed too. Cardiac motion as well as lung motion are currently active research areas [SFP+03], [Rua08], [PUZ+07]. Here, on the opposite of the classical computer vision approach, the main difficulty concern the deformable nature of the object being imaged.

Example of applications in Remote Sensing are: monitoring natural resources, surveillance of nuclear plants, monitoring urban growth, monitoring desertification and deforestation. In Computer Vision, automatic change detection for security monitoring and motion tracking are typical applications. In Medical Imaging there are many important problems falling into this class: dynamic perfusion studies; relating preoperative images and surgical plants to the physical reality of the patient in the operating room during image-guided surgery or in the treatment suite during radiotheraphy; analysis of cardiac motion; monitorning of the tumor growth; digital subtraction angiography (DSA) — registration of images before and after radio isotope injection to characterize functionality; digital subtraction mammography to detect tumors.

Methods employed in this problem can vary depending on the specific applications.

Scene vs model analysis

Images representing *scenes of the same type*, i.e. belonging to the same class of objects, are collected. The aim is to study and represent variations across population and construct a standard model of the scene. In Medical Image Analysis, human organs or anatomical parts of human body constitute the populations studied; the problem is called *intersubject* registration and it is the object of study of an emerging discipline called *computational anatomy* [Mil04]. The challenge is to account for the great variability of human organs, which means dealing with large deformations capable to preserve topological as well as differentiables structures. The first registration method able to cope with that requirement was *fluid registration* [CRM96]. In recent years, a more sophisticated method called *diffeomorphic registration* is employed and make large use of concepts and ideas from the field of differential geometry [BMTY05] [AG04] [CHF02] . In Computer Vision similar goals tackled with similar tools are studied under the name of *shape analysis*.

Multisensor data fusion

A fixed scene is viewed by means of *different kinds of sensors*, providing complementary information about the scene. The aim is the integration and fusion of information supplied by the different sensors in order to gain a larger knowledge about the scene. The problem is called *multi-modal registration*.

In remote sensing, it is performed in order to align images from different electromagnetic bands. e.g. microwave, radar, infrared, visual, or multispectral for improved scene classification such as classifying buildings, roads, vehicles and type of vegetation. In medical image analysis, fusion of *structural* information gathered from CT or MR and *functional* information obtained by PET, SPECT serves to improve significantly diagnosis and locate tumors.

From an analytical point of view, the distinguishing problem here is to find suitable similarity metrics between the two modalities. Metrics based on direct comparison of corresponding pixel values, are not appropriate anymore. For this reason, metrics based on fiducial-points or statistical measure derived from information theory are employed [HCF02], [RMPA98].

1.1.3 The variational framework

In this section we make things more precise and set the problem into a mathematical framework. In particular we clarify the terms of the problem, especially for what concerns the issues of stability and convergence. We confine ourselves to the case of non-parametric

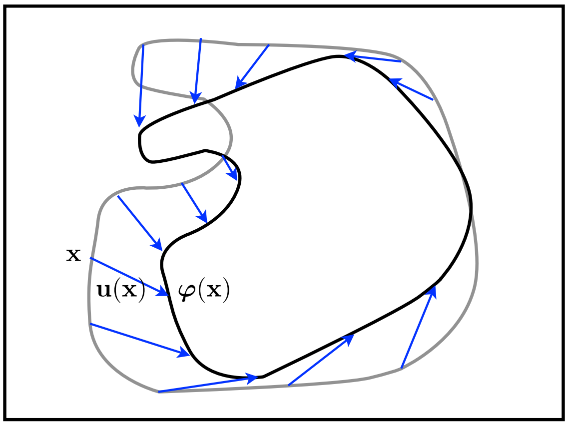

Figure 1.2: Displacement field between two 2D images.

intensity-driven registration methods.

In mathematical terms, the problem of image registration can be described as follows. Given two images, represented by scalar functions $I, I_0 : \Omega \subseteq \mathbb{R}^d \to \mathbb{R}$,[1] the first called *template* image and the second *reference* image, find a *deformation field* (the spatial transformation) $\boldsymbol{\varphi} : \Omega \to \Omega$, such that $I(\boldsymbol{\varphi}(\mathbf{x})) = I_0(\mathbf{x})$. If we introduce the *displacement field*

$$\mathbf{u} : \Omega \to \mathbb{R}^d \qquad \mathbf{u}(\mathbf{x}) = \boldsymbol{\varphi}(\mathbf{x}) - \mathbf{x}$$

then the problem reads as follows

$$I(\mathbf{x} + \mathbf{u}(\mathbf{x})) = I_0(\mathbf{x}), \quad \forall\, \mathbf{x}.$$

This is an equation in the unknown $\mathbf{u}$, the displacement field, which is supposed to be sought in a properly chosen space $U(\Omega, \mathbb{R}^d)$ of mappings from Ω to $\mathbb{R}^d$.

We will show that the problem of image registration turns up as a truly nonlinear inverse problem — actually this aspect has only been sketched in the literature [HW01, PS11]. Given the template image I, one can define an operator from the space of displacement fields $U(\Omega, \mathbb{R}^d)$ into the set $\mathrm{Im}(\Omega)$ of images as follows

$$\begin{aligned} I : U(\Omega, \mathbb{R}^d) &\to \mathrm{Im}(\Omega) \\ \mathbf{u} &\to I(\mathbf{x} + \mathbf{u}(\mathbf{x})) \end{aligned}$$

This operator gives all the warps of the image I and we call it the *warping operator* associated to the image $I \in \mathrm{Im}(\Omega)$. Note that, it is denoted with the same symbol I as for the image: this way, the warping of the image I under the deformation field $\boldsymbol{\varphi}(\mathbf{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x})$ takes the natural notation $I(\mathbf{u})$.

[1] d is the *dimension* of the image; thus we have 2D images for $d = 2$ and 3D images for $d = 3$.

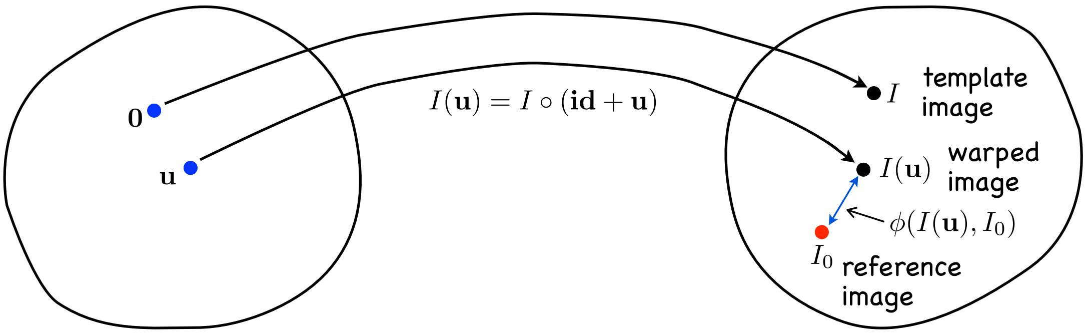

Figure 1.3: The inverse problem of image registration. The warping operator goes from the space of displacement fields into the space of images.

We are now ready to state the problem of image registration in functional language.

Problem 1.1.1. *Given $I_0, I \in \mathrm{Im}(\Omega)$, respectively the* reference *image and the* template *image, solve the functional equation*

$$I(\mathbf{u}) = I_0 \tag{1.1}$$

in the unknown $\mathbf{u} \in U(\Omega, \mathbb{R}^d)$.

The problem is in essence that of inverting the warping operator $I : U(\Omega, \mathbb{R}^d) \to \mathrm{Im}(\Omega)$, and thus it is a nonlinear inverse problem. Usually we do not expect to find (exact) solutions of the equation (1.1), mainly because data (both images I_0, I) are corrupted by noise, but also because the images might come from different sensors, as in the multi-modal case. Therefore, we consider *generalized solutions*[2] of (1.1), that is solutions of the problem

$$\min_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \phi(I(\mathbf{u}), I_0) \tag{1.2}$$

where ϕ is a suitable *distance measure* between images aimed at measuring image dissimilarities. It can be indeed derived by a true metric as in the case $\phi(I_1, I_2) = \|I_1 - I_2\|_q^q$, for some $q \geq 1$ or derived from statistical measures like mutual information or cross correlation [HCF02, RMPA98].

Viewing the operator I as acting between the above function spaces, problem (1.1) shows as a *nonlinear inverse problems between abstract spaces*. Then, *Tikhonov regularization theory*

[2]They are also called *quasi-solutions*.

relies on minimizing a (family of) *Tikhonov functional*

$$\mathscr{T}_\lambda(\mathbf{u}; I_0, I) = \phi(I(\mathbf{u}), I_0) + \lambda J(\mathbf{u}), \quad \lambda > 0$$

where $J : U(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}$ is a properly chosen *regularizer*, assumed positive and λ a regularization parameter weighting the regularization term. This approach is also known, in the related literature, under the name of *variational method* [HCF02, DR04, HW04, PS11]. Generally, the functional J is supposed to affect the smoothness of the displacement field $\mathbf{u}$, depending only on its derivatives. Eventually, the choices of the distance measure ϕ and of the regularizer J determine the registration method: mono-modal, multi-modal, diffusive, elastic, etc. [Mod04, PS11]. Then, the initial (ill-posed) problem (1.1) is replaced by a family of minimization problems

$$\boxed{\min_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \mathscr{T}_\lambda(\mathbf{u}; I_0, I)} \tag{1.3}$$

of parameter $\lambda > 0$.

We remark that both the original problem (1.2) as well as the regularized one (1.3) are nonlinear problems, thus they lack in uniqueness of the solution. However, the introduction of the regularizer J in problem (1.3) gives rise in general to a reduction of the number of solutions. In fact among generalized solutions, Tikhonov's method select the ones that also make the regularizer J minimum.[3] Such solutions are called *J-minimizing* and it is custom to denote them with $\mathbf{u}^\dagger$.

At this stage, one usually go straight on to tackle problem (1.3). However, an important theoretical issue is passed over: Tikhonov's approach needs to be justified. This means that the following problems require to be addressed:

existence: given $I_0, I \in \mathrm{Im}(\Omega)$ and $\lambda > 0$, problem (1.3) admits solutions;

stability (well-posedness): given $\lambda > 0$, solutions of problem (1.3) depend continuously on the data I_0, I; in other words, the multi-map

$$(I_0, I) \to \mathrm{argmin}_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \mathscr{T}_\lambda(\mathbf{u}; I_0, I)$$

is continuous (in a sense to be specified).

convergence: if $I_0' \to I_0$ and $I' \to I$ and $\mathbf{u}_\lambda'$ is a solution of (1.3) with I_0, I replaced respectively by I_0', I', the regularization parameter λ can be chosen (by a parameter choice rule) such that $\lambda \to 0$ and $\mathbf{u}_\lambda' \to \mathbf{u}^\dagger$, where $\mathbf{u}^\dagger$ is a J-minimizing generalized solution of the initial problem (1.1);

[3] This is exactly what the Moore-Penrose pseudoinverse does in the linear case.

We emphasize that all those problems can be hard to solve depending on the choice of the distance measure ϕ and the regularizer J. Even the existence problem can be challenging if non ordinary pairs of ϕ and J are taken — as it is the case, for instance, for the mutual information coupled with the total variation. The questions above are crucial for any regularization method and indeed they have been considered and solved in theoretical studies about general nonlinear inverse problems using different hypotheses, covering many applied problems [EHN96a, SV89, BEN$^+$94, Sch09, Fle10]. Nevertheless, we underline that, to the best of our knowledge, they remain open issues for the problem of image registration. In this thesis we give a comprehensive response to those problems.

1.2 The optical flow estimation problem

In this section we describe the problem of optical flow estimation and discuss the connection with the problem of image registration. Optical flow estimation arises when one is interested in computing the *projected motion field* in sequences of images (movie), i.e. the projection onto the image plane of the 3D motion in physical world. However, what we can actually perceive is just an "apparent" motion, the *optical flow*, which depends only on image intensity variations. In [VP89] many situations where the two quantities are different are discussed. Despite this aspect, optical flow remains a rich source of information about the 3D kinematics of objects.

In the following we shall formalize the problem to better understand the relationship with the image registration. Let be given a (continuous) sequence of images $I(\mathbf{x}, t)$, where $\mathbf{x}$ and t denotes respectively the spatial and temporal variable. In this problem a common and widely used assumption is that the pixel intensities remain constant during the motion. This is the so called *brightness constancy assumption*. Thus, if $\mathbf{x}(t) \in \Omega, t \in [0, 1]$ tracks a given point in the images, it holds

$$I(\mathbf{x}(0), 0) = I(\mathbf{x}(t), t) \qquad \forall\, t$$

Differentiating the relation above, one obtains

$$\dot{\mathbf{x}}(t) \cdot \nabla I(\mathbf{x}(t), t) + \partial_t I(\mathbf{x}(t), t) = 0$$

Therefore at a given instant t, the velocity field $\mathbf{u}(\mathbf{x}(t)) = \dot{\mathbf{x}}(t)$ satisfies the following *optical flow contraint*

$$\mathbf{u}(\mathbf{x}) \cdot \nabla I(\mathbf{x}, t) + \partial_t I(\mathbf{x}, t) = 0 \tag{1.4}$$

In real cases, dealing with (discrete) sequences, two consecutive images I_0, I are usually given and the temporal derivative $\partial_t I$ is approximated by the difference $I - I_0$. Hence one is led to the following minimization problem

$$\boxed{\min_{\mathbf{u}} \|\nabla I \cdot \mathbf{u} - (I_0 - I)\|_q^q := \phi_{OF}(\mathbf{u})} \tag{1.5}$$

If the image I is differentiable with bounded derivatives in Ω, it is easy to show that the operator

$$A : L^p(\Omega, \mathbb{R}^d) \to L^p(\Omega) \text{ with } A\mathbf{u} = \nabla I \cdot \mathbf{u} = \sum_{i=1}^{d} \partial_i I \, u_i \tag{1.6}$$

is well-defined, linear and continuous for $p \geq q$. Thus the optical flow problem 1.5 turns into the following *linear* inverse problem

$$A\mathbf{u} = g$$

where $g = I_0 - I$.

We note that the problem of optical flow estimation (1.5) is very close to the problem of image registration. In fact, it corresponds to a *linearization* of the problem of mono-modal image registration — as we will show in a moment. Starting with the image registration problem

$$\min_{\mathbf{u}} \int_{\Omega} |I(\mathbf{x} + \mathbf{u}(\mathbf{x})) - I_0(\mathbf{x})|^q \, \mathrm{d}\mathbf{x}, \qquad q \geq 1 \tag{1.7}$$

if we linearize the term $I(\mathbf{x} + \mathbf{u}(\mathbf{x}))$ around the point $\mathbf{x}$, by a first order Taylor expansion, it holds

$$I(\mathbf{x} + \mathbf{u}(\mathbf{x})) \approxeq I(\mathbf{x}) + \nabla I(\mathbf{x}) \cdot \mathbf{u}(\mathbf{x})$$

for $\mathbf{u}(\mathbf{x})$ small (for each $\mathbf{x}$). Making this approximation, problem (1.7) transforms into (1.5). Thus the problem of optical flow estimation can be seen as an approximation of the (mono-modal) image registration problem and, on the contrary of image registration, it is a *linear* inverse problem, which is clearly a key advantage. However it is still of ill-posed type and proper regularization is required. Tikhonov regularization again comes up

$$\min_{\mathbf{u}} \|A\mathbf{u} - g\|_q^q + \lambda J(\mathbf{u})$$

with the same choices of regularizers as for the image registration problem.

Actually many authors call (1.7) the optical flow problem [NE86, AWS00, LC01, PBB$^+$06, SPC09], thus they make no difference with the problem of mono-modal image registration and call (1.5) instead the *linearized* optical flow problem. Indeed (1.5) is a valid model only for infinitesimal displacement fields $\mathbf{u}$. In general to cover finite displacements, the so called *warping technique* is employed [PBB$^+$06]. It consists in solving iteratively a sequence of optical flow problems of type (1.5) where at each step the image I is *warped* by the solution obtained at the previous step. Eventually the sequence of these estimates converges possibly towards a solution of (1.7). We give details in the following. If $\mathbf{u}_k$ is a guess for a solution of problem (1.7), one can linearize $I(\mathbf{x} + \mathbf{u}(\mathbf{x}))$ around the point $\mathbf{x} + \mathbf{u}_k(\mathbf{x})$, obtaining

$$I(\mathbf{x} + \mathbf{u}(\mathbf{x})) \approxeq I(\mathbf{x} + \mathbf{u}_k(\mathbf{x})) + \nabla I(\mathbf{x} + \mathbf{u}_k(\mathbf{x})) \cdot (\mathbf{u}(\mathbf{x}) - \mathbf{u}_k(\mathbf{x}))$$

Substituting into (1.7) and setting $\mathbf{v} := \mathbf{u} - \mathbf{u}_k$ one ends up with the following optical flow problem

$$\min_{\mathbf{v}} \|\nabla I(\mathbf{u}_k) \cdot \mathbf{v} - (I_0 - I(\mathbf{u}_k))\|_q^q \tag{1.8}$$

where, using the notations given in section 1.1.3, we set $\nabla I(\mathbf{u}_k) := \nabla I \circ (\mathbf{id} + \mathbf{u}_k)$ and $I(\mathbf{u}_k) := I \circ (\mathbf{id} + \mathbf{u}_k)$. Thus, if $\mathbf{v}_k$ is a solution of this problem, the next guess (approximate solution) for (1.7) is $\mathbf{u}_{k+1} = \mathbf{u}_k + \mathbf{v}_k$. This way an iterative procedure is set up which perhaps converges towards a solution of the original problem (1.7). In fact one can easily see that this procedure (in case $p = q = 2$) corresponds exactly to the well-known *Gauss-Newton* algorithm. In section 4.2.1 we will show that, if the image $I(\mathbf{x})$ is differentiable with bounded derivative and $p \geq q$, the corresponding warping operator $I : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega)$ is Gâteaux differentiable and its derivative at the point $\mathbf{u}_k$ is the linear operator

$$I'(\mathbf{u}_k) : \mathbf{v} \in L^p(\Omega, \mathbb{R}^d) \to \nabla I(\mathbf{u}_k) \cdot \mathbf{v} \in L^q(\Omega)$$

Taking into account this result, the above iterative procedure can be written as follows

$$\begin{aligned} \mathbf{v}_k &= \min_{\mathbf{v}} \|I(\mathbf{u}_k) + I'(\mathbf{u}_k)[\mathbf{v}] - I_0\|_q^q \\ \mathbf{u}_{k+1} &= \mathbf{u}_k + \mathbf{v}_k \end{aligned} \tag{1.9}$$

which clearly shows as a Gauss-Newton procedure for the problem (1.7). Therefore the warping technique, widely used in optical flow computation, is theoretically justified. Nevertheless, it is well-known that Gauss-Newton algorithm converges towards *local* minima and this (local) convergence is guaranteed only if the original problem is *regular*, meaning that the derivative of the underlying operator must be injective with close range [BM04].[4] Unfortunately in case of image registration in infinite dimensional setting those hypotheses are met in no way. Besides, also the linearized problem (1.9) is ill-posed. On the contrary for (low dimensional) parametric transformations the problem is usually regular and the warping technique is effective and it has been indeed used since the beginnings [LK81].

In case of regularized image registration

$$\min_{\mathbf{u}} \|I(\mathbf{u}) - I_0\|_q^q + \lambda J(\mathbf{u}) \tag{1.10}$$

several authors employ the warping technique in the following form [PUZ$^+$07, PBB$^+$06]

$$\mathbf{u}_{k+1} = \operatorname{argmin}_{\mathbf{u}} \|\nabla I(\mathbf{u}_k) \cdot (\mathbf{u} - \mathbf{u}_k) + I(\mathbf{u}_k) - I_0\|_q^q + \lambda J(\mathbf{u}) \tag{1.11}$$

However, for this procedure there is no guarantee of convergence towards any solution of the regularized problem even in finite dimensional settings. Note that in this case the

[4] This agrees with the fact that Gauss-Newton method is known to address overdetermined systems of equations.

linearized problem is regularized — and therefore well-posed — and the procedure makes sense. These arguments motivated us to study generalization of Gauss-Newton method, which takes exactly the form (1.11), to cope with the minimization of Tikhonov functionals arising in non-smooth variational image registration. We were successful to prove good and interesting convergence results, as we will show in Chapter 7, but unfortunately keeping the same hypotheses of the classical Gauss-Newton method, therefore missing irregular (ill-posed) problems. Thus the convergence of algorithm (1.11) remains an open issue and further investigation is required. In Chapter 6 we propose a first-order method to solve problem (1.10) also in the ill-posed case and this time we will able to prove its convergence.

Chapter 2

Mathematical Preliminaries

For the reader's convenience, we introduce here mathematical concepts and methods that will be used and referred throughout the thesis.

In the first section the rationale of the direct methods of the calculus of variations is explained. In Section 2 the fundamental notion of Γ-convergence is given. Section 3 describes Sobolev and BV spaces and recalls the important related compactness' theorems.

2.1 Calculus of variations: the direct methods

Here and in the next section, U will be a Hausdorff topological space. $\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$ shall denote the extended real line.

When dealing with the minimization of a functional $f : U \to \overline{\mathbb{R}}$ there are two approches that can be follows:

- *the classical method* computes the derivative of f and solves the equations $f'(u) = 0$;
- *the direct methods of the calculus of variations* try to establish two properties of the functional f: the lower semicontinuity and the coercivity w.r.t. some topology of the space U.

The two methods are very different. The classical method has been the first one appeared in history. It is due to Euler and Lagrange and consists in solving the *Euler-Lagrange equation*

$$f'(u) = 0$$

Actually that equation, reveals the stationary points of the functional and in infinite dimensional spaces U, it is a partial differential equation. The drawback of this method is that, apart the (Gâteaux) differentiability of the functional, it requires solving a PDE which is often a more difficult problem than the original one.

The direct methods are due mainly to *Tonelli* and nowadays they constitute a standard technique to establish existence's theorems for minimum problems. In the following we give the definitions of the two main ingredients of the theory.

Definition 2.1.1. *Let U be a topological space. A functional $f : U \to \overline{\mathbb{R}}$ is called* sequentially lower semicontinuous *(s.l.s.c.) at $u \in U$ if it holds*

$$u_n \to u \implies f(u) \leq \liminf_{n\to\infty} f(u_n)$$

for every sequence $(u_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$.

There is a corresponding topological notion of lower semicontinuity (l.s.c.) that is not sequential, but in this thesis we shall consider only sequential lower semicontinuity and we shall refer to it simply as lower semicontinuity (l.s.c). The second ingredient is the coercivity.

Definition 2.1.2. *The functional $f : U \to \overline{\mathbb{R}}$ is said to be (sequentially)* coercive *if and only if for every $t \in \mathbb{R}$, there exists $K_t \subseteq U$ (sequentially) compact such that $\{f \leq t\} \subseteq K_t$.*

This means that from every sequence $(u_n)_{n\in\mathbb{N}}$, $u_n \in \{f \leq t\}$, one can extract a convergent subsequence in U.

In the following we give the fundamental theorem on the existence of minimizers; it is actually a generalization of the classical Weierstrass theorem.

Theorem 2.1.3 (Weierstrass). *Let $f : U \to \overline{\mathbb{R}}$ be a l.s.c. and coercive functional over a topological space U. Then the minimum problem*

$$\min_{u\in U} f(u)$$

admits a solution, that is there exists $u_* \in U$ such that $f(u_*) = \inf_U f$.

2.2 Γ-convergence of functionals

In this section we recall the notion of Γ-*convergence* of functionals (also known as *epi-convergence*) and collect the main results. For a detailed treatment of the topic we advice the reader to look at the monographs [Att84, DM93, DZ93]. This is a notion of convergence for sequences of functionals which allows to approach the limit in the corresponding minimization problems. It has found wide application in the *approximation* or *convergence* of variational problems [Att84, DM93, AFP00, AK06], i.e. it serves to approximate a given minimum problem by simpler ones or to study the asymptotic behavior of sequences of minimization problems. In section 3.1, following the same line as [DZ93] chapter IV, we shall use this notion to model general perturbations of minimum problems.

Here and throughout the thesis, we shall never explicitly refer to the topology of U but rather to the convergence of sequences of its points, which we denote by $u_n \to u$. A functional $f : U \to \overline{\mathbb{R}}$ is said to be *proper* if its domain $\operatorname{dom} f := \{u \in U \mid f(u) < +\infty\}$ is not empty.

Definition 2.2.1 (**Γ-convergence**). *Let be given a proper functional $f : U \to \overline{\mathbb{R}}$ and a sequence $(f_n)_{n\in\mathbb{N}}$, $f_n : U \to \overline{\mathbb{R}}$ of proper functionals. We say that the sequence f_n* sequentially Γ-converges *to f, and we write $f_n \xrightarrow{\Gamma} f$, if the following two properties are satisfied:*

(i) for every $u \in U$ and every sequence $(u_n)_{n\in\mathbb{N}}$ converging to u in U it is

$$f(u) \leq \liminf_{n\to\infty} f_n(u_n)$$

(ii) for every $u \in U$ there exists a sequence $(u_n)_{n\in\mathbb{N}}$ converging to u in U such that

$$f(u) = \lim_{n\to\infty} f_n(u_n)$$

If both the two conditions $(i), (ii)$ hold true just for the point $u \in U$, we say f_n sequentially Γ-converges to f at u*.*

It is possible to define a purely topological concept of Γ-convergence which does not rely on any *convergence structure* [DM93]. However, in this thesis we consider only *sequential* Γ-convergence, that for brief we shall simply refer to as Γ-convergence.

We list a series of simple results expressing the main properties of this notion of convergence. We give proofs for reader's convenience and refer to [DM93] for further details. In the sequel, we denote by $\operatorname{argmin} f$ the set al all (global) minimizers of the functional f, that is

$$\operatorname{argmin} f := \big\{u \in U \mid f(u) = \inf f\big\}.$$

Proposition 2.2.2. *Suppose f_n Γ-converges to f. If $u_n \in \operatorname{argmin} f_n$ and for a subsequence $(u_{k_n})_{n\in\mathbb{N}}$, $u_{k_n} \to u \in U$, then $u \in \operatorname{argmin} f$ and $f_{k_n}(u_{k_n}) \to f(u)$.*

Proof. Let $u_{k_n} \to u$. One can easily show that, being $f_n \xrightarrow{\Gamma} f$, it holds $f_{k_n} \xrightarrow{\Gamma} f$. Let $w \in U$. From (ii), there exists $(w_n)_{n\in\mathbb{N}}$ such that $w_n \to w$ and $f_{k_n}(w_n) \to f(w)$. Thus, from the property (i), we have

$$\begin{aligned} f(u) &\leq \liminf_{n\to\infty} f_{k_n}(u_{k_n}) \leq \limsup_{n\to\infty} f_{k_n}(u_{k_n}) \\ &\leq \limsup_{n\to\infty} f_{k_n}(w_n) = f(w) \end{aligned}$$

where we made use of the definition of u_n, to infer $f_{k_n}(u_{k_n}) \leq f_{k_n}(w_n)$. Furthermore, from the above chain of inequalities, written for $w = u$, it follows $f_{k_n}(u_{k_n}) \to f(u)$. □

To ensure that argmin $f_n \neq \varnothing$, it is sufficient to take f_n (sequentially) l.s.c. and f_n (sequentially) coercive for every $n \in \mathbb{N}$ (recall Weierstrass theorem 2.1.3). This allows to define the sequence $(u_n)_{n\in\mathbb{N}}$ in Proposition 2.2.2 above. But, if we want to ensure the existence of a convergent subsequence we need to require more. The following definition and the subsequent proposition tell us how.

Definition 2.2.3. *The sequence $(f_n)_{n\in\mathbb{N}}$ is said to be* equi-coercive *if and only if for every $t \in \mathbb{R}$, there exists $K_t \subseteq U$ (sequentially) compact such that $\{f_n \leq t\} \subseteq K_t$ for every $n \in \mathbb{N}$.*

Proposition 2.2.4. *Let us suppose $(f_n)_{n\in\mathbb{N}}$ equi-coercive. If f_n Γ-converges to f, then each sequence $(u_n)_{n\in\mathbb{N}}$ with $u_n \in \arg\min f_n$, possesses a convergent subsequence.*

Proof. Fix $u \in U$, with $f(u) \in \mathbb{R}$. From property (ii) in the definition of Γ-convergence, there exists $(w_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$ with $w_n \to u$ and $f_n(w_n) \to f(u)$. The sequence $(f_n(w_n))_{n\in\mathbb{N}}$ is bounded and, from the definition of u_n, $f_n(u_n) \leq f_n(w_n)$. Thus, $f_n(u_n)_{n\in\mathbb{N}}$ is bounded above, that is there exixts $t \in \mathbb{R}$ such that $f_n(u_n) \leq t$. Then, it holds $u_n \in \{f_n \leq t\} \subseteq K_t$ and, from the sequential compactness of K_t, there must exists a subsequence $(u_{k_n})_{n\in\mathbb{N}}$ which converges in K_t. □

The next stability result is just the merge of the two previous propositions.

Theorem 2.2.5 (Stability). *Let $f, f_n : U \to \overline{\mathbb{R}}$ be proper and sequentially l.s.c. functionals and suppose f_n Γ-converges to f and $(f_n)_{n\in\mathbb{N}}$ equicoercive. Then, it holds* $\inf f_n \to \inf f$, argmin $f_n \neq \varnothing$ *for every $n \in \mathbb{N}$ and if $(u_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$ with $u_n \in$* argmin f_n*, we have:*

1. *$(u_n)_{n\in\mathbb{N}}$ admits a convergent subsequence;*
2. *if for a subsequence $(u_{k_n})_{n\in\mathbb{N}}$, $u_{k_n} \to u \in U$, then $u \in$* argmin f*, i.e. every cluster point of the sequence $(u_n)_{n\in\mathbb{N}}$ is a minimizer of f.*

Proof. From the two propositions above we get that $(u_n)_{n\in\mathbb{N}}$ admits a convergent subsequence and if $u_{k_n} \to u$ then $u \in \operatorname{argmin} f$ and $f_{k_n}(u_{k_n}) \to f(u) = \inf f$. We shall prove that in fact $f_n(u_n) \to \inf f$. To that purpose, it is enough to prove that each subsequence of $f_n(u_n)_{n\in\mathbb{N}}$ admits a subsequence converging to $\inf f$. Indeed, if $f_{k_n}(u_{k_n})_{n\in\mathbb{N}}$ is any subsequence, then, we can apply the two propositions above to the subsequence $(f_{k_n})_{n\in\mathbb{N}}$ and conclude that $(f_{k_n}(u_{k_n}))_{n\in\mathbb{N}}$ has a subsequence converging to $f(u) = \inf f$. □

We finish the "Γ-trip" by giving a simple criteria for Γ-convergence that will be useful in the sequel.

Proposition 2.2.6. *Let $f : U \to \overline{\mathbb{R}}$ be a proper and sequentially l.s.c. functional and $f_n : U \to \overline{\mathbb{R}}$ be proper with $\mathrm{dom} f_n = \mathrm{dom} f$ for every $n \in \mathbb{N}$. Suppose $f_n(u) \to f(u)$ uniformly over the sets $A \subseteq \mathrm{dom}\, f$ of the form $A = \{u_n \,|\, n \in \mathbb{N}\}$ for any convergent sequences $(u_n)_{n\in\mathbb{N}}$ in U. Then $f_n\,\Gamma$-converges to f.*

Proof. Being $f_n \to f$ pointwise, it is enough to check only the first property of the definition of Γ-convergence. Let $(u_n)_{n\in\mathbb{N}}$, $u_n \in U$ and $u_n \to u \in U$. We have to prove that

$$f(u) \leq \liminf_{n\to\infty} f_n(u_n)$$

Let us reason by contradiction and suppose the above inequality be false. Then, there exists $t \in \mathbb{R}$ and $\varepsilon > 0$ and a subsequence $(u_{k_n})_{n\in\mathbb{N}}$ such that

$$f_{k_n}(u_{k_n}) < t - \varepsilon < t < f(u)$$

for every $n \in \mathbb{N}$. Evidently $u_{k_n} \in \mathrm{dom}\, f_{k_n}$ and we still have $u_{k_n} \to u$. Now, if we set $A := \{u_{k_n} \,|\, n \in \mathbb{N}\} \subseteq \mathrm{dom}\, f$, the hypotheses implies $f_{k_n} \to f$ uniformly on A, thus there exists $\nu \in \mathbb{N}$ such that

$$|f_{k_n}(u') - f(u')| \leq \varepsilon$$

for every $n \geq \nu$ and $u' \in A$. Therefore we have

$$f(u_{k_n}) \leq \varepsilon + f_{k_n}(u_{k_n}) < t < f(u)$$

for every $n \geq \nu$ and this implies $\liminf_n f(u_{k_n}) < f(u)$ which contradicts the hypothesis of lower semicontinuity of f. □

2.3 Function spaces

In this section we recall definitions and main properties of Sobolev and BV spaces. This section is actually quite technical and can be skipped in a first reading. The reader can come back later when these notions are effectively mentioned in the following chapters to look at definitions and statements of theorems.

We shall denote by $\Omega \subseteq \mathbb{R}^d$ an open set. Vectors of $\mathbb{R}^d$ are thought as columns vectors and $|\cdot|$ shall denote the euclidean norm in $\mathbb{R}^d$. Finally $\mathscr{C}_c(\Omega)$ and $\mathscr{C}_c^\infty(\Omega)$ are respectively the space of compactely supported continuous functions on Ω and the space of compactely supported infinitely differentiable functions on Ω.

2.3.1 Sobolev spaces

We recall here some concepts about Sobolev spaces. All definitions and results can be found for instance in [Bré10, AF03].

Definition 2.3.1. *Let $\Omega \subseteq \mathbb{R}^d$ be open, $u \in L^1_{loc}(\Omega)$ and $i \in \mathbb{N}, 1 \le i \le d$. The function u is said to be* wealky differentiable with respect to the i-th variable*, if the i-th distributional derivative of u is a function in $L^1_{loc}(\Omega)$, that is there exists $v \in L^1_{loc}(\Omega)$ such that*

$$\forall\, \phi \in \mathscr{C}_c^\infty(\Omega): \int_\Omega u(\mathbf{x}) \partial_i \phi(\mathbf{x})\, \mathrm{d}x = -\int_\Omega v(\mathbf{x})\phi(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

In such case one can show that v is unique in $L^1_{loc}(\Omega)$ and one defines $\partial_i u := v$ wich takes the name of weak partial derivative of u with respect to the i-th variable.

Definition 2.3.2. *Let $\Omega \subseteq \mathbb{R}^d$ be open and $p \in [1, +\infty]$. The* Sobolev space of type $1, p$, *is the set*

$$W^{1,p}(\Omega) = \big\{ u \in L^p(\Omega) \,\big|\, \forall i,\ u \text{ is weakly differentiable w.r.t. the } i\text{-th var. and } \partial_i u \in L^p(\Omega) \big\}$$

Moreover one set $H^1(\Omega) := W^{1,2}(\Omega)$.

The Sobolev space $W^{1,p}(\Omega)$ contains those functions of $L^p(\Omega)$ having all distributional derivatives also in $L^p(\Omega)$. Clearly $W^{1,p}(\Omega)$ is a subspace of $L^p(\Omega)$ and for each $i \in \mathbb{N}$, $1 \le i \le d$ the partial derivative operator

$$\partial_i : W^{1,p}(\Omega) \to L^p(\Omega)$$

is a linear mapping. If $u \in W^{1,p}(\Omega)$, one defines the *gradient* of u as the function

$$\nabla u : \Omega \to \mathbb{R}^n$$

having as components the partial derivatives $\partial_i u : \Omega \to \mathbb{R}$. Thus by definition $\nabla u \in L^p(\Omega, \mathbb{R}^d)$ and the gradient operator

$$\nabla : W^{1,p}(\Omega) \to L^p(\Omega, \mathbb{R}^d)$$

is a linear mapping. The Sobolev space $W^{1,p}(\Omega)$ is then endowed with the norm

$$\boxed{\|u\|_{1,p} := \|u\|_p + \sum_{i=1}^{d} \|\partial_i u\|_p} \tag{2.1}$$

which makes it a Banach space. It easy to show that the following norms are equivalent to (2.1)

$$\left(\|u\|_p^p + \sum_{i=1}^{d} \|\partial_i u\|_p^p \right)^{1/p} \quad \text{and} \quad \|u\|_p + \|\nabla u\|_p$$

where

$$\|\nabla u\|_p = \left(\int_\Omega |\nabla u(\mathbf{x})|^p \, \mathrm{d}\mathbf{x} \right)^{1/p}$$

Let us consider now the space $W^{1,p}(\Omega, \mathbb{R}^m)$, of (vector) functions

$$\mathbf{u} : \Omega \to \mathbb{R}^m$$

$\mathbf{u} = (u_1, \cdots, u_m)$, such that the components $u_i : \Omega \to \mathbb{R}$ are in $W^{1,p}(\Omega)$[1]. The *derivative of* $\mathbf{u}$ is defined as the function

$$D\mathbf{u} : \Omega \to \mathbb{R}^{m \times d} \quad \text{with} \quad (D\mathbf{u}(\mathbf{x}))_{ij} = \partial_j u_i(\mathbf{x}).$$

or in the same way

$$D\mathbf{u}(\mathbf{x}) = \begin{bmatrix} \nabla u_1(\mathbf{x})^\top \\ \cdots \\ \nabla u_m(\mathbf{x})^\top \end{bmatrix} .$$

Thus $D\mathbf{u}$ is the function having for components the partial derivative $\partial_j u_i : \Omega \to \mathbb{R}$ and it is also called the *Jacobian* of the function $\mathbf{u}$. Therefore

$$D\mathbf{u} \in L^p(\Omega, \mathbb{R}^{m \times d})$$

If we denote again with $|\cdot|$ the euclidean norm in $\mathbb{R}^{m \times d}$ — which is the Frobenius norm — we can consider, on the space $W^{1,p}(\Omega, \mathbb{R}^m)$, the norm

$$\|\mathbf{u}\|_{1,p} := \|\mathbf{u}\|_p + \|D\mathbf{u}\|_p = \left(\int_\Omega |\mathbf{u}(\mathbf{x})|^p \, \mathrm{d}\mu(\mathbf{x}) \right)^{1/p} + \left(\int_\Omega |D\mathbf{u}(\mathbf{x})|^p \, \mathrm{d}\mu(\mathbf{x}) \right)^{1/p}$$

which is equivalent to any of the following one

$$\left(\sum_{i=1}^{m} \|u_i\|_p^p + \sum_{i=1}^{m} \sum_{j=1}^{d} \|\partial_j u_i\|_p^p \right)^{1/p} \quad \text{and} \quad \sum_{i=1}^{m} \|u_i\|_p + \sum_{i=1}^{m} \sum_{j=1}^{d} \|\partial_j u_i\|_p$$

[1] The space $W^{1,p}(\Omega, \mathbb{R}^m)$ is clearly isomorphic to $[W^{1,p}(\Omega)]^m$.

Evidently the derivative

$$D : W^{1,p}(\Omega, \mathbb{R}^m) \to L^p(\Omega, \mathbb{R}^{m\times d})$$

is a linear and bounded operator between Banach spaces. One can prove the following proposition

Proposition 2.3.3. *Let* $\Omega \subseteq \mathbb{R}^d$ *be open,* $1 \le p \le +\infty$. *Then the space* $(W^{1,p}(\Omega, \mathbb{R}^m), \|\cdot\|_{1,p})$ *is separable if* $1 \le p < +\infty$ *and reflexive if* $1 < p < +\infty$.

Together with Kakutani theorem [Bré10], proposition above provides a compactness results for the space $(W^{1,p}(\Omega, \mathbb{R}^m), \|\cdot\|_{1,p})$ in case $1 < p < +\infty$. More precisely for every bounded sequence in $(W^{1,p}(\Omega, \mathbb{R}^m), \|\cdot\|_{1,p})$ one can extract a weakly convergent subsequence.

Definition 2.3.4. *Let* $\Omega \subseteq \mathbb{R}^d$ *be open and* $p \in [1, +\infty]$. *The closure of* $\mathscr{C}^1_c(\Omega, \mathbb{R}^m)$ *in the space* $W^{1,p}(\Omega, \mathbb{R}^m)$ *is denoted by* $W^{1,p}_0(\Omega, \mathbb{R}^m)$.

Intuitively the functions in $W^{1,p}_0(\Omega, \mathbb{R}^m)$ are “roughly” those of $W^{1,p}(\Omega, \mathbb{R}^m)$ that “vanish on $\partial\Omega$”. We recall some important theorems.

Theorem 2.3.5 (Poincaré’s inequality). *Let* $\Omega \subseteq \mathbb{R}^d$ *be a bounded open set and* $1 \le p < +\infty$. *Then there exists* $C > 0$ *(which depends only on* d *and* Ω*) such that*

$$\|\mathbf{u}\|_p \le C\|\nabla \mathbf{u}\|_p \qquad \forall\, \mathbf{u} \in W^{1,p}_0(\Omega, \mathbb{R}^m)$$

Note that the open set Ω is not required to have regular boundary.

Finally we give the *Sobolev and Rellich-Kondrachov embedding theorems.* It is easy to see that, in case of bounded domain Ω, one has the following chain of embeddings (continuous)

$$\mathscr{C}(\overline{\Omega}, \mathbb{R}^m) \subseteq L^\infty(\Omega, \mathbb{R}^m) \subseteq \cdots \subseteq L^q(\Omega, \mathbb{R}^m) \subseteq \cdots \subseteq L^1(\Omega, \mathbb{R}^m)$$

and clearly, for $q = p$, we have

$$W^{1,p}(\Omega, \mathbb{R}^m) \subseteq L^q(\Omega, \mathbb{R}^m) \subseteq \cdots \subseteq L^1(\Omega, \mathbb{R}^m)$$

The Sobolev embedding theorems tell us that we can increase the exponent q (and consequently shrink the spaces L^q) preserving the embeddings of $W^{1,p}(\Omega, \mathbb{R}^m)$. The upper bound for this increase of the exponent q is $p^* := pd/(d-p)$[2] if $p < d$, and $+\infty$ if $p = d$.[3] Moreover in case $p > d$ it is even $W^{1,p}(\Omega, \mathbb{R}^m) \subseteq \mathscr{C}(\overline{\Omega}, \mathbb{R}^m)$. The embeddings are even compact if $q < p^*$.The precise statement is as follows

[2] evidently $p^* = \frac{p}{1-p/d} > p$

[3] note that $p \to d \implies p^* \to \infty$.

Theorem 2.3.6 (Rellich-Kondrakhov and Sobolev). *Let $\Omega \subseteq \mathbb{R}^d$ be a bounded open set with a regular boundary of class $\mathscr{C}^1$. Let $m \geq 1$ and $p \in [1, +\infty[$. Then we have the following compact embeddings:*

(i) if $1 \leq p < d$, then $W^{1,p}(\Omega, \mathbb{R}^m) \hookrightarrow L^q(\Omega, \mathbb{R}^m)$ for every $q \in [1, p^*[$;

(ii) if $p = d$, then $W^{1,p}(\Omega, \mathbb{R}^m) \hookrightarrow L^q(\Omega, \mathbb{R}^m)$ for every $q \in [1, +\infty[$;

(iii) if $p > d$, then $W^{1,p}(\Omega, \mathbb{R}^m) \hookrightarrow \mathscr{C}(\overline{\Omega}, \mathbb{R}^m)$.

For the limiting case $q = p^*$ one has only continuous embedding.

Remark 2.3.7. *The results on the continuous embeddings holds true also for Ω unbounded but with bounded boundary (Sobolev embeddings theorems). Rellich-Kondrakhov theorem actually refer only to the compactness aspect.*

2.3.2 BV spaces

In the applications, most problems require the mathematical model to be discontinuous. In image processing for instance, the model of an image itself must account for discontinuities because they constitute significant and important features. Unfortunately, classical Sobolev spaces do not allow one to take into account such phenomena since the set of points of discontinuity is *essentially* empty. On the other hand, we would not let the discontinuities go "out of control" in order to avoid unrealistic functions. The correct answer to these needs has been developed in the last two decades involving the mathematical community. In a famous paper on image denoising of Rudin, Osher and Fatemi [ROF92a] as well as in the problem of image segmentation formulated by Mumford and Shah [MS89], an appropriate class of functions handling discontinuities is introduced, that is the *functions of bounded variations $BV(\Omega)$*.

They have discontinuities essentially along curves (in the case of functions of two variables) and nevertheless they allow to make sense of the integral

$$\int_\Omega |\nabla u(\mathbf{x})| \, \mathrm{d}\mathbf{x} \tag{2.2}$$

As in case of the Sobolev space, BV functions can be defined in terms of distributional derivaties. More precisely a function $u \in L^1(\Omega)$ is said to be of *bounded variation* if its distributional derivatives are *Radon measure* on Ω. However they can be defined in an equivalent way by means of the notion of *variation* of a function. We will deal directly with vector functions $\mathbf{u} : \Omega \to \mathbb{R}^m$. We recall that $\mathscr{C}_c^1(\Omega, \mathbb{R}^{m \times d})$ is the space of differentiable functions from Ω into $\mathbb{R}^{m \times d}$ with compact support. As usual we denote by $|\cdot|$ the euclidean norm on $\mathbb{R}^{m \times d}$ (the *Frobenius norm*).

Definition 2.3.8. *Let* $\mathbf{u} \in L^1(\Omega, \mathbb{R}^m)$*. The* variation $V_\Omega(\mathbf{u})$ *of* $\mathbf{u}$ *in* Ω *si defined by*

$$V_\Omega(\mathbf{u}) := \sup\left\{ \sum_{i=1}^{m} \int_\Omega u_i \operatorname{div} \phi_i \,\mathrm{d}\mathbf{x} \,\middle|\, \boldsymbol{\phi} \in \mathscr{C}_c^1(\Omega, \mathbb{R}^{m\times d}), \|\boldsymbol{\phi}\|_\infty \le 1 \right\}$$

where $\phi_i : \Omega \to \mathbb{R}^d$ *are the rows of the tensor* $\boldsymbol{\phi} : \Omega \to \mathbb{R}^{m\times d}$ *and* $\|\boldsymbol{\phi}\|_\infty := \sup_{x\in\Omega} |\boldsymbol{\phi}(\mathbf{x})|$*.*

One can prove [AFP00] that the variation in Ω

$$V_\Omega : L^1(\Omega, \mathbb{R}^m) \to \mathbb{R} \cup \{+\infty\}$$

is a lower semicontinuous functional in the (strong) topology of $L^1(\Omega, \mathbb{R}^m)$. Then, the space of function of bounded variation is naturally

$$\boxed{BV(\Omega, \mathbb{R}^m) := \left\{ \mathbf{u} \in L^1(\Omega, \mathbb{R}^m) \,\middle|\, V_\Omega(\mathbf{u}) < +\infty \right\}}$$

If $\mathbf{u} \in BV(\Omega, \mathbb{R}^m)$, then one set $|D\mathbf{u}|(\Omega) := V_\Omega(\mathbf{u})$[4] which is called the *total variation of* $\mathbf{u}$. One can prove that

$$W^{1,1}(\Omega, \mathbb{R}^m) \subseteq BV(\Omega, \mathbb{R}^m)$$

and for $\mathbf{u} \in W^{1,1}(\Omega, \mathbb{R}^m)$, it holds

$$|D\mathbf{u}|(\Omega) = \int_\Omega |D\mathbf{u}(\mathbf{x})| \,\mathrm{d}\mathbf{x}\,.$$

Thus the total variation is a generalization of the L^1 norm of the derivative for functions which do not have a L^1 derivative (in the sense of Sobolev).

The space $BV(\Omega, \mathbb{R}^m)$ is then endowed with the following norm

$$\|\mathbf{u}\|_{BV} := \|\mathbf{u}\|_1 + |D\mathbf{u}|(\Omega)$$

which make it a Banach space. It is also possible to define another topology on $BV(\Omega, \mathbb{R}^m)$, which is called the *weak*-$*$ topology and denoted by $\overset{*}{\rightharpoonup}$. We do not recall here the definition. It is important just to recall some simple facts. The weak-$*$ topology is weaker than the topology of the norm $\|\cdot\|_{BV}$ and stronger than the topology of the L^1 norm. Furthermore the following simple criterion for weak-$*$ convergence holds

Theorem 2.3.9. *Let* $\mathbf{u}_k, \mathbf{u} \in BV(\Omega, \mathbb{R}^m)$*. Then* $\mathbf{u}_k \overset{*}{\rightharpoonup} \mathbf{u}$ *iff* $\sup_{k\in\mathbb{N}} \|\mathbf{u}_k\|_{BV} < +\infty$ *and* $\mathbf{u}_k \to \mathbf{u}$ *in* $L^1(\Omega, \mathbb{R}^m)$*.*

[4]The notation $|D\mathbf{u}|(\Omega)$ comes from the other definition we refered to at the beginning of the section. Indeed one can define a *derivative* $D\mathbf{u}$ of the function $\mathbf{u}$, which is in fact a (Radon) vector-valued measure and $|D\mathbf{u}|$ is its variation, which is a scalar measure.

From this theorem it follows that the total variation $|D\cdot|(\Omega) : BV(\Omega, \mathbb{R}^m) \to \mathbb{R}$ is weakly-$*$ lower semicontinuous.

The following compactness theorem for BV functions is very useful in connection with variational problems. Since the Sobolev space $W^{1,1}(\Omega, \mathbb{R}^m)$ has no similar compactness property, this provides also a justification for the introduction of BV spaces.

Theorem 2.3.10 (Compactness in BV). *Let Ω be a bounded open set with Lipschitz boundary. If $(\mathbf{u}_k)_{k\in\mathbb{N}}$, $\mathbf{u}_k \in BV(\Omega, \mathbb{R}^m)$ with $\sup_{k\in\mathbb{N}}\|\mathbf{u}_k\|_{BV} < +\infty$, then there exists a subsequence $(\mathbf{u}_{k_n})_{n\in\mathbb{N}}$ weakly-$*$ convergent in $BV(\Omega, \mathbb{R}^m)$. In other words bounded sets (in norm) of $BV(\Omega, \mathbb{R}^m)$ are sequentially relatively compact for the weak-$*$ topology.*

The theorem above tell us that the norm $\|\cdot\|_{BV}$ is sequentially coercive for the weak-$*$ topology. Next, taking into account that the weak-$*$ topology is stronger than the topology of L^1, it results that the canonical embedding

$$\iota : BV(\Omega, \mathbb{R}^m) \to L^1(\Omega, \mathbb{R}^m)$$

(which is linear and continuous) transforms weak-$*$ convergent sequences into strong convergent sequences in $L^1(\Omega, \mathbb{R}^m)$. Actually one can prove more (see [AFP00], Theorem 3.49 p. 152).

Theorem 2.3.11 (Compact embedding). *Let Ω be a bounded open set with Lipschitz boundary. Then the following compact embeddings hold true*

$$BV(\Omega, \mathbb{R}^m) \hookrightarrow L^p(\Omega, \mathbb{R}^m)$$

for $1 \le p < 1^* = d/(d-1)$. The embedding is only continuous if $p = 1^*$.

Theorem 2.3.12 (Poincaré's inequality). *Let Ω be a bounded open set with Lipschitz boundary. Then for $1 \le p \le 1^*$, it holds*

$$\left\| \mathbf{u} - \frac{1}{|\Omega|} \int_\Omega \mathbf{u}(x)\,\mathrm{d}\mathbf{x} \right\|_p \le C|D\mathbf{u}|(\Omega) \qquad \forall\, \mathbf{u} \in BV(\Omega, \mathbb{R}^m)$$

Part I

The Theory of Variational Regularization

In this part we present an analysis of variational regularization techniques in abstract spaces and then we apply the theory to the image registration problem. Our theory covers both mono-modal as well as multi-modal image registration and gives stability and convergence results for a number of significant regularization methods.

Chapter 3

Generalized Tikhonov Regularization

In this chapter we extend the classical theory of Tikhonov regularization to a more general framework. We shall study a notion of Hadamard *well-posedness* for general *minimum problems* based on the concept of Γ-convergence of functionals — which we recalled in section 2.2. We also show the link between such concept of well-posedness and Tikhonov regularization. Next, we propose a general framework for regularizing nonlinear ill-posed inverse problems, taking into account *distance measure* more general than norms and perturbations of both the operator and the data.

The chapter is structured in two sections. The first one deals with regularization of minimum problem, while in the second section the regularization of nonlinear inverse problems is addressed.

3.1 Regularizing minimum problems

In this section we present the theory of Tikhonov regularization for general *minimization problems*

$$\boxed{\min_{u \in U} f(u)} \tag{3.1}$$

where U is a Hausdorff topological space and $f : U \to \overline{\mathbb{R}}$ is a proper and sequentially lower semicontinuous (l.s.c.) functional. The set of solutions of problem (3.1) is

$$\operatorname{argmin} f := \big\{ u \in U \,\big|\, f(u) = \inf f \big\}, \tag{3.2}$$

which, in general, may contain more then one point[1]. We assume problem (3.1) possibly unstable under perturbation of the functional f, meaning that if we change slightly f (in

[1] Thus, we do not make the hypothesis of uniqueness in problem (3.1)

a sense to be specified) we might end with a completely different solution set: that is the phenomenon called *ill-posedness* in the sense of *Hadamard*.

The study of *Hadamard well-posedness* for general minimization problems has been pursued in [DZ93], where the concept of Γ-convergence of functionals is re-interpreted to provide a framework for treating perturbations of a given minimization problem. Here we assume the same point of view and we consider Γ-convergent perturbations. In order to study the behavior of the set of minimizer (3.2), we need a notion of set convergence. We shall use the following one which is actually common in inverse problems [SV89, HKPS07, Sch09].

Definition 3.1.1. *Given a sequence of subset $(A_n)_{n\in\mathbb{N}}, A_n \subseteq U$ and $A \subseteq U$, we say that* A_n converges to A *and we write $A_n \to A$ iff for every sequence $(u_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$ with $u_n \in A_n$, it is*

1. *$(u_n)_{n\in\mathbb{N}}$ admits a convergent subsequence;*
2. *if for a subsequence $(u_{k_n})_{n\in\mathbb{N}}$, $u_{k_n} \to u \in U$, then $u \in A$.*

This means that for each sequence $(u_n)_{n\in\mathbb{N}}$, with $u_n \in A_n$, the set of its cluster points is nonvoid and contained in A.

In section 2.2 we saw the main properties of Γ-convergence for functionals and Theorem 2.2.5 can be viewed as a (Hadamard) well-posedness result for problem 3.1 under Γ-convergent perturbations. Indeed, taking into account Definition (3.1.1), it can be rephrased as

$$f_n \xrightarrow{\Gamma} f \text{ and } (f_n)_{n\in\mathbb{N}} \text{ equi-coercive } \implies \operatorname{argmin} f_n \to \operatorname{argmin} f$$

The following proposition makes clear a possible cause of ill-posedness in minimization problems.

Proposition 3.1.2. *If $(f_n)_{n\in\mathbb{N}}$ is equi-coercive and f_n Γ-converges to f, then f is coercive too.*

Proof. Fix $t \in \mathbb{R}$ and take $s \in \mathbb{R}$, $s > t$. If $f(u) \leq t$ we have $f(u) < s$ and there exists $(u_n)_{n\in\mathbb{N}}$, $u_n \to u$, $f_n(u_n) \to f(u)$. Then, $\exists\, \nu \in \mathbb{N}$ such that for $n \geq \nu$ $f_n(u_n) < s$. Thus, $u_n \in \{f_n \leq s\} \subseteq K_s$ for every $n \geq \nu$. Being $u_n \to u$ and K_s sequentially closed, we have $u \in K_s$. In the end we proved $\{f \leq t\} \subseteq K_s$ which is sequentially compact. □

The proposition above shows that, if in problem (3.1) the functional f is not coercive, we may not hope to find any equi-coercive perturbations $(f_n)_{n\in\mathbb{N}}$ which Γ-converges to f and get any stability results based upon Theorem 2.2.5. In other words the lack of the coercivity property for the functional f is a source of ill-posedness for the minimization problem (3.1).

In order to cure ill-posedness of problem (3.1), Tikhonov theory introduces a *regularization functional* (also called a *stabilizing functional* [TA77])

$$J : U \to \overline{\mathbb{R}}, \text{ (seq.) l.s.c., } \operatorname{dom} J \cap \operatorname{dom} f \neq \varnothing \tag{3.3}$$

which is weighted by a positive scalar $\lambda > 0$ and added back to the original functional f just in order to gain the coercivity property. Eventually, one replaces problem (3.1) with the following minimization problem

$$\boxed{\min_{u \in U} f(u) + \lambda J(u)} \tag{3.4}$$

depending on the *regularization parameter* $\lambda > 0$, where the functional J is chosen in such a way $f + \lambda J$ be coercive. The parameter λ plays the role of a weight which tunes the amount of regularization.

We already mentioned, in section 2.2, that Γ convergence is designed to express the convergence of minimum problems. Here, we applied the theory to study the asymptotic behavior of Tikhonov's minimum problems (3.4) as the regularization parameter tends to zero and the perturbed data tend to the exact data. To the best of our knowledge, the connection between Tikhonov regularization and Γ-convergence has been only analyzed in [DZ93, Zol00], but there, stronger assumptions on the regularizer and on the convergence of perturbed problems are required.

We shall asses the stability of problem (3.4), for fixed λ, by considering the behavior of solutions for appropriate perturbations of the functional f. In order to rely on the general Theorem 2.2.5, we need to consider perturbations f_n of f which guarantee that $f_n + \lambda J$ Γ-converges to $f + \lambda J$. This turns out to require Γ-convergence as well as *pointwise convergence* for the sequence of perturbations $(f_n)_{n \in \mathbb{N}}$. In general Γ-convergence and pointwise convergence are independent properties (see Example 4.4 in [DM93]). However, we highlight that if $f_n \to f$ pointwise, then just the check of property (i) in Definition 2.2.1 is enough to guarantee Γ-convergence of the functionals f_n towards f, being (ii) trivially satisfied. The following proposition is preliminary for the subsequent stability result — see also Proposition 6.25 in [DM93].

Proposition 3.1.3. *Let $f, f_n : U \to \overline{\mathbb{R}}$ be proper functionals, $J : U \to \overline{\mathbb{R}}$ as in* (3.3) *and $\lambda > 0$. If f_n Γ-converges and converges pointwise to f, then the sequence $f_n + \lambda J$ Γ-converges and converges pointwise to $f + \lambda J$.*

Proof. Since obiously $f_n + \lambda J$ converges pointwise to $f + \lambda J$, we need just to check the first property of Γ-convergence. Let $u \in U$ and $(u_n)_{n \in \mathbb{N}}$ such that $u_n \to u$. Then, from (i)

and lower semicontinuity of J, we have

$$f(u) \leq \liminf_{n\to\infty} f_n(u_n) \quad J(u) \leq \liminf_{n\to\infty} J(u_n)$$

Thus,

$$f(u) + \lambda J(u) \leq \liminf_{n\to\infty} f_n(u_n) + \lambda J(u_n)\,. \qquad \square$$

Theorem 3.1.4 (Stability). *Let $f, f_n : U \to \overline{\mathbb{R}}$ be proper and sequentially l.s.c., J be as in (3.3) and $\lambda > 0$. Suppose f_n Γ-converges and converges pointwise to f and $(f_n + \lambda J)_{n\in\mathbb{N}}$ be equi-coercive. Then $\inf(f_n + \lambda J) \to \inf(f + \lambda J)$, $\arg\min(f_n + \lambda J) \neq \varnothing$ for every $n \in \mathbb{N}$ and $\arg\min(f_n + \lambda J) \to \arg\min(f + \lambda J)$.*

In the following, a simple criteria of equi-coercivity is given.

Proposition 3.1.5. *If $J : U \to \overline{\mathbb{R}}$ is coercive and $f_n : U \to \overline{\mathbb{R}}$ are equi-bounded from below, then $(f_n + \lambda J)_{n\in\mathbb{N}}$ is equi-coercive for every $\lambda > 0$.*

Proof. Let $\alpha \in \mathbb{R}$ such that $\alpha \leq f_n$ for every $n \in \mathbb{N}$. Then $\alpha + \lambda J \leq f_n + \lambda J$ and for every $t \in \mathbb{R}$ we have

$$f_n(u) + \lambda J(u) \leq t \implies J(u) \leq (t - \alpha)/\lambda$$

hence

$$\{f_n + \lambda J \leq t\} \subseteq \{J \leq (t - \alpha)/\lambda\} \subseteq K$$

for every $n \in \mathbb{N}$. $\square$

Remark 3.1.6. *If $f, J : U \to \overline{\mathbb{R}}$ are proper and bounded from below, and $f + \lambda J$ is coercive for some $\lambda > 0$, then $f + \mu J$ is coerceve for every $\mu > 0$.*
Indeed if $\mu \geq \lambda$, let $\alpha \in \mathbb{R}$ be such that $\alpha \leq J$, hence $0 \leq J - \alpha$. Then $\lambda(J - \alpha) \leq \mu(J - \alpha) \implies f + \lambda J \leq f + \mu J + \alpha(\lambda - \mu)$. Thus for $t \in \mathbb{R}$, we have

$$\{f + \mu J \leq t\} \subseteq \{f + \lambda J \leq t + \alpha(\lambda - \mu)\}$$

Next, if $\mu \leq \lambda$, let $\beta \in \mathbb{R}$ such that $\beta \leq f$, hence $0 \leq f - \beta$. Then $\lambda/\mu \geq 1$ and $f - \beta + \lambda J \leq (\lambda/\mu)(f - \beta) + \lambda J = (\lambda/\mu)(f + \mu J - \beta)$. Therefore for $t \in \mathbb{R}$

$$\{f + \mu J \leq t\} \subseteq \{f + \lambda J \leq (\lambda/\mu)(t - \beta) + \beta\}$$

Tikhonov regularization is based on the idea to substitute problem (3.1) — unstable — with problem (3.4) which can turn to be stable for suitable choices of the regularization functional. However, the link between the original problem (3.1) still lacks. Thus, we shall investigate the case where λ can vary, more precisely we select a sequence $(\lambda_n)_{n\in\mathbb{N}}$, $\lambda_n > 0$ in problem (3.4) and let $\lambda_n \to 0$ studying the convergence of the sets

$$\boxed{\operatorname{argmin}(f_n + \lambda_n J) \to \operatorname{argmin} f}$$

The study of this problem has been considered in [Att96] for the case $f_n = f$ (no perturbations). The general case of $f_n \neq f$ has been considered only in [DZ93, Zol00] but with stronger hypothesis on J or under different notions of perturbations[2]. Following [Att96] we introduce rescaled functions that change the problem in an equivalent form. Let $f_n, f, J : U \to \overline{\mathbb{R}}$ be proper functionals with $\operatorname{dom} f \cap \operatorname{dom} J \neq \varnothing$ and $(\lambda_n)_{n\in\mathbb{N}}$, $\lambda_n > 0$ be given with $\lambda_n \to 0$. Suppose $\overline{f} := \inf f \in \mathbb{R}$ and set

$$\begin{aligned} &\varphi_n = \frac{1}{\lambda_n}(f_n - \overline{f}) + J \\ &\varphi : U \to \overline{\mathbb{R}}, \quad \varphi(u) = \begin{cases} J(u) & \text{if } u \in \operatorname{argmin} f \\ +\infty & \text{otherwise} \end{cases} \end{aligned} \tag{3.5}$$

Clearly $\lambda_n\varphi_n + \overline{f} = f_n + \lambda_n J$, hence $\operatorname{argmin}(f_n + \lambda_n J) = \operatorname{argmin}\varphi_n$ and one can study the behavior of $\operatorname{argmin}\varphi_n$ instead. As a result, we will study the minimum problem $\min\varphi$ and the Γ-convergence of the sequence φ_n towards φ. Three propositions shall be provided.

The following proposition tell us that among all the solutions of problem (3.1), we can always find one $u^\dagger$, which makes minimum the regularization functional J. Such solutions are called *J-minimizing*.

Proposition 3.1.7. *Let $f, J : U \to \overline{\mathbb{R}}$ be proper and sequentially l.s.c. and let $S = \operatorname{argmin} f$ be the set of solutions of problem (3.1). Suppose $S \cap \operatorname{dom} J \neq \varnothing$ and $f + \lambda J$ sequentially coercive for some $\lambda > 0$. Then there exists $u^\dagger \in S$ with $J(u^\dagger) = \min_{u\in S} J(u)$.*

Proof. Let $\overline{f} = \inf f$. Since f is proper and $\operatorname{argmin} f \neq \varnothing$, it holds $\overline{f} \in \mathbb{R}$. Let $t \in \mathbb{R}$ and using the function φ defined above, it is simple to prove that

$$\{\varphi \le t\} = \operatorname{argmin} f \cap \{J \le t\} = \{f \le \overline{f}\} \cap \{J \le t\}$$

Since f, J are sequentially l.s.c, it follows that $\{\varphi \le t\}$ is sequentially closed. Furthermore

$$\begin{aligned} \varphi(u) \le t &\implies f(u) = \overline{f} \text{ and } J(u) \le t \\ &\implies f(u) + \lambda J(u) \le \overline{f} + \lambda t \end{aligned}$$

Thus $\{\varphi \le t\} \subseteq \{f + \lambda J \le \overline{f} + \lambda t\}$, the last set being contained in a sequentially compact subset K. We proved that the function φ is sequentially l.s.c. and sequentially coercive, hence it has a minimizer $u^\dagger$, which of course is a solution of the problem $\min_S J$. □

[2] In particular they study perturbations under uniform convergence and Attouch-Wets convergence.

Proposition 3.1.8. *Suppose $f_n \to f$ pointwise and moreover $(f_n(u)-\overline{f})/\lambda_n \to 0$ for every $u \in \arg\min f$. Then $\varphi_n \to \varphi$ pointwise.*

Proof. Let $u \in \operatorname{argmin} f$. Then, from the hypothesis, $\varphi_n(x) = (f_n(u) - \overline{f})/\lambda_n + J(u) \to J(u) = \varphi(u)$. In case $u \notin \operatorname{argmin} f$, then $f_n(u) - \overline{f} \to f(u) - \overline{f} > 0$ and, being $\lambda_n \to 0$, we have $\varphi_n(x) = (f_n(u) - \overline{f})/\lambda_n + J(u) \to +\infty = \varphi(u)$. □

The following is the analogue of Proposition 3.1.3.

Proposition 3.1.9. *Let the functionals f_n Γ-converge and converge pointwise to f and J satisfy (3.3). If $(f_n - \overline{f})/\lambda_n$ Γ-converges and converges pointwise to 0 at each point of $\operatorname{argmin} f$, meaning that for each $u \in \operatorname{argmin} f$ it holds:*

1. $(f_n(u) - \overline{f})/\lambda_n \to 0$;
2. $u_n \in X$, $u_n \to u \implies 0 \leq \liminf_{n\to\infty}(f_n(u_n) - \overline{f})/\lambda_n$,

then $\varphi_n \xrightarrow{\Gamma} \varphi$ and $\varphi_n \to \varphi$ pointwise.

Proof. The previous proposition gives pointwise convergence of φ_n towards φ. We therefore need to show just the property (i) of Γ-convergence. Let $u \in U$ and $(u_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$ with $u_n \to u$. If $u \in \arg\min f$, then

$$0 \leq \liminf_n \frac{f_n(u_n) - \overline{f}}{\lambda_n}, \quad \varphi(u) = J(u) \leq \liminf_n J(u_n)$$

therefore, $\varphi(u) \leq \liminf_n[(f_n(u_n) - \overline{f})/\lambda_n + J(u_n)] = \liminf_n \varphi_n(u_n)$. In case $u \notin \operatorname{argmin} f$, then $f(u) > \overline{f}$ and $\varphi(u) = +\infty$. Let $\varepsilon > 0$ be such that $f(u) > \overline{f} + \varepsilon$. Thus $\overline{f} + \varepsilon < f(u) \leq \liminf_n f_n(u_n)$. Therefore there exists $\nu \in \mathbb{N}$ such that for all $n \in \mathbb{N}$, $n \geq \nu$ it holds $f_n(u_n) > \overline{f} + \varepsilon$ and hence $(f_n(u_n) - \overline{f})/\lambda_n > \varepsilon/\lambda_n$. This implies $\liminf_n(f_n(u_n) - \overline{f})/\lambda_n = +\infty$ and taking into account that $(J(u_n))_{n\in\mathbb{N}}$ is bounded from below (since $J(u) \leq \liminf_n J(u_n)$), we get $\liminf_n \varphi_n(u_n) = +\infty = \varphi(u)$. □

Remark 3.1.10. *In Proposition 3.1.9, the condition $0 \leq \liminf_n(f_n(u_n) - \overline{f})/\lambda_n$ can be replaced with the condition $0 \leq \liminf_n(f_n(u_n) - f_n(u))/\lambda_n$, for every sequence $(u_n)_{n\in\mathbb{N}}$, $u_n \to u \in \operatorname{argmin} f$. Indeed*

$$\frac{f_n(u_n) - \overline{f}}{\lambda_n} = \frac{f_n(u_n) - f_n(u)}{\lambda_n} + \frac{f_n(u) - \overline{f}}{\lambda_n}$$

Therefore, since we have assumed $(f_n(u) - \overline{f})/\lambda_n \to 0$ for every $u \in \operatorname{argmin} f$, if $0 \leq \liminf_n(f_n(u_n) - f_n(u))/\lambda_n$, we get $0 \leq \liminf_n(f_n(u_n) - \overline{f})/\lambda_n$. In fact both conditions are equivalent.

Remark 3.1.11. *In case $f_n = f$ for every $n \in \mathbb{N}$, the condition $f_n\,\Gamma$-converges and converges pointwise to f, means f sequentially l.s.c and moreover the two conditions given in Proposition 3.1.9 about the sequence $(f_n - \overline{f})/\lambda_n$ are trivially satisfied. Therefore, if f is l.s.c., we have that φ_n converges and converges pointwise to φ. Our result generalizes Theorem 2.1 and Theorem 2.6 in [Att96].*

We thus conclude by providing the following

Theorem 3.1.12 (Convergence). *Let $f, f_n : U \to \overline{\mathbb{R}}$ be proper and seq. l.s.c. and J satisfying (3.3). Suppose $\operatorname{argmin} f \cap \operatorname{dom} J \neq \varnothing$. Let $(\lambda_n)_{n\in\mathbb{N}}$, $\lambda_n > 0$ and $\lambda_n \to 0$. Suppose $f_n\,\Gamma$-converges and converges pointwise to f and $(f_n - \overline{f})/\lambda_n\,\Gamma$-converges and converges pointwise to 0 at each point $u \in \operatorname{argmin} f$. If $(\varphi_n)_{n\in\mathbb{N}}$ is equi-coercive, then $\operatorname{argmin}(f_n + \lambda_n J) \neq \varnothing$ for every $n \in \mathbb{N}$ and*

1. $\operatorname{argmin}(f_n + \lambda_n J) \to \operatorname{argmin}\{J(u) \,|\, u \in \operatorname{argmin} f\} \neq \varnothing$;
2. *for every* $u_n \in \operatorname{argmin}(f_n + \lambda_n J)$ *it is* $\lim_{n\to\infty} J(u_n) \to \min\{J(u) \,|\, u \in \operatorname{argmin} f\}$.

The first property means that cluster points of the sequences $u_n \in \operatorname{argmin}(f_n + \lambda_n J)$ are solutions of our original problem (3.1), that is if for a subsequence $(u_{k_n})_{n\in\mathbb{N}}$, $u_{k_n} \to u^\dagger \in U$, then $u^\dagger \in \arg\min f$, and they are J-minimizing too. The second property tell us that $\lim_{n\to\infty} J(u_n) = J(u^\dagger)$.

Proof. We need just to prove the last statement in the theorem. From the general theory we know that

$$\varphi_n(u_n) \to \inf \varphi = \inf_{\operatorname{argmin} f} J = J(u^\dagger).$$

If $u_{k_n} \to u^\dagger$, then $0 \leq \liminf_{n\to\infty}(f_n(u_{k_n}) - \overline{f})/\lambda_n$. Thus, if $\varepsilon > 0$, there exists $\nu \in \mathbb{N}$ such that

$$-\varepsilon \leq \frac{f_n(u_{k_n}) - \overline{f}}{\lambda_n}$$

for each $n \geq \nu$ and taking into account that $u_{k_n} \in \operatorname{argmin} \varphi_{k_n}$, we have

$$\begin{aligned} -\varepsilon + J(u_{k_n}) &\leq \frac{f_{k_n}(u_{k_n}) - \overline{f}}{\lambda_{k_n}} + J(u_{k_n}) \\ &\leq \frac{f_{k_n}(u^\dagger) - \overline{f}}{\lambda_{k_n}} + J(u^\dagger) \end{aligned}$$

still, for each $n \geq \nu$. Being $(f_{k_n}(u^\dagger) - \overline{f})/\lambda_{k_n} \to 0$, we have

$$\limsup_{n\to\infty} J(u_{k_n}) \leq J(u^\dagger) + \varepsilon$$

Since $\varepsilon > 0$ is arbitrary we get

$$J(u^\dagger) \leq \liminf_n J(u_{k_n}) \leq \limsup_n J(u_{k_n}) \leq J(u^\dagger)$$

that is $J(u_{k_n}) \to J(u^\dagger)$. We proved that for each subsequence such that $u_{k_n} \to u^\dagger$, it holds $J(u_{k_n}) \to J(u^\dagger)$. This in fact implies $J(u_n) \to J(u^\dagger)$. If this is not the case, then there exists a subsequence $(x_{r_n})_{n\in\mathbb{N}}$ such that $J(x_{r_n}) \notin V$ for $n \geq \nu$, where V is a neighborhood of $J(u^\dagger)$. This means that no subsequence of $J(x_{r_n})_{n\in\mathbb{N}}$ can converge to $J(u^\dagger)$. However, the sequence $(x_{r_n})_{n\in\mathbb{N}}$ is relatively compact and there must exist a converging subsequence, say $(x_{r_{os(n)}})_{n\in\mathbb{N}}$, which is of course a converging subsequence of $(u_n)_{n\in\mathbb{N}}$ and from what we proved, $J(x_{r_{os(n)}}) \to J(u^\dagger)$ which gives a contradiction. □

Remark 3.1.13. *A simple condition to make $(\varphi_n)_{n\in\mathbb{N}}$ equi-coercive is to require $(f_n - \overline{f})/\lambda_n$ bounded from below and J coercive. Indeed if $\alpha \in \mathbb{R}$ and $\alpha \leq (f_n - \overline{f})/\lambda_n$, then $\alpha + J \leq \varphi_n$ and hence*

$$\{\varphi_n \leq t\} \subseteq \{J \leq t - \alpha\} \leq K_{\alpha - t}.$$

We can weaken the hypothesis of equi-coercivity of $(\varphi_n)_{n\in\mathbb{N}}$ and require just the sequence $(u_n)_{n\in\mathbb{N}}$ to be sequentially relatively compact. That condition can be achieved if we suppose the sequence $(f_n(u_n) - \overline{f})/\lambda_n$ bounded from below, say by α, and J coercive. Indeed taken $u \in \operatorname{argmin} f \cap \operatorname{dom} J$, it is $\varphi_n(x) \to \varphi(u) = J(u) < +\infty$. Then, for $t > J(u)$ there exists $\nu \in \mathbb{N}$ such that $\varphi_n(x) < t$ for all $n \in \mathbb{N}$, $n \geq \nu$. Therefore we have

$$\alpha + J(u_n) \leq \frac{f_n(u_n) - \overline{f}}{\lambda_n} + J(u_n) = \varphi_n(u_n) \leq \varphi(u) < t$$

Thus $u_n \in \{J \leq t - \alpha\} \subseteq K_{t-\alpha}$ for every $n \in \mathbb{N}$.

3.2 Regularizing ill-posed Inverse Problems

In this section, we extend the classical theory of Tikhonov regularization for abstract inverse problem [SV89, HKPS07, Sch09], to include the image registration problem, for both mono-modal and multi-modal case. From a theoretical point of view, our framework introduces two main novelties: first, a general "distance" for the data fit term; second, perturbations in the operator. Apart from that, statements of the provided theorems follow classical results in variational regularization methods in Banach spaces and we refer to the above cited references for an account of the theory. Finally, we analyze the case of norm powers as distance, recovering known results [Sch09].

We consider a nonlinear equation of the form

$$\boxed{F(u) = v} \tag{3.6}$$

where $F : D(F) \subseteq U \to V$ is a (nonlinear) operator between a Hausdorff topological space U and a subset $V \subseteq \hat{V}$ of a normed space $(\hat{V}, \|\cdot\|)$ and $v \in V$ is a given data. $D(F)$ and $R(F)$ shall denote respectively the domain and range of F.

Often the topology of U is the weak topology of a Banach space, but this is not always the case — as we will see — and anyway we chose to denote convergence of sequences in U by $u_n \to u$. We note that V is endowed with a metric topology and a weak topology which are both inherited from those of $\hat{V}$.

In dealing with problem (3.6) we do not require the existence of any exact solution, but alternatively we search for *generalized solutions*, solving the following minimization problem

$$\boxed{\min_{u \in D(F)} \phi(F(u), v)} \tag{3.7}$$

where $\phi : V \times V \to \mathbb{R}$ is a function playing the role of a generalized distance on V. Thus, we are actually dealing with the so called *non-attainable case* [BEN$^+$94].

In general problem (3.7) may be *ill-posed*, meaning that if we consider perturbations of the data (F, v)

$$F_n : D(F_n) \subseteq U \to V, \quad v_n \in V, \quad n \in \mathbb{N} \tag{3.8}$$

the perturbed problems

$$\min_{u \in D(F_n)} \phi(F_n(u), v_n) \tag{3.9}$$

might have solutions far away from those of (3.7), even if the perturbations (F_n, v_n) approach (in some sense) the given data (F, v) as $n \to +\infty$.

The theory of *Tikhonov regularization*, also known as *variational regularization* [Sch09], copes with ill-posedness solving a neighboring problem of the following form

$$\min_{u \in D(F)} \phi(F(u), v) + \lambda J(u) \qquad \lambda > 0 \tag{3.10}$$

where $J : U \to \overline{\mathbb{R}}$ is a suitable functional which possibly turns the problem into a well-posed one — for this reason called a *stabilizing* functional [TA77].

Our program is first of all, to asses well-posedness of problem (3.10) for fixed λ, meaning to establish existence of solutions and their continuous dependence from the data (F, v). Next, we address the convergence issue by taking a sequence of regularization parameters $\lambda_n > 0$, $\lambda_n \to 0$ and checking that the solutions of the corresponding problems

$$\min_{u \in D(F_n)} \phi(F_n(u), v_n) + \lambda_n J(u) \tag{3.11}$$

converge towards the solutions of the original problem (3.7) as $n \to +\infty$.

We underline that our theory introduces a general distance measure ϕ not necessarily defined by the norm of the space V. This contrasts with the assumptions of the large majority of papers on variational regularization [EKN89, SV89, BEN+94, RS06, HKPS07, Sch09] — only recently more general "misfit" has been considered [Fle10, FH10], but they are still not appropriate for multi-modal image registration. Moreover, possible errors in the operator F are taken into account.

3.2.1 The general theory

Although ϕ does not need to satisfy the axioms of distances, we shall require it to satisfy the following two conditions.

Assumption 3.2.1. *on the "distance" function ϕ:*

(i) *ϕ is weakly sequentially lower semicontinuous (l.s.c.) in the first variable.*

(ii) *ϕ is (jointly) Lipschitz continuous on bounded sets of V,*

The first condition meaning

$$\phi(v, w) \leq \liminf_{n\to\infty} \phi(v_n, w)$$

for every $v_n, v \in V$, $v_n \rightharpoonup v$ and $w \in V$. The last condition meaning that for every $W \subseteq V$, W bounded, it holds

$$|\phi(v_1, v_2) - \phi(w_1, w_2)| \leq C_W(\|v_1 - w_1\| + \|v_2 - w_2\|)$$

for every $(v_1, v_2), (w_1, w_2) \in W \times W$ and for a suitable constant $C_W \geq 0$. Clearly, ϕ is jointly continuous on the whole domain $V \times V$. Moreover, very often ϕ will be also simmetric.

We now make a list of assumptions about the operator F, the regularizer J and the kind of allowed perturbations.

Assumption 3.2.2. *on the operator F:*

$D(F)$ is sequentially closed and F is sequentially continuous w.r.t. the topology of U and the weak topology of V, that is $u_n \to u \implies F(u_n) \rightharpoonup F(u)$.

Assumption 3.2.3. *on the regularizer J:*

$J : U \to \overline{\mathbb{R}}$ is proper l.s.c. and $\operatorname{dom} J \cap D(F) \neq \varnothing$

The following first result is a direct application of the Weierstrass theorem 2.1.3 on the existence of minimum points. It will require the function J to be coercive (see Definition 2.1.2). We also note that if J is proper l.s.c. and coercive, then J is bounded from below.

Theorem 3.2.4 (**Existence**). *Let ϕ, F and J meet assumptions 3.2.1, 3.2.2, 3.2.3 and suppose J coercive. Then problem* (3.10) *admits solutions.*

We consider perturbations of the operator F and the data v as in (3.8) and satisfying the following assumptions.

Assumption 3.2.5. *on the kind of allowed perturbations:*

(i) $v_n \to v$,

(ii) F_n *satisfy Assumption 3.2.2 and* $D(F_n) = D(F)$,

(iii) $F_n(u) \to F(u)$ *uniformly over the sets A of the form* $A = \{u_n \,|\, n \in \mathbb{N}\}$ *for any convergent sequence* $(u_n)_{n\in\mathbb{N}}$ *of* $D(F)$.

In the next result we use for brief the notation $\phi(F, v)$ for the function $u \to \phi(F(u), v)$ (defined $+\infty$ for $u \notin D(F)$) and the same for $\phi(F_n, v_n)$.

Theorem 3.2.6 (**Stability**). *Let ϕ, F, J and v_n, F_n meet assumptions 3.2.1, 3.2.2, 3.2.3, 3.2.5 and suppose $\phi(F_n, v_n)$ equi-bounded from below and J coercive. Then, it holds*

$$\inf_U \phi(F_n, v_n) + \lambda J \to \inf_U \phi(F, v) + \lambda J$$

Moreover, $\operatorname{argmin}(\phi(F_n, v_n) + \lambda J) \neq \varnothing$ *for every $n \in \mathbb{N}$ and*

$$\operatorname{argmin}(\phi(F_n, v_n) + \lambda J) \to \operatorname{argmin}(\phi(F, v) + \lambda J).$$

This theorem says that cluster points of the sequences $(u_n)_{n\in\mathbb{N}}$, $u_n \in \operatorname{argmin}(\phi(F_n, v_n) + \lambda J)$ minimize the Tikhonov functional (3.10).

Remark 3.2.7. *We note that the assumption "$\phi(F_n, v_n)$ equi-bounded form below" is often met, either because ϕ itself if bounded from below or because the operators F_n are equi-bounded (as it is the case for the warping operators).*

We now tackle the issue of convergence of Tikhonov regularization method for problem (3.7), letting the regularization parameter λ vary. To that purpose, we need to make a stronger assumption on the kind of perturbations.

Assumption 3.2.8. *on the allowed perturbations:*

(i) $\|v - v_n\| \leq \delta_n$, *with* $\delta_n \geq 0$ *and* $\delta_n \to 0$.

(ii) F_n *satisfy Assumption 3.2.2 and* $D(F_n) = D(F)$,

(iii) $\|F_n(u) - F(u)\| \leq \eta_n$ *for every* $u \in D(F)$, *with* $\eta_n \geq 0$ *and* $\eta_n \to 0$[3].

We recall that a solution $u^\dagger$ of problem (3.7) is called *J-minimizing* if it makes $J(u)$ minimum among all the solutions, that is

$$J(u^\dagger) = \min\{J(u) \,|\, u \in \operatorname{argmin} \phi(F, v)\}$$

Theorem 3.2.9 (Convergence). *Let* ϕ, F, J *and* v_n, F_n *satisfy Assumptions 3.2.1, 3.2.2, 3.2.3, 3.2.8. Suppose there exists a solution* u *of* (3.7) *with* $J(u) < +\infty$ *and* J *coercive. Suppose either* F *be bounded or* ϕ *globally Lipschitz continuous on* $V \times V$. *If* $(\lambda_n)_{n\in\mathbb{N}}$, $\lambda_n > 0$ *is such that*

$$\lambda_n \to 0 \quad \textit{and} \quad (\eta_n + \delta_n)/\lambda_n \to 0 \tag{3.12}$$

then, $\operatorname{argmin}(\phi(F_n, v_n) + \lambda_n J) \neq \varnothing$ *for every* $n \in \mathbb{N}$ *and*

1. $\operatorname{argmin}(\phi(F_n, v_n) + \lambda_n J) \to \operatorname{argmin}\{J(u) \,|\, u \in \operatorname{argmin} \phi(F, v)\} \neq \varnothing$;
2. *if* $u_n \in \operatorname{argmin}(\phi(F_n, v_n) + \lambda_n J)$, *it is* $\lim_{n\to\infty} J(u_n) = \min\{J(u) \,|\, u \in \operatorname{argmin} \phi(F, v)\}$.

Hypothesis (3.12) says that the parameters λ_n's should tend to zero not too fast, slower then the error sequence $(\eta_n + \delta_n)_{n\in\mathbb{N}}$.

Remark 3.2.10. *Condition* (3.12) *in Theorem 3.2.9 seams stronger then the corresponding one given in Banach space settings (using a data fit term based on some power of the norm) where the condition* $\delta_n^q/\lambda_n \to 0$ *appears (see Theorem 3.5 in [HKPS07]. However we highlight that we are treating the non-attainable case, i.e. we are not assuming the existence of any exact solution of problem* (3.6). *On the contrary we make the waker assumption that problem* (3.7) *has solutions. In fact our results is in line with the one given in Theorem 3.5 in [BEN+94].*

3.2.2 Proofs of the main theorems

We now provide proofs of the two theorems above. Our analysis is based on the general theory presented in section 3.1 and henceforth, we shall refer to definitions and results given there.

We set

$$f(u) = \begin{cases} \phi(F(u), v) & \text{if } u \in D(F) \\ +\infty & \text{if } x \notin D(F) \end{cases}. \tag{3.13}$$

[3] Thus $F_n \to F$ uniformly on $D(F)$.

and

$$f_n(u) = \begin{cases} \phi(F_n(u), v_n) & \text{if } u \in D(F_n) \\ +\infty & \text{if } x \notin D(F_n) \end{cases}. \tag{3.14}$$

where v_n and F_n satisfy Assumption 3.2.5[4].

From these definitions, the assumption on the perturbations and the continuity of ϕ, it follows that $f_n \to f$ pointwise. In fact we can get also Γ-convergence, as the following result shows

Proposition 3.2.11. *If ϕ, F and v_n, F_n meet the assumptions 3.2.1, 3.2.2, 3.2.5 and f, f_n are defined as in* (3.13)-(3.14)*, then f_n Γ-converges and converges pointwise to f.*

Proof. We apply Proposition 2.2.6. We set $\|F\|_{A,\infty} := \sup_{u\in A}\|F(u)\|$, the seminorm of the uniform topology on A, and the condition on uniform convergence on A can be expressed as $\|F_n - F\|_{A,\infty} \to 0$. Let $A = \{u_n \mid n \in \mathbb{N}\} \subseteq D(F)$, with $(u_n)_{n\in\mathbb{N}}$ a convergent sequence in U. Because of Assumption 3.2.2 and 3.2.5, $F(A)$ and $F_n(A)$ are equi-bounded, therefore we can chose $W \subseteq V$, W bounded such that $v_n, v \in W$ and $F(A), F_n(A) \subseteq W$ for every $n \in \mathbb{N}$. Then

$$\begin{aligned} |f(u) - f_n(u)| &= |\phi(F(u), v) - \phi(F_n(u), v_n)| \\ &\le C_W(\|F(u) - F_n(u)\| + \|v - v_n\|) \\ &\le C_W(\|F - F_n\|_{A,\infty} + \|v - v_n\|) \end{aligned}$$

for every $u \in A$ and $n \in \mathbb{N}$. It follows $f \to f_n$ uniformly on the set A. Furthermore $f(u) = \phi(F(u), v)$ is l.s.c. Indeed, from Assumption 3.2.2, $\operatorname{dom} f$ is closed and if $u_n, u \in \operatorname{dom} f$ and $u_n \to u$, then $F(u_n) \rightharpoonup F(u)$ and therefore $\phi(F(u), v) \le \liminf_n \phi(F(u_n), v)$, since we supposed $\phi(\cdot, v)$ weakly l.s.c. □

Remark 3.2.12. *We can drop hypothesis* (i) *in Assumption 3.2.1 if we suppose the operator $F : D(F) \subseteq U \to V$ continuous. This way we obtain again $f(u) = \phi(F(u), v)$ is l.s.c. and Proposition 3.2.11 is still true.*

Proof of Theorem 3.2.6. The previous proposition together with the stability theorem 3.1.4, shows that for an ill-posed inverse problem, Tikhonov regularization makes the problem well-posed under perturbations of the kind allowed by Assumption 3.2.5 as soon as $(f_n + \lambda J)_{n\in\mathbb{N}}$ is equi-coercive. Since, from the hypotheses, $(f_n)_{n\in\mathbb{N}}$ are equi-bounded from below and J is coercive, Proposition 3.1.5 applies and this concludes the proof. ■

We now treat the convergence's theorem and define the rescaled functions φ_n, φ as in (3.5), and suppose $\overline{f} := \inf_U f \in \mathbb{R}$. The problems $\min_U \varphi_n$ are of course equivalent to (3.11) and we have the following result

[4]The functions f, f_n are nothing but the functions $\phi(F, v)$ and $\phi(F_n, v_n)$ considered before.

Proposition 3.2.13. *Let us make Assumptions 3.2.1, 3.2.2 and suppose the perturbations* (3.8) *satisfy:*

(i) $\|v - v_n\| \le \delta_n$, *with* $\delta_n \ge 0$ *and* $\delta_n \to 0$,

(ii) $D(F_n) = D(F)$ *for every* $n \in \mathbb{N}$,

(iii) $\|F_n(u) - F(u)\| \le \eta_n \omega(u)$ *for every* $u \in D(F)$, *with* $\eta_n \ge 0$, $\eta_n \to 0$ *and* $\omega : D(F) \to \mathbb{R}_+$ *a function bounded on sets of the form* $A = \{u_n \,|\, n \in \mathbb{N}\}$, *for any sequence* $(u_n)_{n\in\mathbb{N}}$ *of* $D(F)$ *convergent in* U.

If we choose $\lambda_n > 0$ *such that* $(\delta_n + \eta_n)/\lambda_n \to 0$, *then* $\varphi_n \xrightarrow{\Gamma} \varphi$ *and* $\varphi_n \to \varphi$ *pointwise.*

Proof. We are going to meet the hypotheses of Proposition 3.1.9. Let $u \in \operatorname{argmin} f$ and let $W \subseteq V$, W bounded, such that $F(u), F_n(u), v, v_n \in W$, then

$$\begin{aligned} |f(u) - f_n(u)| &= |\phi(F(u), v) - \phi(F_n(u), v_n)| \\ &\le C_W(\|F(u) - F_n(u)\| + \|v - v_n\|) \\ &\le C_W(\eta_n \omega(u) + \delta_n) \\ &\le C_W(\eta_n + \delta_n)(\omega(u) + 1) \end{aligned}$$

Therefore

$$\frac{|f(u) - f_n(u)|}{\lambda_n} \le C_W \frac{\eta_n + \delta_n}{\lambda_n}(\omega(u) + 1) \tag{3.15}$$

hence $(f(u) - f_n(u))/\lambda_n \to 0$. Next, let $(u_n)_{n\in\mathbb{N}}$, $u_n \in U$ with $u_n \to u$. We have to prove $0 \le \liminf_{n\in\mathbb{N}}(f_n(u_n) - f_n(u))/\lambda_n$. Suppose, by contradiction, that this is not true. Then there exists $\varepsilon > 0$ and a subsequence $(u_{k_n})_{n\in\mathbb{N}}$ such that

$$\frac{f_{k_n}(u_{k_n}) - f_{k_n}(u)}{\lambda_{k_n}} < -\varepsilon \qquad \text{for every } n \in \mathbb{N}. \tag{3.16}$$

Clearly $u_{k_n} \to u$ and $A := \{u_{k_n} \,|\, n \in \mathbb{N}\} \subseteq D(F)$. Thus, being $F_{k_n} \to F$ uniformly on A, there exists $W \subseteq V$, W bounded, such that $F(A), F_{k_n}(A) \subseteq W$ and $v, v_{k_n} \in W$ for every $n \in \mathbb{N}$ and it holds

$$\begin{aligned} f(u_{k_n}) - f_{k_n}(u_{k_n}) &\le |\phi(F(u_{k_n}), v) - \phi(F_{k_n}(u_{k_n}), v_{k_n})| \\ &\le C_W(\|F(u_{k_n}) - F_{k_n}(u_{k_n})\| + \|v - v_{k_n}\|) \\ &\le C_W(\eta_{k_n} \omega(u_{k_n}) + \delta_{k_n}) \\ &\le C_W(\eta_{k_n} + \delta_{k_n})\big(\sup \omega(A) + 1\big) \end{aligned}$$

From (3.15)

$$f_{k_n}(u) - f(u) \le C_W(\eta_{k_n} + \delta_{k_n})(\omega(u) + 1)$$

Summing the previous two inequalities, we get

$$\begin{aligned} f_{k_n}(u) - f_{k_n}(u_{k_n}) &\leq f(u) - f(u_{k_n}) + C(\eta_{k_n} + \delta_{k_n}) \\ &\leq C(\eta_{k_n} + \delta_{k_n}) \end{aligned}$$

where we took into account that $f(u) - f(u_{k_n}) \leq 0$, since $u \in \operatorname{argmin} f$. Finally we obtain

$$-C\frac{\eta_{k_n} + \delta_{k_n}}{\lambda_{k_n}} \leq \frac{f_{k_n}(u_{k_n}) - f_{k_n}(u)}{\lambda_n}$$

and the left hand side converges to 0. Then, for n sufficiently large, we have

$$-\varepsilon \leq \frac{f_{k_n}(u_{k_n}) - f_{k_n}(u)}{\lambda_n}$$

which, together with (3.16), gives a contradictions. □

Concerning the hypotheses on the perturbations considered in the proposition above, it is worth noting that in case $F_n \to F$ uniformly on the whole domain $D(F)$, it is straighforward to find such η_n and ω: one can choose $\eta_n = \|F - F_n\|_\infty$ and $\omega(u) = 1$; another simple case is when both F_n and F are linear operators: in that case $\eta_n = \|F - F_n\|$ and $\omega(u) = \|u\|$.

Proof of Theorem 3.2.9. In view of Theorem 3.1.12 and the previous proposition, we need just to guarantee $(\varphi_n)_{n\in\mathbb{N}}$ to be equi-coercive. In case F is bounded, the inequality (3.15) holds true for every $u \in D(F)$, with W such that $W \supseteq R(F), \cup_{n\in\mathbb{N}} R(F_n)$. Then for every $u \in D(F)$

$$-C\frac{\eta_n + \delta_n}{\lambda_n} \leq \frac{f_n(u) - f(u)}{\lambda_n} \leq \frac{f_n(u) - \overline{f}}{\lambda_n}$$

Thus, being $((\eta_n + \delta_n)/\lambda_n)_{n\in\mathbb{N}}$ bounded from above, we have $(f_n - \overline{f})/\lambda_n$ bounded from below and we can relies on Remark 3.1.13. Obviously the same reasoning is valid if we assume ϕ globally Lipschitz continuous, dropping the hypothesis of boundness of F. □

3.2.3 The special case of L^q distance measures

We finish this section by applying the general convergence results just described, to the case of the distance measure

$$\boxed{\phi(v_1, v_2) = \|v_1 - v_2\|^q} \tag{3.17}$$

where $\|\cdot\|$ is the norm of $\hat{V}$ and $1 \leq q < +\infty$. Before doing so, let us recall the notion of the duality map of a normed space [Chi09]. Let $(\hat{V}, \|\cdot\|)$ be a normed space, $q \geq 1$ and consider the *q-duality map* $j_q = \partial(1/q\|\cdot\|^q)$, that is

$$j_q : \hat{V} \to \mathfrak{P}(\hat{V}^*) \quad j_q(v) = \partial \left(\frac{1}{q} \|\cdot\|^q \right)(v) \subseteq \hat{V}^*$$

where ∂ is the subdifferential operator in the sense of convex analysis [Zăl02]. One can show that

$$j_q(v) = \{v^* \in \hat{V}^* \mid \langle v, v^* \rangle = \|v\|^q, \|v^*\| = \|v\|^{q-1}\} \neq \varnothing$$

Furthermore, from the definition of subgradient, it follows directly

$$\|v\|^q \leq \|w\|^q + q\langle v - w, v^* \rangle \qquad v^* \in j_q(v) \tag{3.18}$$

and therefore it holds

$$\|v\|^q \leq \|w\|^q + q\|v - w\| \|v\|^{q-1} \tag{3.19}$$

for every $v, w \in V$. Exchanging the role of v, w, we get

$$|\|v\|^q - \|w\|^q| \leq q\|v - w\| \max\{\|v\|^{q-1}, \|w\|^{q-1}\}$$

This inequality clearly shows that if we define ϕ as in (3.17), then ϕ satisfy the second condition in Assumption 3.2.1; the other one follows directly from the weak lower semi-continuity of the norm. The general theory developed above can indeed be applied to this case.

In the following a simple equi-coercivity result, for the case (3.17), is established.

Lemma 3.2.14. *If $1 \leq q < +\infty$, it holds*

$$f(u) \leq 2^{q-1} \left[f_n(u) + (\|F(u) - F_n(u)\| + \|v - v_n\|)^q \right]$$

for every $u \in U$. See Lemma 3.21 in [Sch09].

Lemma 3.2.15. *If $F_n \to F$ uniformly on the whole domain $D(F)$, J is bounded from below and $f + \lambda J$ is sequentially coercive, then $(f_n + \lambda J)_{n \in \mathbb{N}}$ is sequentially equi-coercive.*

Proof. From the lemma, it follows

$$f + \lambda J \leq 2^{q-1}(f_n + \varepsilon_n^q) + \lambda J$$

where we set $\varepsilon_n(u) = \|F(u) - F_n(u)\| + \|v - v_n\|$. Because $v_n \to v$ and $F_n \to F$ uniformly, $\varepsilon_n(u)$ is bounded. Since J is bounded from below, there exists $\alpha \in \mathbb{R}$ such that $\alpha \leq \lambda J$, hence $0 \leq \lambda J - \alpha$. Then $\lambda J - \alpha \leq 2^{q-1}(\lambda J - \alpha)$ and

$$f + \lambda J \leq 2^{q-1}(f_n + \varepsilon_n^q) + 2^{q-1}(\lambda J - \alpha) + \alpha \leq a(f_n + \lambda J) + b$$

for every $n \in \mathbb{N}$, with $a > 0$ and $b \in \mathbb{R}$ constants independent from $n \in \mathbb{N}$. Thus if $t \in \mathbb{R}$, then

$$f_n(u) + \lambda J(u) \leq t \implies f(u) + \lambda J(u) \leq at + b$$

Being $f + \lambda J$ sequentially coercive, there exists K_{at+b} sequentially compact such that $\{f + \lambda J \leq at + b\} \subseteq K_{at+b}$ and hence

$$\{f_n + \lambda J \leq t\} \subseteq K_{at+b}$$

for every $n \in \mathbb{N}$. $\square$

The following proposition can be used instead of the equi-coercivity requirement for $(\varphi_n)_{n\in\mathbb{N}}$ and allow to weaken the hypotheses of Theorem 3.2.9 keeping the same conclusions.

Proposition 3.2.16. *Let ϕ be defined by* (3.17) *and F, J and v_n, F_n satisfy Assumptions 3.2.2, 3.2.3, 3.2.8 and f, f_n be defined as in* (3.13)-(3.14). *Suppose* $\operatorname{argmin} f \cap \operatorname{dom} J \neq \varnothing$*, J bounded from below and $f + \lambda J$ coercive for some $\lambda > 0$. Let $(\lambda_n)_{n\in\mathbb{N}}$, $\lambda_n > 0$ be such that*

$$\lambda_n \to 0 \quad \textit{and} \quad (\eta_n + \delta_n)/\lambda_n \to 0 \tag{3.20}$$

Then, $\arg\min(f_n + \lambda_n J) \neq \varnothing$ *for every $n \in \mathbb{N}$ and if one chooses $u_n \in \arg\min(f_n + \lambda_n J)$, the sequence $(u_n)_{n\in\mathbb{N}}$ is sequentially relatively compact.*

Proof. Let us fix $u \in D(F) \cap \operatorname{dom} J$. From the definition of u_n, it holds

$$f_n(u_n) + \lambda_n J(u_n) \leq f_n(u) + \lambda_n J(u) \leq C(u) \tag{3.21}$$

J is bounded from below, say $\alpha \leq J$ for an $\alpha \in \mathbb{R}$. Then

$$f_n(u_n) + \lambda_n \alpha \leq f_n(u_n) + \lambda J(u_n) \leq C(u)$$

Thus, $(f_n(u_n))_{n\in\mathbb{N}}$ is bounded from above. From (3.21) it follows

$$J(u_n) \leq \frac{f_n(u) - f_n(u_n)}{\lambda_n} + J(u)$$

We are going to prove that the term $(f_n(u) - f_n(u_n))/\lambda_n$ is bounded from above. From lemma 3.2.14, we have $f(u_n) \leq 2^{q-1}[f_n(u_n) + (\|F(u_n) - F_n(u_n)\| + \|v - v_n\|)^q]$, the right term being of course bounded. Thus $(f(u_n))_{n\in\mathbb{N}}$ is bounded. As done before and using (3.19), we have

$$\begin{aligned} f(u_n) - f_n(u_n) &= \|F(u_n) - v\|^q - \|F_n(u_n) - v_n\|^q \\ &\leq q(\eta_n + \delta_n) f(u_n)^{\frac{q-1}{q}} \end{aligned}$$

and

$$f_n(u) - f(u) = \|F_n(u) - v_n\|^q - \|F(u) - v\|^q$$
$$\leq q(\eta_n + \delta_n) f_n(u)^{\frac{q-1}{q}}$$

Summing the two inequalities we find

$$f_n(u) - f_n(u_n) \leq f(u) - f(u_n) + q(\eta_n + \delta_n)(f(u_n)^{\frac{q-1}{q}} + f_n(u)^{\frac{q-1}{q}})$$
$$\leq q(\eta_n + \delta_n)(f(u_n)^{\frac{q-1}{q}} + f_n(u)^{\frac{q-1}{q}})$$

where we used the fact that $u \in \operatorname{argmin} f$. Being both sequences $(f(u_n))_{n\in\mathbb{N}}$, $(f_n(u))_{n\in\mathbb{N}}$ bounded, we get

$$\frac{f_n(u) - f_n(u_n)}{\lambda_n} \leq q \frac{\eta_n + \delta_n}{\lambda_n} C$$

Thus, since $(\eta_n + \delta_n)/\lambda_n \to 0$, we have

$$J(u_n) \leq C + J(u)$$

showing that the sequence $(J(u_n))_{n\in\mathbb{N}}$ is bounded too. Thus the sequence $(f(u_n)+\lambda J(u_n))_{n\in\mathbb{N}}$ is bounded and because $f + \lambda J$ is coercive, one can extract a convergent subsequence. □

Chapter 4

The Inverse Problem of Image Registration

In this chapter the mathematical foundations of image registration problem are investigated in depth. In particular, the problem of image registration is studied as a nonlinear ill-posed inverse problem between abstract spaces. A nonlinear operator underlying the process of image registration (which we call *warping operator*) is formally defined as well as different function spaces for the admissible deformations: Lebesgue, Sobolev and BV function spaces. Topological and differential properties of the warping operator are studied in order to apply methods used in the field of inverse problems. Using q-norms and mutual information based distance measures and different kinds of regularizers (among them p-norms of the Jacobian, polyconvex hyperelastic potentials and total variation), hypoteses for the validity of the general theory of Tikhonov regularization developed in the previous chapter are checked and existence, stability and convergence results are obtained. This provides justification for many variational methods in image registration in the mono-modal as well as multi-modal case.

The rest of the chapter is organized as follows. In section 4.1 we set up function spaces with topologies and define the warping operator. Topological and differential properties of the warping operator are studied in section 4.2. In section 4.3 we apply the general theory developed in section 3.2 to the problem of image registration getting well-posedness and convergence results for several variational methods.

4.1 Basic function spaces and operators

In this section we make explicit the basic players involved in the problem of image registration. This means introducing spaces of functions with topologies and operators acting among them.

Let us begin with the *space of images*. In all the following chapter Ω shall denote an open bounded and convex domain in $\mathbb{R}^d$ with Lipschitz boundary which plays the role of a region containing properly the rectangular domain where images are supposed to be defined. The Lebesgue measure of Ω shall be denoted by $|\Omega|$. The space of images $\mathrm{Im}(\Omega)$ will be a subset of the space of essentially bounded (scalar) functions over Ω, i.e. $\mathrm{Im}(\Omega) \subseteq L^\infty(\Omega)$,

$$L^\infty(\Omega) = \big\{ I : \Omega \to \mathbb{R} \,\big|\, I \text{ measurable and } \|I\|_\infty < +\infty \big\}.$$

It is worth recalling that, being Ω bounded, the following chain holds true among all the Lebesgue spaces over Ω

$$L^\infty(\Omega) \subseteq \cdots L^{q_2}(\Omega) \subseteq L^{q_1}(\Omega) \subseteq \cdots L^1(\Omega),$$

$1 \leq q_1 \leq q_2 \leq +\infty$. Therefore, each q-norm $\|I\|_q = \big(\int_\Omega |I(\mathbf{x})|^q \,\mathrm{d}\mathbf{x}\big)^{1/q}$ is suitable for defining a metric among images. Furthermore, it holds

$$\|I\|_{q_1} \leq |\Omega|^{(1/q_1 - 1/q_2)} \|I\|_{q_2},$$

meaning that the embedding $L^{q_2}(\Omega) \hookrightarrow L^{q_1}(\Omega)$ is in fact continuous. We will consider the space of images $\mathrm{Im}(\Omega)$ as a subset of the Banach space $(L^q(\Omega), \|\cdot\|_q)$ for some $q \geq 1$: i.e. we consider it endowed with the topology of the q-norm $\|\cdot\|_q$.

Next, we set a *space of admissible displacement fields* $U(\Omega, \mathbb{R}^d)$ (the members being mappings $\mathbf{u} : \Omega \to \mathbb{R}^d$) and we suppose $U(\Omega, \mathbb{R}^d) \subseteq L^p(\Omega, \mathbb{R}^d)$ for some $p \geq 1$. The choices we are going to consider are the following

$$U(\Omega, \mathbb{R}^d) = \begin{cases} L^p(\Omega, \mathbb{R}^d) & \text{(strong topology)} \\ W^{1,p}(\Omega, \mathbb{R}^d) & \text{(weak topology)} \\ BV(\Omega, \mathbb{R}^d) & \text{(weak-}\ast\text{ topology)} \end{cases}$$

respectively, the Lebesgue space of p-summable mappings, the Sobolev space of mappings having p-summable weak first derivatives, and the space of mappings of bounded variation. See [Bré10, AFP00] for the definitions of those concepts.

Finally, given an image $I \in \mathrm{Im}(\Omega)$, we introduce an operator associated to it. First, we extend the image I to all of $\mathbb{R}^d$ trivially, setting $I(\mathbf{x}) = 0$ outside Ω. Next, we suppose that the warped image $I(\mathbf{x}+\mathbf{u}(\mathbf{x}))$ still belongs to the space of images $\mathrm{Im}(\Omega)$ for every admissible displacement field $\mathbf{u} \in U(\Omega, \mathbb{R}^d)$. Then, we define the *warping operator* as

$$\begin{aligned} I : U(\Omega, \mathbb{R}^d) \subseteq L^p(\Omega, \mathbb{R}^d) &\to \mathrm{Im}(\Omega) \subseteq L^q(\Omega), \\ \mathbf{u} &\to \; I(\mathbf{u}) = I \circ (\mathbf{id} + \mathbf{u}) \end{aligned}$$

where $1 \leq p, q < +\infty$ and $\mathbf{id}$ denotes the identity mapping on the set Ω. It is worth noting that, the warping operator is a nonlinear operator of a known type in mathematics: it is in fact a *Nemitskii operator* (also called *superposition operator* or *composite operator*) — see [Vai64, AP93, Ber77, AZ90][1].

4.2 The study of the warping operator

In this section topological and differential properties of the warping operator are studied in the Lebesgue spaces. We also study the restriction of the operator to Sobolev and BV spaces. Although the results are classical in the mathematical community and are based on the study of superposition operators [Vai64, AZ90], here they are explicitely presented in the context of image registration. Hereafter a template image $I \in L^\infty(\mathbb{R}^d)$ is given.

4.2.1 The warping operator in Lebesgue spaces

We consider the warping operator as acting on the whole space $L^p(\Omega, \mathbb{R}^d)$, that is

$$I : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega), \quad I(\mathbf{u}) = I \circ (\mathbf{id} + \mathbf{u}) \tag{4.1}$$

where $p, q \geq 1$. More explicitely $I(\mathbf{u}) : \Omega \to \mathbb{R}$ is the image defined as $I(\mathbf{u})(\mathbf{x}) = I(\mathbf{x}+\mathbf{u}(\mathbf{x}))$ where $\mathbf{u} : \Omega \to \mathbb{R}^d$ is a p-summable displacement field. Evidently we have

$$|I(\mathbf{u})(\mathbf{x})| = |I(\mathbf{x}+\mathbf{u}(\mathbf{x}))| \leq \|I\|_\infty$$

and hence $\|I(\mathbf{u})\|_q \leq |\Omega|^{1/q} \|I\|_\infty$. Then, the warping operator (4.1) is bounded. We give two theorems, respectively about topological and differential properties of the warping operator. These follow from more general results about superposition operators [Vai64, AP93] and we provide proofs for completeness.

Theorem 4.2.1. *The warping operator* (4.1) *is well-defined for each $p, q \in [1, +\infty[$, it is bounded and moreover:*

[1] Actually, our convention to denote the image and its warping operator with the same symbol follows the one in [AP93]

1. *it is continuous (in the corresponding L-norms), if the image $I : \mathbb{R}^d \to \mathbb{R}$ is continuous;*

2. *it is Hölder continuous with exponent $\alpha \leq 1$ and constant $[I]_{0,\alpha}|\Omega|^{\frac{1}{q}-\frac{\alpha}{p}}$, if the image $I : \mathbb{R}^d \to \mathbb{R}$ is Hölder continuous with exponent α and constant $[I]_{0,\alpha}$, and $p \geq \alpha q$.*

Proof. If we suppose the image $I : \mathbb{R}^d \to \mathbb{R}$ continuous and $1 \leq q < +\infty$, then the warping operator (4.1) is continuous too. Indeed if $\mathbf{u}_n \to \mathbf{u}$ in $(L^p(\Omega, \mathbb{R}^d), \|\cdot\|_p)$, then, up to a subsequence, $\mathbf{u}_n(\mathbf{x}) \to \mathbf{u}(\mathbf{x})$ for a.e. $u \in \Omega$. Thus, from the continuity of I, it follows $I(\mathbf{u}_n) \to I(\mathbf{u})$ a.e. in Ω and being $|I(\mathbf{u}_n)| \leq \|I\|_\infty < +\infty$, the dominated convergence theorem allows us to conclude $I(\mathbf{u}_n) \to I(\mathbf{u})$ in $(L^q(\Omega), \|\cdot\|_q)$.

Next, assuming the image $I : \Omega \to \mathbb{R}$ Hölder continuous with exponent $\alpha \in]0, 1]$, we have

$$\begin{aligned}|I(\mathbf{u}_1)(\mathbf{x}) - I(\mathbf{u}_2)(\mathbf{x})| &= |I(x + \mathbf{u}_1(\mathbf{x})) - I(\mathbf{x} + \mathbf{u}_2(\mathbf{x}))| \\ &\leq [I]_{0,\alpha}|\mathbf{u}_1(\mathbf{x}) - \mathbf{u}_2(\mathbf{x})|^\alpha\end{aligned}$$

hence

$$\int_\Omega |I(\mathbf{u}_1)(\mathbf{x}) - I(\mathbf{u}_2)(\mathbf{x})|^{\frac{p}{\alpha}}\, \mathrm{d}x \leq ([I]_{0,\alpha})^{\frac{p}{\alpha}} \int_\Omega |\mathbf{u}_1(\mathbf{x}) - \mathbf{u}_2(\mathbf{x})|^p\, \mathrm{d}\mathbf{x}$$

and it follows

$$\|I(\mathbf{u}_1) - I(\mathbf{u}_2)\|_{\frac{p}{\alpha}} \leq [I]_{0,\alpha}\|\mathbf{u}_1 - \mathbf{u}_2\|_p^\alpha$$

(recall that $L^\infty(\Omega) \subseteq L^p(\Omega)$). If now $p/\alpha \geq q$, then $L^{\frac{p}{\alpha}}(\Omega) \hookrightarrow L^q(\Omega)$. Therefore

$$\|I(\mathbf{u}_1) - I(\mathbf{u}_2)\|_q \leq |\Omega|^{\frac{1}{q}-\frac{\alpha}{p}}[I]_{0,\alpha}\|\mathbf{u}_1 - \mathbf{u}_2\|_p^\alpha$$

that is, the warping operator is Hölder continuous with the same exponent α and constant $[I]_{0,\alpha}|\Omega|^{\frac{1}{q}-\frac{\alpha}{p}}$. □

Remark 4.2.2. *Continuing our discussion on topological properties, one can prove an important result about the weak continuity of the warping operator I. Indeed from Theorem 3.9 in [AZ90], it follows that, as a superposition operator, $I : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega)$ is never weakly continuous (that is continuous for the weak topologies of $L^p(\Omega, \mathbb{R}^d)$ and $L^q(\Omega)$) unless $I : \mathbb{R}^d \to \mathbb{R}$ is an affine function. This means also that there is no hope to apply the Tikhonov regularization theory to the case of the operator $I : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega)$ using the weak topology of $L^p(\Omega, \mathbb{R}^d)$. See section 3.2.*

We now deal with the differential properties. We consider *Gâteaux* and *Fréchet* differentiability and, especially in infinite dimensional spaces, the distinction between the two notions matters. Definitions can be found for instance in [IT79].

Theorem 4.2.3. *Let us suppose the image $I : \mathbb{R}^d \to \mathbb{R}$ differentiable with bounded gradient in $\mathbb{R}^d$, i.e. $\|\nabla I(\mathbf{x})\| \le L_I$ for every $\mathbf{x} \in \mathbb{R}^d$. Then, for every $p, q \in [1, +\infty[$, the operator* (4.1) *is:*

1. *Gâteaux differentiable, if $p \ge q$. In that case for all $\mathbf{u} \in L^p(\Omega, \mathbb{R}^d)$*

$$\boxed{I'(\mathbf{u}) : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega) \quad I'(\mathbf{u})[\mathbf{v}] = \nabla I(\mathbf{u}) \cdot \mathbf{v}}$$

   where $\nabla I(\mathbf{u}) := \nabla I \circ (\mathbf{id} + \mathbf{u})$ and $(\nabla I(\mathbf{u}) \cdot \mathbf{u})(\mathbf{x}) = \nabla I(x + \mathbf{u}(\mathbf{x})) \cdot \mathbf{v}(\mathbf{x})$; furthermore it holds

$$\boxed{\|I'(\mathbf{u}_1) - I'(\mathbf{u}_2)\| \le \|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)\|_r}$$

   and $\|I'(\mathbf{u})\| \le \|\nabla I(\mathbf{u})\|_r$, where $r \ge 1$ and $1/r = 1/q - 1/p$;

2. *of class $\mathscr{C}^1$, hence Fréchet differentiable, if the image I is of class $\mathscr{C}^1(\mathbb{R}^d)$ and $p > q$. Furthermore it has derivative*

$$I' : L^p(\Omega, \mathbb{R}^d) \to \mathbb{L}(L^p(\Omega, \mathbb{R}^d), L^q(\Omega))^2$$

   α-Hölder continuous, if the gradient of the image ∇I is α-Hölder continuous and $p \ge (1 + \alpha)q$.

3. *never (that is at no point) Fréchet differentiable unless the image $I : \mathbb{R}^d \to \mathbb{R}$ is an affine (linear) function, if the image I is of class $\mathscr{C}^1(\mathbb{R}^d)$ and $p = q$.*

Proof. Suppose $I : \mathbb{R}^d \to \mathbb{R}$ Gâteaux differentiable and Lipschitz continuous and we will show that for $p \ge q$, the warping operator (4.1) is Gâteaux differentiable. Indeed if $\mathbf{u}, \mathbf{v} \in L^p(\Omega, \mathbb{R}^d)$, for all $t \ne 0$ we have

$$\frac{I(\mathbf{u} + t\mathbf{v}) - I(\mathbf{u})}{t}(\mathbf{x}) = \frac{I(x + \mathbf{u}(\mathbf{x}) + t\mathbf{v}(\mathbf{x})) - I(x + \mathbf{u}(\mathbf{x}))}{t}$$

and the right-hand side tends towards $\partial_{\mathbf{v}(\mathbf{x})} I(x + \mathbf{u}(\mathbf{x})) = \nabla I(x + \mathbf{u}(\mathbf{x})) \cdot \mathbf{v}(\mathbf{x})$ for $t \to 0$, for every $u \in \Omega$. Following the same notation as done before for the warping operator, we define

$$\nabla I(\mathbf{u}) : \Omega \to \mathbb{R}^d \qquad \nabla I(\mathbf{u})(\mathbf{x}) = \nabla I(x + \mathbf{u}(\mathbf{x}))$$

and then

$$\nabla I(\mathbf{u}) \cdot \mathbf{v} : \Omega \to \mathbb{R} \qquad (\nabla I(\mathbf{u}) \cdot \mathbf{v})(\mathbf{x}) = \nabla I(\mathbf{u})(\mathbf{x}) \cdot \mathbf{v}(\mathbf{x})$$

Thus, we have proved that for $t \to 0$

$$\frac{I(\mathbf{u} + t\mathbf{v}) - I(\mathbf{u})}{t} \to \nabla I(\mathbf{u}) \cdot \mathbf{v} \quad \text{(pointwise)}$$

[2] $\mathbb{L}(L^p(\Omega, \mathbb{R}^d), L^q(\Omega))$ denotes the space of bounded linear operators from $L^p(\Omega, \mathbb{R}^d)$ to $L^q(\Omega)$ endowed with the *operator norm* $T = \sup_{\|u\| \le 1} \|T[u]\|$.

Furthermore, the Lipschitz continuity of $I : \mathbb{R}^d \to \mathbb{R}$ implies that for each $\mathbf{x} \in \Omega$ it holds

$$\begin{aligned}\left|\frac{I(\mathbf{x}+\mathbf{u}(\mathbf{x})+t\mathbf{v}(\mathbf{x}))-I(\mathbf{x}+\mathbf{u}(\mathbf{x}))}{t}\right| &\leq \frac{1}{|t|}|I(\mathbf{x}+\mathbf{u}(\mathbf{x})+t\mathbf{v}(\mathbf{x}))-I(\mathbf{x}+\mathbf{u}(\mathbf{x}))| \\ &\leq \frac{1}{|t|}\mathrm{Lip}(I)|t\mathbf{v}(\mathbf{x})| = \mathrm{Lip}(I)|\mathbf{v}(\mathbf{x})|\end{aligned}$$

and $|\mathbf{v}| \in L^p(\Omega) \subseteq L^q(\Omega)$. Therefore, from the dominated convergence theorem, we get $\nabla I(\mathbf{u}) \cdot \mathbf{v} \in L^q(\Omega)$ and

$$\frac{I(\mathbf{u}+t\mathbf{v})-I(\mathbf{u})}{t} \to \nabla I(\mathbf{u}) \cdot \mathbf{v} \text{ in } (L^q(\Omega), \|\cdot\|_q)$$

We highlight that $\nabla I(\mathbf{u}) \cdot \mathbf{v} \in L^q(\Omega)$ also because

$$|(\nabla I(\mathbf{u}) \cdot \mathbf{v})(\mathbf{x})| = |\nabla I(\mathbf{u})(\mathbf{x}) \cdot \mathbf{v}(\mathbf{x})| \leq |\nabla I(x+\mathbf{u}(\mathbf{x}))||\mathbf{v}(\mathbf{x})| \leq \|\nabla I\|_\infty |\mathbf{v}(\mathbf{x})|$$

and $\|\nabla I(\mathbf{u}) \cdot \mathbf{v}\|_q \leq \|\nabla I\|_\infty \|\mathbf{v}\|_q \leq \|\nabla I\|_\infty |\Omega|^{\frac{1}{q}-\frac{1}{p}} \|\mathbf{v}\|_p$. We notice that $\|\nabla I\|_\infty < +\infty$ because I is Lipschitz continuous: actually $\|\nabla I\|_\infty = \mathrm{Lip}(I)$. This shows that the operator

$$\mathbf{v} \in L^p(\Omega, \mathbb{R}^d) \to \nabla I(\mathbf{u}) \cdot \mathbf{v} \in L^q(\Omega)$$

which is of course linear, is also bounded. In summary, we proved that the warping operator is Gâteaux differentiable and its derivative is as follows

$$I'(\mathbf{u}) : L^p(\Omega, \mathbb{R}^d) \to L^q(\Omega) \qquad I'(\mathbf{u})[\mathbf{v}] = \nabla I(\mathbf{u}) \cdot \mathbf{v}$$

and we have also $\|I'(\mathbf{u})\| \leq |\Omega|^{\frac{1}{q}-\frac{1}{p}} \|\nabla I\|_\infty$. Next, if $\mathbf{u}_1, \mathbf{u}_2, \mathbf{v} \in L^p(\Omega, \mathbb{R}^d)$, then

$$(I'(\mathbf{u}_1) - I'(\mathbf{u}_2))[\mathbf{v}] = (\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)) \cdot \mathbf{v}$$

and

$$\begin{aligned}\int_\Omega |(\nabla I(\mathbf{u}_1)(\mathbf{x}) - \nabla I(\mathbf{u}_2)(\mathbf{x})) \cdot \mathbf{v}(\mathbf{x})|^q \,\mathrm{d}\mathbf{x} &\leq \int_\Omega |\nabla I(\mathbf{u}_1)(x) - \nabla I(\mathbf{u}_2)(x)|^q |\mathbf{v}(x)|^q \,\mathrm{d}\mathbf{x} \\ &\leq \Big(\int_\Omega |\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)|^r \,\mathrm{d}\mathbf{x}\Big)^{q/r} \Big(\int_\Omega |v|^p \,\mathrm{d}\mathbf{x}\Big)^{q/p} \\ &= \|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)\|_r^q \|\mathbf{v}\|_p^q\end{aligned}$$

where $r \geq 1$ and $1/r = 1/q - 1/p$. The inequality above is nothing but the Hölder inequality applied to $|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)|^q$ and $|v|^q$, taking into account that

$$|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)|^q \in L^\infty(\Omega) \subseteq L^{r/q}(\Omega),\ |\mathbf{v}|^q \in L^{p/q}(\Omega)$$

and that p/q and $r/q = p/(p-q)$ are conjugate exponents. Thus, we have

$$\|(\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)) \cdot \mathbf{v}\|_q \leq \|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)\|_r \|\mathbf{v}\|_p$$

Note that the same conclusion holds if $p = q$: in that case $r = \infty$. Summarizing we get

$$\|I'(\mathbf{u}_1) - I'(\mathbf{u}_2)\| \leq \|\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2)\|_r$$

With the same reasoning one can prove

$$\|\nabla I(\mathbf{u}) \cdot \mathbf{v}\|_q \leq \|\nabla I(\mathbf{u})\|_r \|\mathbf{v}\|_p$$

This way one can obtain a better estimate of the norm of $I'(\mathbf{u})$ then before, that is $\|I'(\mathbf{u})\| \leq \|\nabla I(\mathbf{u})\|_r$. The inequality above shows that the continuity properties of the derivative I' of the operator I depends on those of the operator

$$\nabla I : L^p(\Omega, \mathbb{R}^d) \to L^r(\Omega, \mathbb{R}^d), \quad \nabla I(\mathbf{u}) = \nabla I \circ (\mathbf{id} + \mathbf{u}) \tag{4.2}$$

In case $p > q$, that is $r < +\infty$, and with the further hypothesis $\nabla I : \mathbb{R}^d \to \mathbb{R}^d$ be continuos (hence $I \in \mathscr{C}^1(\mathbb{R}^d)$), one sees that the operator (4.2) is continuous. Indeed if $\mathbf{u}_n \to \mathbf{u}$ in $(L^p(\Omega, \mathbb{R}^d), \|\cdot\|_p)$, then, up to a subsequence, $\mathbf{u}_n(\mathbf{x}) \to \mathbf{u}(\mathbf{x})$ for a.e $u \in \Omega$. Thus, $\nabla I(\mathbf{u}_n) \to \nabla I(\mathbf{u})$ a.e. in Ω and $|\nabla I(\mathbf{u}_n)| \leq a$ with $a \in L^\infty(\Omega) \subseteq L^r(\Omega)$ (take $a = \|\nabla I\|_\infty$). The dominated convergence theorem implies $\nabla I(\mathbf{u}_n) \to \nabla I(\mathbf{u})$ in $(L^r(\Omega, \mathbb{R}^d), \|\cdot\|_r)$. Then in this case the derivative

$$I' : L^p(\Omega, \mathbb{R}^d) \to \mathbb{L}(L^p(\Omega, \mathbb{R}^d), L^q(\Omega, \mathbb{R}^d))$$

is continuous and hence the warping operator is Fréchet differentiable. As done for the case of the operator I, one sees that the operator (4.2) is Hölder continuous with exponent α if so the function $\nabla I : \Omega \to \mathbb{R}^d$ and $p/\alpha \geq r$ (which is equivalent to $p \geq (1+\alpha)q$). It is worth to notice that, unless the image $I : \Omega \to \mathbb{R}$ "degenerates", in the case $p = q$, the warping operator

$$I : L^p(\Omega, \mathbb{R}^d) \to L^p(\Omega)$$

is never Fréchet differentiable at any point of $L^p(\Omega, \mathbb{R})$. In fact, one can prove that if the gradient ∇I of the image is bounded and the operator I is Fréchet differentiable in $\mathbf{u} \in L^p(\Omega, \mathbb{R}^d)$, then

$$I(\mathbf{x} + \mathbf{u}) = a(\mathbf{x}) + \mathbf{b}(\mathbf{x}) \cdot \mathbf{u} \text{ for a.e. } \mathbf{x} \in \Omega \text{ and all } \mathbf{u} \in \Omega$$

with $a : \Omega \to \mathbb{R}$ and $\mathbf{b} : \Omega \to \mathbb{R}^d$. Thus, the image $I : \Omega \subseteq \mathbb{R}^d \to \mathbb{R}$ would be an affine function [AZ90]. $\square$

4.2.2 The warping operator in Sobolev and BV spaces

We now move on to the study of the restriction of the warping operator to Sobolev spaces $W^{1,p}$ and the space of functions of bounded variations BV.

Let us deal first with Sobolev spaces. Since clearly $W^{1,p}(\Omega, \mathbb{R}^d) \hookrightarrow L^p(\Omega, \mathbb{R}^d)$, we can consider the restriction of the warping operator

$$I : W^{1,p}(\Omega, \mathbb{R}^d) \to L^q(\Omega) \tag{4.3}$$

Recalling the Rellich-Kondrakhov Theorem 2.3.6, we have the following compact embeddings:

$$W^{1,p}(\Omega, \mathbb{R}^d) \hookrightarrow L^s(\Omega, \mathbb{R}^d) \quad \text{for every } s \in [1, p^*[\tag{4.4}$$

where $p^* = pd/(d-p)$ if $p < d$ and $p^* = +\infty$ if $p \geq d$ (in any case $p^* > p$). For $s = p^*$ only continuous embedding holds (see Theorem 2.3.6). Then, one can prove the following result

Theorem 4.2.4. *The restriction of the warping operator to the Sobolev space* (4.3) *is*

1. *completely continuous (it transforms weakly convergent sequences into strongly convergent sequences) for any $p, q \geq 1$, if $I : \mathbb{R}^d \to \mathbb{R}$ is continuous;*
2. *Gâteaux differentiable, if $q \leq p^*$ and the image I is differentiable with bounded gradient;*
3. *Fréchet differentiable with compact derivative, if $q < p^*$ and the image I is of class $\mathscr{C}^1(\mathbb{R}^d)$ with bounded gradient;*
4. *with α-Hölder continuous derivative I', if $(1+\alpha)q \leq p^*$ and ∇I is α-Hölder continuous.*

Proof. From (4.4), it follows that the embedding $W^{1,p}(\Omega, \mathbb{R}^d) \hookrightarrow L^p(\Omega, \mathbb{R}^d)$ is compact and taking into account the conclusion of Theorem 4.2.1, it follows that the operator (4.3) is completely continuous for any $p, q \geq 1$. Next, if $q < p^*$ we can take $s \in \mathbb{R}$, with $q < s < p^*$ and consider the composition of maps

$$W^{1,p}(\Omega, \mathbb{R}^d) \hookrightarrow L^s(\Omega, \mathbb{R}^d) \xrightarrow{I} L^q(\Omega) \tag{4.5}$$

From (4.4), (4.5) and Theorem 4.2.3 (point 2), it follows that the operator (4.3) is Fréchet differentiable with compact derivative. In case $q = p^* < +\infty$, the embedding $W^{1,p}(\Omega, \mathbb{R}^d) \hookrightarrow L^{p^*}(\Omega, \mathbb{R}^d)$ is only continuous and the warping operator $I : L^{p^*}(\Omega, \mathbb{R}^d) \to L^q(\Omega)$ is only Gâteaux differentiable. As a result, one can only say that, in case $q = p^*$, the warping operator (4.3) is Gâteaux differentiable. Finally, again from the chain (4.5) and Theorem 4.2.3 (point 2), if ∇I is α-Hölder continuous, $0 < \alpha \leq 1$ and $(1+\alpha)q \leq p^*$, then the derivative of the operator (4.3) is α-Hölder continuous too (again, simply chose $s \in \mathbb{R}$ with $(1+\alpha)q \leq s \leq p^*$). $\square$

Just as example, let us discuss some particular cases. Suppose that the gradient of the image ∇I is Lipschitz continuous. If $p = d = 2$, then $p^* = +\infty$ and, thanks to Theorem 4.2.4, the operator (4.3) is Fréchet differentiable with a Lipschitz continuous derivative and a compact derivative $I'(\mathbf{u})$ for any $q \geq 1$. In case $d = 3$ and $p = 2$, it is $p^* = 6$ and the warping operator (4.3) is Fréchet differentiable for $q < 6$ and it has Lipschitz derivative for $q \leq 3$. In case $p = 1$, it is $p^* = d/(d-1)$ and it holds $1 < p^* \leq 2$ ($p^* = 2$ iff $d = 2$). Then the operator (4.3) is Fréchet differentiable if $q < p^*$. The derivative I' is Lipschitz continuous if $q \leq p^*/2$ and this happens only for $d = 2$ and $q = 1$. Moreover it has α-Hölder continuous derivative I', if ∇I is α-Hölder continuous.

The case of the functions of bounded variations is analog to that of $W^{1,1}$, it is enough to recall Theorem 2.3.11 which states that the following embeddings hold true

$$BV(\Omega, \mathbb{R}^d) \hookrightarrow L^q(\Omega) \quad \text{for every } s \in [1, d/(d-1)[$$

(for $s = d/(d-1)$ it is only continuous). In the same way, one can prove the following theorem about the restriction of the warping operator

$$I : BV(\Omega, \mathbb{R}^d) \to L^q(\Omega) \tag{4.6}$$

Theorem 4.2.5. *The restriction of the warping operator to the BV space* (4.6) *is*

1. *completely continuous for any $q \geq 1$, if $I : \mathbb{R}^d \to \mathbb{R}$ is continuous;*
2. *Gâteaux differentiable, if $q \leq d/(d-1)$ and the image $I : \mathbb{R}^d \to \mathbb{R}$ is differentiable with bounded gradient;*
3. *Fréchet differentiable with compact derivative, if $q < d/(d-1)$ and I is of class $\mathscr{C}^1$ with bounded gradient;*
4. *with α-Hölder continuous derivative I', if $(1+\alpha)q \leq d/(d-1)$ and ∇I is α-Hölder continuous.*

4.3 Well-posedness and convergence

In this section we apply the general theory of section 3.2 to the image registration problem (1.1). We provide first an analysis of two different distance measures widely used in applications. Next, we give stability and convergence results. Finally, we list several popular regularizers and show that they are compliant to the theory.

4.3.1 Distance measures: mono and multi-modal case

L^q based distance. In case the L^q norm is used for evaluating the distance between images, we set $\mathrm{Im}(\Omega) := L^\infty(\Omega)$ and

$$\phi : \mathrm{Im}(\Omega) \times \mathrm{Im}(\Omega) \subseteq L^q(\Omega) \times L^q(\Omega) \to \mathbb{R}, \qquad \phi(I_1, I_2) = \|I_1 - I_2\|_q^q$$

We studied this kind of distances, in general settings, in section 3.2.3. We saw that ϕ is (jointly) continuous in the whole domain and (jointly) Lipschitz continuous on bounded sets of $\mathrm{Im}(\Omega) \times \mathrm{Im}(\Omega)$ (in the L^q norm). Thus Assumption 3.2.1 are satisfied.

Mutual Information based distance. The second kind of measure between images, considered here, is based on the notion of mutual information. Let us recall the definition [FH02, FH04, HCF02, PS11]. Given an image

$$I : \Omega \to \mathbb{R}\,,$$

which we assume for the moment measurable, the probability density of its intensity values (gray levels) is being estimated by the *Parzen window* method. If we chose a Gaussian window with standard deviation $\sigma > 0$

$$g_\sigma(i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-i^2/(2\sigma^2)},$$

we set

$$p_I(i) = \frac{1}{|\Omega|} \int_\Omega g_\sigma(I(\mathbf{x}) - i)\,\mathrm{d}\mathbf{x},$$

the variable i denoting the intensity of the image. The function p_I is defined by integrals and it is continuous on $\mathbb{R}$.[3] Next, clearly $p_I(i) > 0$ — otherwise it would be $g_\sigma(I(\mathbf{x}) - i) = 0$ for a.e. $x \in \Omega$ and hence g_σ would be zero at some point of $\mathbb{R}$, which gives a contradiction. Moreover it is a probabilty density function on $\mathbb{R}$, i.e. its integral is 1.

Note that the definition of p_I requires only the measurability of the image $I : \Omega \to \mathbb{R}$. In case of two images I_1, I_2 one can consider the vector image (two-channels)

$$\mathbf{I} : \Omega \to \mathbb{R}^2 \text{ con } \mathbf{I}(\mathbf{x}) = (I_1(\mathbf{x}), I_2(\mathbf{x}))$$

and the *joint probability density function* of the intensity values of the images I_1 and I_2, shall be defined in the same manner

$$p_{I_1,I_2}(\mathbf{i}) = \frac{1}{|\Omega|} \int_\Omega G_\sigma(\mathbf{I}(\mathbf{x}) - \mathbf{i})\,\mathrm{d}\mathbf{x} \tag{4.7}$$

[3] Since the function $g_\sigma(I(\mathbf{x}) - i)$ is continuous in the variable i and $|g_\sigma(I(\mathbf{x}) - i)| \leq g_\sigma(0)$, which is integrable over Ω, the conclusion follows from the Lebesgue dominated convergence theorem.

where this time G_σ is a bivariate Gaussian

$$G_\sigma(\mathbf{i}) = g_\sigma(i_1)g_\sigma(i_2) = \frac{1}{2\pi\sigma^2}e^{-|\mathbf{i}|^2/(2\sigma^2)}$$

It is easy to see that the marginal densities p_{I_1} and p_{I_2} (defined as above) can be obtained by partial integration

$$p_{I_1}(i_1) = \int_{\mathbb{R}} p_{I_1,I_2}(i_1,i_2)\,\mathrm{d}i_2 \quad \text{and} \quad p_{I_1}(i_2) = \int_{\mathbb{R}} p_{I_1,I_2}(i_1,i_2)\,\mathrm{d}i_1$$

Finally, the *mutual information* between I_1 and I_2 is defined as follows

$$\boxed{\mathbf{MI}(I_1,I_2) := \int_{\mathbb{R}^2} p_{I_1,I_2}(\mathbf{i}) \log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\,\mathrm{d}\mathbf{i}.} \tag{4.8}$$

It is a measure of the distance between the distributions $p_{I_1,I_2}(i_1,i_2)$ and $p_{I_1}(i_1)p_{I_2}(i_2)$, and thus account for the level of statistical dependency of the two random variables associated to the intensities of the images I_1 and I_2. Mutual information $\mathbf{MI}(I_1,I_2)$ is always well-defined for measurable images I_1, I_2, since in fact it is equal to the Kullback-Leibler distance $D(p_{I_1,I_2}\|p_{I_1}p_{I_2})$ (this definition is recalled in Appendix A, see also corollary A.2.3, noting that p_{I_1,I_2} and $p_{I_1}p_{I_2}$ are two strictly positive and continuous probability density on $\mathbb{R}^2$). Furthermore it holds

$$\mathbf{MI}(I_1,I_2) \geq 0, \quad \mathbf{MI}(I_1,I_2) = \mathbf{MI}(I_2,I_1)$$

and $\mathbf{MI}(I_1,I_2) = 0$ iff the random variables of the intensities of the two images are indipendent one of each other.

The following theorems establish topological and differential properties of the mutual information. They are slight generalizations of the results given in [FH02, FH04] and we provide proofs in Appendix A. First of all, the mutual information (4.8) is indeed finite if at least one of the two images is (essentially) bounded as the following proposition states

Proposition 4.3.1. *Let $I_1, I_2 : \Omega \to \mathbb{R}$ be two measurable images. If $\|I_1\|_\infty \leq A$ or $\|I_2\|_\infty \leq A$, then it holds $M(I_1,I_2) \leq C(A)$ — where $C(A)$ is a constant which does not depend directly on I_1, I_2, but just on the bound A.*

Next, the following result shows a continuity property for the mutual information.

Proposition 4.3.2. *Let I_1^k, I_2^k, $k \in \mathbb{N}$ and I_1, I_2 measurable images and suppose that $\|I_1^k\|_\infty, \|I_1\|_\infty \leq A$. Then*

$$I_1^k(\mathbf{x}) \to I_1(\mathbf{x}) \text{ and } I_2^k(\mathbf{x}) \to I_2(\mathbf{x}) \text{ for a.e. } \mathbf{x} \in \Omega \implies \mathbf{MI}(I_1^k, I_2^k) \to \mathbf{MI}(I_1, I_2)$$

Corollary 4.3.3. *For $I_1 \in L^\infty(\Omega)$ and $q \geq 1$, the functional $\mathbf{MI}(I_1, \cdot) : L^q(\Omega) \to \mathbb{R}$ is continuous for the L^q norm and also $\mathbf{MI}$ is jointly continuous in the L^q norm on bounded sets of $L^\infty(\Omega) \times L^\infty(\Omega)$ (in the norm $\|\cdot\|_\infty$).*

Proof. Let $I, I^k \in L^q(\Omega)$ with $I^k \to I$ in $L^q(\Omega)$. Then there exists a subsequence $(I^{n_k})_{k\in\mathbb{N}}$ such that $I^{n_k}(\mathbf{x}) \to I(\mathbf{x})$ for a.e. $\mathbf{x} \in \Omega$. One can then applied the previous proposition (with $A = \|I_1\|_\infty$) and get $\mathbf{MI}(I_1, I^{n_k}) \to \mathbf{MI}(I_1, I)$. Next if $I_1^k, I_2^k, I_1, I_2 \in L^q(\Omega)$ with $\|I_i^k\|_\infty, \|I_i\|_\infty \leq A$ and $I_i^k \to I_i$ in $L^q(\Omega)$ for $i = 1, 2$, then there exist subsequences $(I_1^{n_k})_{k\in\mathbb{N}}, (I_2^{n_k})_{k\in\mathbb{N}}$ such that $I_1^{n_k}(\mathbf{x}) \to I_1(\mathbf{x})$ and $I_2^{n_k}(\mathbf{x}) \to I_2(\mathbf{x})$ for a.e. $\mathbf{x} \in \Omega$. From Proposition 4.3.2 it follows $\mathbf{MI}(I_1^{n_k}, I_2^{n_k}) \to \mathbf{MI}(I_1, I_2)$. This concludes the proof. □

Finally, let us give a theorem about the partial differentiability of $\mathbf{MI}(I_1, I_2)$ w.r.t. one variable, say I_2.

Theorem 4.3.4. *Let $I_1 \in L^\infty(\Omega)$. Then the functional*

$$\mathbf{MI}(I_1, \cdot) : L^q(\Omega) \to \mathbb{R} \tag{4.9}$$

is Fréchet differentiable with continuous derivative $\nabla\mathbf{MI}(I_1, \cdot) : L^q(\Omega) \to L^{q'}(\Omega)$ and for every $I_2 \in L^q(\Omega)$ it holds

$$\nabla\mathbf{MI}(I_1, \cdot)(I_2) = \frac{1}{|\Omega|}(\partial_2 G_\sigma * L_{I_1,I_2}) \circ \mathbf{I} \in L^{q'}(\Omega)$$

where q' is the conjugate exponent of q and the function $L_{I_1,I_2} : \mathbb{R}^2 \to \mathbb{R}$ is defined as

$$L_{I_1,I_2}(i_1, i_2) = \log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)} + 1$$

Moreover $\|\nabla\mathbf{MI}(I_1, \cdot)(I_2)\|_{q'} \leq C(A)$ — where $C(A)$ is a constant which does not depend on I_2 and neither on I_1 but just on $A = \|I_1\|_\infty$. Hence the mapping (4.9) is Lipschitz continuous with a Lipschitz which depend on A alone.

Thus, in case of mutual information, let $A > 0$ (large), set $\mathrm{Im}(\Omega) = \{I \in L^\infty(\Omega) \,|\, \|I\|_\infty \leq A\}$ and

$$\phi : \mathrm{Im}(\Omega) \times \mathrm{Im}(\Omega) \subseteq L^q(\Omega) \times L^q(\Omega) \to \mathbb{R}, \quad \phi(I_1, I_2) = -\mathbf{MI}(I_1, I_2)$$

Then the function ϕ is bounded and (jointly) Lipschitz continuous on the whole domain (in the L^q norm) since

$$\begin{aligned} |\mathbf{MI}(I_1^1, I_2^1) - \mathbf{MI}(I_1^2, I_2^2)| &\leq |\mathbf{MI}(I_1^1, I_2^1) - \mathbf{MI}(I_1^1, I_2^2)| + |\mathbf{MI}(I_1^1, I_2^2) - \mathbf{MI}(I_1^2, I_2^2)| \\ &\leq C(A)(\|I_2^1 - I_2^2\|_q + \|I_1^1 - I_1^2\|_q) \end{aligned}$$

Thus Assumption 3.2.1 are satisfied. Moreover the set $\mathrm{Im}(\Omega)$ is stable under warping operations, meaning that if $I \in \mathrm{Im}(\Omega)$ and $\mathbf{u} \in L^p(\Omega, \mathbb{R}^d)$, than $I \circ (\mathbf{id} + \mathbf{u}) \in \mathrm{Im}(\Omega)$ — this allows to define the warping operator properly.

4.3.2 Main result

We can now treat the problem of image registration for general distance measures in a unified manner. Let us consider $\mathrm{Im}(\Omega)$ and $\phi : \mathrm{Im}(\Omega) \times \mathrm{Im}(\Omega) \to \mathbb{R}$ as defined in the two cases described above. The following theorem holds true

Theorem 4.3.5. *Let $I_0, I \in \mathrm{Im}(\Omega)$ be a reference and template image. Let $U(\Omega, \mathbb{R}^d)$ be a subspace of $L^p(\Omega, \mathbb{R}^d)$ endowed with a topology such that the embedding*

$$U(\Omega, \mathbb{R}^d) \hookrightarrow L^p(\Omega, \mathbb{R}^d)$$

is continuous and let $J : U(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}$ be a convex seq. l.s.c. and coercive functional. Then, for fixed $\lambda > 0$, the problem

$$\min_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \phi(I(\mathbf{u}), I_0) + \lambda J(\mathbf{u}) \tag{4.10}$$

is well-posed. More precisely if $I_0^n, I^n \in \mathrm{Im}(\Omega)$ such that

(i) *$I_0^n \to I_0$ in the norm L^q;*

(ii) *I, I^n are continuous and $I^n \to I$ uniformly on $\mathbb{R}^d$,*

then, for the problem

$$\min_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \phi(I^n(\mathbf{u}), I_0^n) + \lambda J(\mathbf{u}), \quad \lambda > 0$$

the conclusions of Theorem 3.2.6 hold. Moreover, under the same perturbations (i) – (ii) above, if

$$\|I_0^n - I_0\|_q \leq \delta_n, \quad \|I^n - I\|_\infty \leq \eta_n$$

and $\lambda_n \to 0$ with $(\delta_n + \eta_n)/\lambda_n \to 0$, then the problem

$$\min_{\mathbf{u} \in U(\Omega, \mathbb{R}^d)} \phi(I^n(\mathbf{u}), I_0^n) + \lambda_n J(\mathbf{u})$$

will converge to the problem (4.10), in the sense that the conclusions of Theorem 3.2.9 hold.

Proof. From the inequality

$$\begin{aligned}\|I(\mathbf{u}) - I^n(\mathbf{u})\|_q &\leq |\Omega|^{\frac{1}{q}} \|I(\mathbf{u}) - I^n(\mathbf{u})\|_\infty \\ &\leq |\Omega|^{\frac{1}{q}} \|I - I^n\|_\infty\end{aligned}$$

it follows that the sequence of the warping operators $I^n : L^p(\Omega, \mathbb{R}^d) \to \mathrm{Im}(\Omega)$ converges uniformly to the warping operator $I : L^p(\Omega, \mathbb{R}^d) \to \mathrm{Im}(\Omega)$ and moreover they are all bounded and continuous operators. Therefore, assumptions 3.2.1-3.2.2-3.2.8 in section 3.2 are satisfied a fortiori for the restrictions to $U(\Omega, \mathbb{R}^d)$ of the warping operators I, I^n and Theorems 3.2.4-3.2.6 and 3.2.9 apply. □

Theorem 4.3.5 shows that we can indeed get existence, stability and convergence results for variational methods in image registration. However it leaves open the choice of the space $U(\Omega, \mathbb{R}^d)$ and the regularizer J which are required to meet to the hypotheses of the theorem — in particular reffering to the coercivity property. This task is often facilitated by shrinking the space of allowed displacement fields to a Banach space $U(\Omega, \mathbb{R}^d)$ such that the embedding $U(\Omega, \mathbb{R}^d) \hookrightarrow L^p(\Omega, \mathbb{R}^d)$ is *compact* and endowing $U(\Omega, \mathbb{R}^d)$ with the weak topology. The change to weak topology makes the search for a coercive functional $J : U(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}$ easier. However, it is remarkable that one can have coercivity for an important regularizer in the whole space $L^p(\Omega, \mathbb{R}^d)$ using the strong topology, as we will see soon.

4.3.3 Regularizing the image registration problem

In this final section, we now describe several regularization functionals quite popular in image registration literature. They are shown to be l.s.c. and coercive in the space $U(\Omega, \mathbb{R}^d)$. Therefore, according to Theorem 4.3.5, if we use them coupled with the two distance measures defined in section 4.3.1, we get well-posed and convergent methods for image registration. We emphasize that we have provided here just some notable examples. Other regularizers might be considered and, according to the theory, they lead to stable and convergent methods as soon as they are coercive and l.s.c.

4.3.3.1 Regularizers in $W^{1,p}(\Omega)$

Here we consider the case $U(\Omega, \mathbb{R}^d) = W^{1,p}(\Omega, \mathbb{R}^d)$ endowed with the weak topology. We shall treat functionals of the following form

$$J(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \varphi(\mathbf{x}, D\mathbf{u}(\mathbf{x}))\,\mathrm{d}\mathbf{x} & \text{if } \mathbf{u} \in W_0^{1,p}(\Omega, \mathbb{R}^d); \\ +\infty & \text{otherwise} \end{cases} \tag{4.11}$$

where $W_0^{1,p}(\Omega, \mathbb{R}^d)$ is the subspace of mappings which are zero on the boundary of Ω (zero trace) and the function $\varphi : \Omega \times \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ is measurable and satisfies the following conditions

(*i*) φ is bounded from below and $\varphi(\mathbf{x}, \cdot) : \mathbb{R}^{d\times d} \to \mathbb{R} \cup \{+\infty\}$ is l.s.c. for a.e. $\mathbf{x} \in \Omega$;

(*ii*) $\varphi(\mathbf{x}, \cdot) : \mathbb{R}^{d\times d}$ is convex for a.e. $\mathbf{x} \in \Omega$;

(*iii*) $p > 1$ and $\varphi(\mathbf{x}, \mathbf{H}) \geq a(\mathbf{x}) + b|\mathbf{H}|^p$ for every $(\mathbf{x}, \mathbf{H}) \in \Omega \times \mathbb{R}^{d\times d}$ and suitable $a \in L^1(\Omega)$ and $b > 0$.

The first condition ensures that definition (4.11) is well-posed and the functional

$$J : W^{1,p}(\Omega, \mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$$

is (strongly) lower semicontinuous for every $p \geq 1$ [Dac08]. In fact we shall need the *weak lower semicontinuity* property which can be obtained if we require also condition (*ii*). As regards the *weak coerciveness* of J, it can be easily shown as soon as (*iii*) is satisfied. Indeed for $\mathbf{u} \in W_0^{1,p}(\Omega, \mathbb{R}^d)$, condition (*iii*) implies $J(\mathbf{u}) \geq \|a\|_1 + b\|D\mathbf{u}\|_p^p$ and using *Poincaré's inequality* 2.3.5, we get $J(\mathbf{u}) \geq \|a\|_1 + \frac{b}{C^p}\|\mathbf{u}\|_{1,p}^p$. This condition gives the required weak coerciveness, taking into account that for $p > 1$ the Banach space $W^{1,p}(\Omega, \mathbb{R}^d)$ is reflexive.

Dirichlet functional. The first choice is just to take the norm of the Jacobian of the mapping $\mathbf{u} : \Omega \to \mathbb{R}^d$, i.e.

$$\boxed{J(\mathbf{u}) = \|D\mathbf{u}\|_p^p = \int_\Omega |D\mathbf{u}|^p \,\mathrm{d}\mathbf{x}, \qquad p > 1} \tag{4.12}$$

This functional has the form (4.11) with $\varphi(\mathbf{x}, \mathbf{H}) = |\mathbf{H}|^p$ and conditions (*i*), (*ii*), (*iii*) above are satisfied. Thus, it gives rise to a weakly l.s.c. and weakly coercive functional. In case $p = 2$, this regularizer coupled with the L^2 distance measure yields the so called *diffusive registration* [Mod04].

Nagel-Enkelman functional. This regularizer assumes $p = 2$ and it is a slight generalization of the Dirichlet functional (for the case $p = 2$), still of diffusive-type but which introduces anisotropy in the smoothness properties [NE86, AWS00, HCF02]. It is defined as

$$\boxed{J(\mathbf{u}) = \int_\Omega \mathrm{tr}(D\mathbf{u}(\mathbf{x})\mathbf{T}_{I_0}(\mathbf{x})D\mathbf{u}(\mathbf{x})^\top)\,\mathrm{d}\mathbf{x}} \tag{4.13}$$

where $\mathbf{T}_{I_0} : \Omega \to \mathbb{R}^{d\times d}$ is a tensor field on Ω defined as

$$\mathbf{T}_{I_0}(\mathbf{x}) = \frac{(\lambda + |\nabla I_0(\mathbf{x})|^2)\mathbf{Id}_d - \nabla I_0(\mathbf{x})\nabla I_0(\mathbf{x})^\top}{(d-1)|\nabla I_0(\mathbf{x})|^2 + \lambda d}$$

and $\mathbf{Id}_d$ denotes the identity matrix of order d. It is of type (4.11), with

$$\varphi(\mathbf{x}, \mathbf{H}) = \mathbf{H}\mathbf{T}_{I_0}(\mathbf{x})\mathbf{H}^\top$$

and evidently $\varphi(\mathbf{x}, \cdot) : \mathbb{R}^{d\times d} \to \mathbb{R}$ is a positive quadratic form, therefore conditions $(i), (ii)$ are satisfied. Condition (iii) can be met as soon as we bound from below the eigenvalues of $\mathbf{T}_{I_0}(\mathbf{x})$ uniformly in $\mathbf{x}$ and this can be achieved if the image I_0 is Lipschitz continuous. Eventually, the regularizer (4.13) is weakly l.s.c. and weakly coercive in $W^{1,2}(\Omega, \mathbb{R}^d)$ [AWS00, HCF02].

Linearized elasticity potential. It assumes $p = 2$ and

$$\boxed{J(\mathbf{u}) = \int_\Omega \lambda \mathrm{tr}(\mathbf{e}(\mathbf{u}))^2 + 2\mu|\mathbf{e}(\mathbf{u})|^2 \, \mathrm{d}\mathbf{x}} \tag{4.14}$$

where $\mathbf{e}(\mathbf{u}) = (D\mathbf{u} + D\mathbf{u}^\top)/2$ is the *infinitesimal strain tensor* and $\lambda, \mu \geq 0$ are the Lamé constants [Cia88]. This choice yields the *elastic registration method* [Mod04]. It can be deduced again by the scheme (4.11), taking

$$\varphi(\mathbf{x}, \mathbf{H}) = \lambda\Big[\mathrm{tr}\Big(\frac{\mathbf{H}+\mathbf{H}^\top}{2}\Big)\Big]^2 + 2\mu \mathrm{tr}\Big[\Big(\frac{\mathbf{H}+\mathbf{H}^\top}{2}\Big)^2\Big]$$

Clearly $\varphi(x, \cdot)$ is a positive quadratic form, but one can show that it is not positive definite, hence condition (ii) can not be satisfied. Therefore coerciveness has to be proved directly. Using *Korn's inequality* [Cia88]

$$\|D\mathbf{u}\|_2 \leq C_K \|\mathbf{e}(\mathbf{u})\|_2, \qquad \mathbf{u} \in W_0^{1,2}(\Omega, \mathbb{R}^d)$$

and again from Poincaré's inequality 2.3.5, one gets

$$J(\mathbf{u}) \geq 2\mu\|\mathbf{e}(\mathbf{u})\|_2^2 \geq \frac{2\mu}{C^2 C_K^2}\|\mathbf{u}\|_{1,2}^2$$

which shows the (weak) coerciveness of J as soon as $\mu > 0$.

Hyperelastic, polyconvex potential. This regularizer has been used for image registration in [DR04]. For semplicity we assume $d = 3$. This case weakens the convexity hypothesis (ii) and instead requires a *polyconvex* condition. More precisely one set [Cia88, Dac08]

$$\boxed{J(\mathbf{u}) = \int_\Omega \mathbb{W}(\mathbf{x}, \mathbf{Id}_3 + D\mathbf{u}(\mathbf{x}), \operatorname{cof}(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})), \det(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})))\, \mathrm{d}\mathbf{x}} \tag{4.15}$$

where

- $(i)'$ $\mathbb{W} : \Omega \times \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is measurable;
- $(ii)'$ $\mathbb{W}(\mathbf{x}, \cdot) : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is l.s.c. and convex for a.e. $\mathbf{x} \in \Omega$;
- $(iii)'$ $\mathbb{W}(\mathbf{x}, \mathbf{F}, \mathbf{G}, t) = +\infty$ for $t \leq 0$.
- $(iv)'$ $p > 3$ and $\mathbb{W}(\mathbf{x}, \mathbf{F}, \mathbf{G}, t) \geq a(\mathbf{x}) + b|\mathbf{F}|^p$ for every $\mathbf{F}, \mathbf{G} \in \mathbb{R}^{3\times 3}$, $t \in \mathbb{R}$ and for suitable $a \in L^1(\Omega)$, $b > 0$.

Thus, it is definded according to (4.11) with

$$\varphi(\mathbf{x}, \mathbf{H}) = \mathbb{W}(\mathbf{x}, \mathbf{Id}_3 + \mathbf{H}, \operatorname{cof}(\mathbf{Id}_3 + \mathbf{H}), \det(\mathbf{Id}_3 + \mathbf{H}))$$

We highlight that, because of the lack of property (ii), the regularizer (4.15) is no longer convex. From the hypotheses above, one can show

$$\mathbb{W}(\mathbf{x}, \mathbf{F}, \mathbf{G}, t) \to +\infty \text{ per } t \to 0^+. \tag{4.16}$$

Indeed if $t_n \to 0$, then $(\mathbf{F}, \mathbf{G}, t_n) \to (\mathbf{F}, \mathbf{G}, 0)$ and hence, from the lower semicontinuity, it is $+\infty = \mathbb{W}(\mathbf{x}, \mathbf{F}, \mathbf{G}, 0) \leq \liminf_{n\to\infty} \mathbb{W}(\mathbf{x}, \mathbf{F}, \mathbf{G}, t_n)$. In the context of elasticity theory, φ is called the *stored energy function* and the matrix $\mathbf{F}$ represents the gradient of the deformation $\boldsymbol{\varphi} = \mathbf{id} + \mathbf{u}$. The behavior (4.16) reflects the idea that "infinite stress should accompany extreme strains" [Cia88]. Clearly $(iv)' \implies (iii)$, thus the (weak) coerciveness of J follows easily. The weak lower semicontinuity is much more difficult to prove and we refer to sections 8.3.2-8.4.2 in [Dac08] for details. Moreover the domain of J fulfills

$$\operatorname{dom}(J) \subseteq \left\{ \mathbf{u} \in W_0^{1,p}(\Omega, \mathbb{R}^3) \,\middle|\, \det(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})) > 0 \text{ q.o. in } \Omega \right\}$$

and all the displacement fields $\mathbf{u}$ gives rise to one-to-one deformation fields $\boldsymbol{\varphi} = \mathbf{id} + \mathbf{u} : \overline{\Omega} \to \overline{\Omega}$[4]

Finally, lower semicontinuity and coerciveness of J can be still guaranteed if condition $(iv)'$ is replaced with the following one:

[4]Recall that for $p > d$ it holds $W^{1,p}(\Omega, \mathbb{R}^d) \subseteq \mathscr{C}(\overline{\Omega}, \mathbb{R}^d)$. See also section 5.5 in [Cia88].

$(iv)''$ $p \geq 2$ and $\mathbb{W}(\mathbf{x}, \mathbf{F}, \operatorname{cof}(\mathbf{F}), \det(\mathbf{F})) \geq a(\mathbf{x}) + b(|\mathbf{F}|^p + |\operatorname{cof}(\mathbf{F})|^q + |\det(\mathbf{F})|^r)$ for every $\mathbf{F} \in \mathbb{R}^{3\times 3}$ with $\det(\mathbf{F}) > 0$, for a.e. $\mathbf{x} \in \Omega$ and for suitable $a \in L^1(\Omega)$, $b > 0, q \geq \frac{p}{p-1}$ and $r > 1$.

and in this case one has

$$\begin{aligned}\operatorname{dom}(J) \subseteq \big\{\mathbf{u} \in W_0^{1,p}(\Omega, \mathbb{R}^d) \,\big|\, &\operatorname{cof}(\mathbf{Id}_3 + D\mathbf{u}) \in L^q(\Omega, \mathbb{R}^{3\times 3}),\\ &\det(\mathbf{Id}_3 + D\mathbf{u}) \in L^r(\Omega) \text{ and } \det(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})) > 0 \text{ a.e. in } \Omega\big\}\end{aligned}$$

The existence theory in hyperelasticity with polyconvex stored energy functions is due to J. Ball. See again section 8.4.2 in [Dac08] or chap. 7 in [Cia88].

As an instance of the above regularizer we cite the one given in [DR04] Example 3.1, where

$$J(\mathbf{u}) = \int_\Omega a|\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})|^p + b|\operatorname{cof}(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x}))|^q + \Gamma(\det(\mathbf{Id}_3 + D\mathbf{u}(\mathbf{x})))\,\mathrm{d}\mathbf{x}$$

and $\Gamma(t) \geq c|t|^r$ for $r > 1$. In nonlinear elasticity such material laws have been proposed by Ogden [Ogd97] and for $p = q = 2$ we obtain the Mooney-Rivlin model [Cia88].

4.3.3.2 Regularizers in $BV(\Omega)$

As a further regularizer — well-know for other image processing problems like denoising, impainting, or optical flow estimation [AK06, Ves01, HSSW02], but not yet well-studied in connection with the problem of image registration — we consider the total variation. Thus, we set $U(\Omega, \mathbb{R}^d) = BV(\Omega, \mathbb{R}^d)$ the space of mappings $\mathbf{u} : \Omega \to \mathbb{R}^d$ of bounded variation, endowed with the weak-$*$ topology, and take as regularizer the *total variation* [AFP00, AK06]

$$\boxed{J(\mathbf{u}) = |D\mathbf{u}|(\Omega)} \tag{4.17}$$

where

$$|D\mathbf{u}|(\Omega) = \sup\Big\{\int_\Omega \langle \mathbf{u}, \operatorname{div}\boldsymbol{\phi}\rangle\,\mathrm{d}\mathbf{x} \,\Big|\, \boldsymbol{\phi} \in \mathscr{C}_c^1(\Omega, \mathbb{R}^{d\times d}), |\boldsymbol{\phi}(\mathbf{x})| \leq 1\Big\}$$

In section 2.3.2, we mentioned that the functional $J : BV(\Omega, \mathbb{R}^m) \to \mathbb{R}$ is (seq.) lower semicontinuous w.r.t. the L^1 topology and thus w.r.t. the weak-$*$ topology. This functional is clearly not coercive on $BV(\Omega, \mathbb{R}^d)$ (w.r.t. the weak-$*$ topology) and, as in the Sobolev case, boundary conditions are needed. However, in this case the Dirichlet boundary condition does not work. Setting $\mathbf{u}_{|\partial\Omega} = 0$ does non force the function to have large derivatives in Ω, since the function is allowed to have jumps. The goal is achieved by taking $\Omega_0 \subseteq \Omega$ open, connected, with Lipschitz boudary, and $\overline{\Omega_0} \subseteq \Omega$ (with $|\Omega \setminus \Omega_0| < \varepsilon$, ε small) that still contains the square where images are supposed to be defined and considering the space

$$U_{\Omega_0}(\Omega, \mathbb{R}^d) := \big\{\mathbf{u} \in BV(\Omega, \mathbb{R}^d) \,\big|\, \mathbf{u} = 0 \text{ on } \Omega \setminus \Omega_0\big\}$$

This space is sequentially closed for the L^1 topology and a fortiori for the weak-$*$ topology of $BV(\Omega, \mathbb{R}^d)$. Using the extension theorems for BV functions, one can show (see [AFP00] Theorem 3.87, p. 180) that

$$|D\mathbf{u}|(\Omega) = |D\mathbf{u}|(\Omega_0) + \int_{\partial\Omega_0} |\mathbf{u}| \,\mathrm{d}\mathscr{H}^{d-1}$$

where $\mathscr{H}^{d-1}$ is the Hausdorff measure on $\mathbb{R}^d$ of dimension $d-1$[5]. Next, the following *Poincaré's inequality* holds true (see [BMM95] p. 209)

$$\|\mathbf{u}\|_1 = \|\mathbf{u}\|_{\Omega_0,1} \leq C\left[|D\mathbf{u}|(\Omega_0) + \int_{\partial\Omega_0} |\mathbf{u}| \,\mathrm{d}\mathscr{H}^{d-1}\right]$$

Thus, for every $\mathbf{u} \in U(\Omega, \mathbb{R}^d)$

$$\|\mathbf{u}\|_{BV} = \|\mathbf{u}\|_1 + |D\mathbf{u}|(\Omega) \leq (C+1)|D\mathbf{u}|(\Omega) \tag{4.18}$$

From (4.18), it follows that the functional

$$J : U(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}, \;\; J(\mathbf{u}) = \begin{cases} |D\mathbf{u}|(\Omega) & \text{if } \mathbf{u} \in U_{\Omega_0}(\Omega, \mathbb{R}^d) \\ +\infty & \text{otherwise} \end{cases}$$

is sequentially coercive for the weak-$*$ topology; moreover, it is also weak-$*$ lower semicontinuous.

The total variation regularization can be treated also in the space $L^p(\Omega, \mathbb{R}^d)$. Indeed, consider the same space $U_{\Omega_0}(\Omega, \mathbb{R}^d) \subseteq BV(\Omega, \mathbb{R}^d)$ defined before, and let

$$J : L^p(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}, \;\; J(\mathbf{u}) = \begin{cases} |D\mathbf{u}|(\Omega) & \text{if } \mathbf{u} \in U_{\Omega_0}(\Omega, \mathbb{R}^d) \\ +\infty & \text{otherwise} \end{cases}$$

which is actually a trivial extension of the previous functional. Using the compact embeddings $BV(\Omega, \mathbb{R}^d) \hookrightarrow L^p(\Omega, \mathbb{R}^d)$ for $p < d/(d-1)$, one can show that, if $1 \leq p < d/(d-1)$, the functional J is coercive in the (strong) topology of $L^p(\Omega, \mathbb{R}^d)$. Moreover it is also lower semicontinuous in the topology of $L^p(\Omega, \mathbb{R}^d)$.

This means that, using this regularizer, the inverse problem of image registration can be treated also in the whole space $U(\Omega, \mathbb{R}^d) = L^p(\Omega, \mathbb{R}^d)$ endowed with the strong topology.

[5] the function inside the boundary integral $\int_{\partial\Omega_0}$ is the euclidean norm of the trace of $\mathbf{u}_{|\Omega_0}$ on $\partial\Omega_0$.

Part II

Minimizing the Tikhonov Functional: Algorithms

Tikhonov regularization theory drives naturally to the study of optimization problem of following type

$$\min_{u \in U} f(u) + g(u) \tag{$\mathcal{P}$}$$

where the objective function is composed by the sum of a *data term* f (equals to $\phi(I(\cdot), I_0)$ in image registration) and a *penalty term* g (λJ in image registration).

For the cases treated in this thesis, the data term f is always smooth (taking I and ϕ regular enough) and in general non-convex. Therefore, if the penalty term g is also smooth — as it is the case for the four regularizers (4.12),(4.13),(4.14),(4.15) described in section 4.3.3 — one can pick out into a large collection of methods in the field of nonlinear smooth optimization (gradient descent, Newton-type methods, etc.) or also relies on classical variational techniques [Mod04, FH04], solving the corresponding *Euler-Lagrange equation*. However, total variation regularization is much more involved, because in that case the regularization term (4.17) is convex, but non-smooth.

In the second part of the thesis we deal with the problem of minimizing general Tikhonov functionals arising in *non-smooth variational regularization*. This means solving optimization problems of type ($\mathcal{P}$) where the data term f is always smooth and the penalty term g is *convex but possibly non-smooth*. As a result, ($\mathcal{P}$) is a non-smooth and non-convex optimization problem and calls for non-smooth optimization techniques. Among the different possibilities we choose *proximal type methods* [CW05, CP11], which use the *proximity operator* associated to the convex function g in the iterative process.

We analyze problem ($\mathcal{P}$) under different hypotheses for the function f and the function spaces involved. We shall consider three cases, treated respectively in the following three chapters:

1. f is smooth convex on a Hilbert space U;
2. f is smooth possibly non-convex on a Banach space U;
3. $f(u) = \|F(u) - v\|^2$ with $F : U \to V$ a nonlinear differentiable operator between Hilbert spaces U and V;

The first case relates in fact to linear inverse problems. Accelerated and inexact forward-backward splitting algorithms are studied.

The second case is the most general one. The basic forward-backward splitting algorithm is studied, following the same line as in [BK09].

The third case corresponds to a penalized least squares problem. A proximal Gauss-Newton procedure is studied. It covers only well-posed problems (*regular problems* in [BM04]), since the derivative $F'(x)$ is required to be injective and with close range.

Chapter 5

Accelerated Inexact Forward-backward Algorithms for Convex Problems

In this chapter we propose a convergence analysis of accelerated forward-backward splitting methods for minimizing composite functions, when the proximity operator is not available in closed form, and is thus computed up to a certain precision. We prove that the $1/k^2$ convergence rate for the function values can be achieved if the admissible errors are of a certain type and satisfy a sufficiently fast decay condition. Our analysis is based on the machinery of estimate sequences first introduced by Nesterov for the study of accelerated gradient descent algorithms. An experimental analysis aiming at validating the obtained rates is also presented.

The chapter has the follows layout. Sections 1 states the problem, describe the related literature and highlight the main contributions. In Section 2, we give a notion of admissible approximation of proximal points and discuss its applicability. Section 3 reviews the framework of estimate sequences of Nesterov and gives a general updating rule for recursively constructing estimate sequences for convex problems. In Section 4, we present the main results of the chapter: a new general accelerated scheme for forward-backward splitting algorithms and a convergence theorem under admissible approximations of proximal points. Section 5 discusses a backtracking procedure for the proposed algorithm. In Section 6, we rewrite the algorithm in equivalent forms, which encompass other popular algorithms. In Section 7, we discuss a relevant class of functions g for which most algorithms yield admissible approximations of the proximal points. Finally, Section 8 contains a numerical evaluation of the effect of errors in the computation of the proximal points on to the forward-backward algorithm (5.1).

5.1 Problem setting and main contribution

Let $\mathcal{H}$ be a Hilbert space and consider the optimization problem

$$\boxed{\inf_{x\in\mathcal{H}} f(x) + g(x) =: \varphi(x),} \tag{$\mathcal{P}$}$$

where

H1) $g : \mathcal{H} \to \overline{\mathbb{R}}$ is a proper, lower semicontinuous (l.s.c.) and convex function

H2) $f : \mathcal{H} \to \mathbb{R}$ is convex differentiable and ∇f is L-Lipschitz continuous on $\mathcal{H}$ with $L > 0$, namely
$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|, \quad \forall x, y \in \mathcal{H}.$$

We denote by φ_* the infimum of φ. We do not require in general the infimum to be attained, neither to be finite. It is well-known that problem ($\mathcal{P}$) covers a wide range of signal recovery problems (see [CW05] and references therein), including constrained and regularized least-squares problems [FNW07, Eic92, SP98, DTV07], (sparse) regularization problems in image processing, such as total variation denoising and deblurring (see e.g. [ROF92b, CL97, Cha04, BBFAC04]), as well as machine learning tasks involving nondifferentiable penalties (see e.g. [DS09, MRS$^+$10]).

The variety of applications to real life problems stimulated the search of simple first-order methods to solve ($\mathcal{P}$), which can be applied to large scale problems. In this area, a significant amount of research has been devoted to *forward–backward splitting methods*, that allow to decouple the contributions of the functions f and g in a gradient descent step determined by f and in a backward implicit step induced by g [CW05, LM79, Pas79]. These schemes are also known under the name of *proximal gradient methods* [Tse10], since the implicit step relies on the computation of the so called proximity operator, introduced by Moreau in [Mor62, Mor63, Mor65]. Though appealing for their simplicity, gradient-based methods often exhibit a slow speed of convergence. For this reason, resorting to the ideas contained in the work of Nesterov [Nes83], there has recently been an active interest in accelerations and modifications of the classical forward-backward splitting algorithm [Tse10, Nes09, BT09b, G$\ddot{9}$2]. We will study the following general accelerated scheme

$$\left| \begin{aligned} & x_{k+1} = \mathrm{prox}_{\lambda_k g}(y_k - \lambda_k \nabla f(y_k)), \\ & y_{k+1} = c_{1,k}x_{k+1} + c_{2,k}x_k + c_{3,k}y_k, \end{aligned} \right. \tag{5.1}$$

for suitably chosen constants $c_{i,k}$, ($i = 1, 2, 3, k \in \mathbb{N}$) and parameters $\lambda_k > 0$ — where $\mathrm{prox}_{\lambda_k g} : \mathcal{H} \to \mathcal{H}$ denotes the *proximity operator* associated to $\lambda_k g$. In particular, choosing $c_{3,k} = 0$, the procedure (5.1) has become very popular under the name of *Fast Iterative*

Shrinkage Thresholding Algorithm (FISTA) and the optimal (in the sense of [NY83]) $1/k^2$ convergence rate for the objective values $\varphi(x_k)-\varphi_*$ has been proved in [BT09b]. In the case of $c_{3,k} \neq 0$, the procedure (5.1) yields an infinite-memory algorithm [Tse10]. Furthermore, the effectiveness of such accelerations has been tested empirically on several key scientific problems (see e.g. [BBC09]).

Unfortunately, the proximity operator is in general not available in exact form. Just to mention some examples, this happens when applying proximal methods to image deblurring with total variation [SGG+09, Cha04, BBFAC04, BT09a, EZC10], or to structured sparsity regularization problems in machine learning and inverse problems [ZRY08, JOV09, Bac08, For10, MRS+10, MVVR10, RMSS+10, MGV+11, AMP+11]. In those cases, the proximity operator is usually computed using ad hoc algorithms, and therefore inexactly. Eventually the whole procedure for solving problem $(\mathcal{P})$ is constituted by two nested loops: an external one of type (5.1) and an internal one which serves to compute the proximal operator occurring in the first row of (5.1). Hence, the problem of studying the convergence of the algorithms under possible perturbations of proximal points arises.

On one hand, the problem of errors in the computation of proximal points for non accelerated schemes has been addressed, under various hypotheses, in several papers [Roc76b, CW05, SS00a, SS00b, SS00c, SS01, BS01, Zas10, ABI97]. On the other hand, the convergence of the accelerated forward-backward algorithms has been proved only when the proximity operator is evaluated exactly. To the best of our knowledge, accelerated schemes under inexact evaluation of the proximity operator have been devised only for the classical *proximal point algorithm*, which corresponds to the case $f = 0$ in (5.1), in the paper [Gü92] and very recently in [SV12a]. As regards the general case $f \neq 0$, the problem of errors in the computations has been raised in [BT09a] for the deblurring problem, where the authors propose a monotone version of the accelerated procedure and empirically observe better convergence properties, though no theoretical analysis of the computational errors is carried out.

Main contributions. From a theoretical point of view, the contribution of this chapter is threefold: first, we show that by considering a suitable notion of admissible approximation of the proximal point [ABI97, SV12a] — different from those in [Roc76b] and [Gü92] — it is possible to get quadratic convergence of the inexact version of the accelerated forward-backward scheme (5.1). In particular, we prove that the proposed algorithm shares the $1/k^2$ convergence rate if the computation of the proximity operator in (5.1) at the k-th step is performed up to a precision ε_k, with $\varepsilon_k = O(1/k^q)$ and $q > 3/2$. This assumption clearly implies summability of the errors, which is a common requirement in papers concerning convergence in the inexact case even if classical proximal point algorithm is considered (see e.g. [Roc76b]). We underline, however, that if solely convergence is needed, summability of the errors can be avoided, and requiring $\varepsilon_k = O(1/k^q)$, with $q > 1/2$ is enough. Secondly, we show that our concept of error is suitable for different algorithms tailored to compute the proximal point, as for instance the popular one in [Cha04]. This closes the issue of convergence regarding the whole two-loops algorithm mentioned above for many relevant cases in the applications.

The third contribution concerns the techniques we employ to obtain the result. In fact, the derivation of the algorithm relies on the machinery of the estimate sequences, as first proposed by Nesterov [Nes83]. Leveraging on the ideas developed in [SV12a], we propose a flexible method to build estimate sequences, that can be easily adapted to deal with inexact forward-backward algorithms. For instance, this allows to recast the well-known algorithm FISTA [BT09b] within this framework.

Finally, we performed a series of numerical experiments aiming at evaluating the behavior of the algorithm (5.1) under different levels of accuracy in the computation of the proximity operator.

5.2 A notion of inexact proximal point

The algorithms analyzed in this chapter are based on the computation of the proximity operator of a convex function, introduced by Moreau [Mor62, Mor63, Mor65], and then made popular in the optimization literature by Martinet [Mar70] and Rockafellar [Roc76b, Roc76a]. Let $\overline{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$ be the extended real line. For a proper, convex and l.s.c. function $g : \mathcal{H} \to \overline{\mathbb{R}}$, $\lambda > 0$ and $y \in \mathcal{H}$, *the proximal point of y with respect to λg* is defined by setting

$$\operatorname{prox}_{\lambda g}(y) := \operatorname{argmin}_{x\in\mathcal{H}} \left\{ g(x) + \frac{1}{2\lambda}\|x-y\|^2 \right\}$$

and the mapping $\operatorname{prox}_{\lambda g} : \mathcal{H} \to \mathcal{H}$ is called the *proximity operator of λg*. If we let $\Phi_\lambda(x) = g(x) + \frac{1}{2\lambda}\|x-y\|^2$, the first order optimality condition for a convex minimum problem yields

$$z = \operatorname{prox}_{\lambda g}(y) \iff 0 \in \partial\Phi_\lambda(z) \iff \frac{y-z}{\lambda} \in \partial g(z), \tag{5.2}$$

where ∂ denotes the subdifferential operator. The last equivalence also shows that $\operatorname{prox}_{\lambda g}(y) = (I + \lambda\partial g)^{-1}(y)$.

We already noted that, from a practical point of view, it is essential to replace the proximal point with an approximate version of it. We introduce here a concept of approximation of the proximal point that has been used successfully in [Lem92, CL93, Com97, BIS97, ABI97, SV12a] and it is based on the notion of ε-subdifferential.

We recall that, for $\varepsilon \geq 0$, the *ε-subdifferential of g at the point $z \in \operatorname{dom} g$* is the set

$$\partial_\varepsilon g(z) = \{\xi \in \mathcal{H} \,:\, g(x) \geq g(z) + \langle x - z, \xi\rangle - \varepsilon, \forall x \in \mathcal{H}\}. \tag{5.3}$$

The notion of approximation is based on the relaxation of condition (5.2) characterizing the proximal point and up to our knowledge first considered in [Lem92, CL93].

Definition 5.2.1. *Let $\varepsilon \geq 0$. We say that $z \in \mathcal{H}$ is an* approximation of $\operatorname{prox}_{\lambda g}(y)$ with ε-precision *and we write $z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y)$ if and only if*

$$\frac{y-z}{\lambda} \in \partial_{\frac{\varepsilon^2}{2\lambda}} g(z). \tag{5.4}$$

Note that if $z \approx_\varepsilon \operatorname{prox}_{\lambda g}(y)$, then necessarily $z \in \operatorname{dom} g$. Therefore, the allowed approximations are always feasible. The condition (5.4) can be equivalently written as

$$y \in z + \lambda \partial_{\frac{\varepsilon^2}{2\lambda}} g(z) \iff z \in (I + \lambda \partial_{\frac{\varepsilon^2}{2\lambda}} g)^{-1}(y).$$

Recalling that the proximity operator of λg is defined as $(I + \lambda \partial g)^{-1}$, the admissible approximations can be seen as a sort of "ε-enlargement" of the proximity operator. A similar concept of error has been very recently proposed for non accelerated proximal algorithms in the preprint [MS10].

Other notions of approximations of the proximity operator have been considered in the literature. One of the first is due to Rockafellar in [Roc76b], and treated by Güler too in [Gÿ92], where the following definition is employed

$$d(0, \partial \Phi_\lambda(z)) \leq \frac{\varepsilon}{\lambda}. \tag{5.5}$$

For other notions of approximations in the context of proximal point algorithms see also [CW05, BIS97, SS00a, SS00b, SS00c, SS01, BS01, Zas10]. The paper [SV12a] presents a general study and comparison of different types of error, also including the one considered here. In Section 5.7, we will show that a whole class of problems can be treated with the error criterion (5.4).

Example 5.2.2. *To clarify what kind of approximations are covered by our definition, we describe the case where g is the indicator function of a closed and convex set C, and the proximal operator is consequently the projection onto C, denoted by P_C. Given $y \in \mathcal{H}$, it holds*

$$z \approxeq_\varepsilon P_C(y) \iff z \in C \text{ and } \langle x - z, y - z\rangle \leq \frac{\varepsilon^2}{2} \quad \forall x \in C. \tag{5.6}$$

Recalling that the projection $P_C(y)$ of a point y is the unique point $z \in C$ which satisfies $\langle x - z, y - z\rangle \leq 0$ for all $x \in C$, approximations of this type are therefore the points enjoying a relaxed formulation of this property. From a geometric point of view, the characterization of projection ensures that the convex set C is entirely contained in the half-space determined

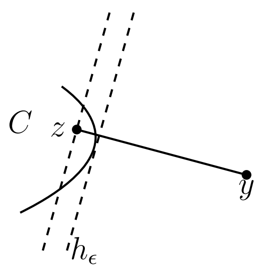

Figure 5.1: Admissible approximation of $P_C(y)$

by the tangent hyperplane at the point $P_C(y)$*, namely* $C \subseteq \{x \in X : \langle x - P_C(y), y - P_C(y)\rangle \leq 0\}$*. Figure 5.2.2 depicts an admissible approximation of* $P_C(y)$*. To check that* z *satisfies condition* (5.6)*, it is enough to verify that* C *is entirely contained in the negative half-space determined by the (affine) hyperplane of equation*

$$h_\varepsilon : \quad \langle x - z, \frac{y-z}{\|y-z\|}\rangle = \frac{\varepsilon^2}{2\|y-z\|}.$$

which is normal to $y - z$ *and at distance* $\varepsilon^2/(2\|y-z\|)$ *from* z*.*

We remark that if C *is bounded, an approximation in the sense of Rockafellar* (5.5) *can be regarded as an approximation of our type. More precisely:*

$$z \approxeq_\varepsilon P_C(y) \text{ in the sense of } (5.5) \implies z \approxeq_\eta P_C(y) \text{ in the sense of } (5.4)$$

with $\eta = \sqrt{2\mathrm{diam}(C)\varepsilon}$*.*

In general, verifying whether a point is an admissible approximation of the proximal point may be complicated. The next proposition shows that there exists a class of functions g for which approximations in the sense of Definition 5.2.1 can be easily obtained. For $t \in \mathcal{H}$ and $\delta > 0$, we denote by $B_\delta(t)$ the closed ball of centre t and radius δ in $\mathcal{H}$.

Proposition 5.2.3. *Let* $g : \mathcal{H} \to \overline{\mathbb{R}}$ *be a proper, convex and l.s.c. function. Let* $y \in \mathcal{H}$ *and* $t = \mathrm{prox}_{\lambda g}(y)$*. Suppose* $\mathrm{dom}\, g$ *be bounded (in norm) and* g *be locally Lipschitz continuous in* t*, meaning that there exists* $\delta > 0$ *such that* g *is* M*-Lipschitz continuous on* $B_\delta(t) \cap \mathrm{dom}\, g$ *for some* $M \geq 0$*. For any* $\varepsilon > 0$*, if* $0 < \sigma \leq \delta$ *with* $\sigma(\mathrm{diam}(\mathrm{dom}\, g) + \|y-t\| + \lambda M) \leq \varepsilon^2/2$*, then*

$$\|z - t\| \leq \sigma \implies z \approxeq_\varepsilon \mathrm{prox}_{\lambda g}(y)$$

for every $z \in \mathrm{dom}\, g$*.*

Proof. Being $t = \mathrm{prox}_{\lambda g}(y)$, it holds $(y-t)/\lambda \in \partial g(t)$ or, equivalently

$$t \in \mathrm{dom}\, g \quad \text{and} \quad g(x) - g(t) \geq \langle x - t, (y-t)/\lambda\rangle \;\forall\, x \in \mathcal{H}$$

Let $z \in \text{dom } g$ with $\|z - t\| \leq \sigma$ and σ chosen as in the statement above. We have to prove that $(y - z)/\lambda \in \partial_{\frac{\varepsilon^2}{2\lambda}} g(z)$ or, equivalently

$$g(x) - g(z) \geq \langle x - z, \frac{y - z}{\lambda} \rangle - \frac{\varepsilon^2}{2\lambda} \quad \forall x \in \text{dom } g$$

Indeed, for every $x \in \text{dom } g$, we have

$$\begin{aligned}
g(x) - g(z) &= g(x) - g(t) + g(t) - g(z) \\
&\geq \langle x - t, (y - t)/\lambda \rangle + g(t) - g(z) \\
&= \langle x - z, (y - z)/\lambda \rangle + \langle x - z, (z - t)/\lambda \rangle + \langle z - t, (y - t)/\lambda \rangle + g(t) - g(z) \\
&\geq \langle x - z, (y - z)/\lambda \rangle - \|x - z\| \|z - t\|/\lambda - \|z - t\| \|y - t\|/\lambda - M\|t - z\| \\
&\geq \langle x - z, (y - z)/\lambda \rangle - \sigma(\text{diam}(\text{dom } g)/\lambda + \|y - t\|/\lambda + M) \\
&\geq \langle x - z, (y - z)/\lambda \rangle - \varepsilon^2/(2\lambda)
\end{aligned}$$

We emphasize that Proposition 5.2.3 implies that

$$\forall \varepsilon > 0 \, \exists \sigma > 0 \text{ such that } \forall z \in \text{dom}\, g : \|z - t\| \leq \sigma \implies z \approxeq_\varepsilon \text{prox}_{\lambda g}(y) \tag{5.7}$$

This statement allows to conclude that if some algorithm produces a sequence $(z_n)_{n \in \mathbb{N}}$ with $z_n \in \text{dom } g$ and $\|z_n - \text{prox}_{\lambda g}(y)\| \to 0$, then whatever $\varepsilon > 0$ we choose, we can find $n \in \mathbb{N}$ (large enough) such that $z_n \approxeq_\varepsilon \text{prox}_{\lambda g}(y)$.

Remark 5.2.4. *We point out that the hypothesis* dom g *be bounded in Proposition 5.2.3 cannot be dropped. In fact, we will show a simple example of a function g which is Lipschitz continuous in its domain, with unbounded domain and which does not meet the statement* (5.7). *To this purpose, let $g = \delta_K$, where $K = [0, +\infty[\subseteq \mathbb{R}$. One can easily show that for each $z \in K$ and $\varepsilon > 0$, it holds $\partial_{\frac{\varepsilon^2}{2}} g(z) \subseteq \,]-\infty, 0]$, therefore, given $y \in \mathbb{R}$,*

$$\{z \in K \mid z \approxeq_\varepsilon \text{prox}_g(y)\} \subseteq [y, +\infty[\,.$$

Thus, if (5.7) *held true for g, then $B_\sigma(t) \cap K \subseteq [y, +\infty[$ for some $\sigma > 0$. But for $y \in K$, $y > 0$, one has $t = \text{prox}_g(y) = y$ and hence $B_\sigma(t) \cap K \not\subseteq [y, +\infty[$ which leads to a contradiction.*

Another possibility for getting approximations in the sense of Definition 5.2.1 is to use the duality technique, an approach that is quite common in signal recovery and image processing applications [CW05, Cha04, CDV10]. The starting point is the *Moreau decomposition formula* [Mor65, CW05]

$$\text{prox}_{\lambda g}(y) = y - \lambda \, \text{prox}_{g^*/\lambda}(y/\lambda), \tag{5.8}$$

where $g^* : \mathcal{H} \to \overline{\mathbb{R}}$ is the (Fenchel) *conjugate functional* of g defined as $g^*(y) = \sup_{x\in\mathcal{H}}(\langle x, y\rangle - g(x))$.

In the cases where the proximity operator of g^* is easy to compute, formula (5.8) provides a convenient method to find the proximity operator of λg. A remarkable property of inexact proximal points based on the criterion (5.4) is that, in a sense, the Moreau decomposition still holds. In fact, if $y, z \in \mathcal{H}$ and $\varepsilon, \lambda > 0$, then letting $\eta = \varepsilon/\lambda$, it is

$$z \approxeq_\eta \operatorname{prox}_{g^*/\lambda}(y/\lambda) \iff y - \lambda z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y)\ . \tag{5.9}$$

This arises immediately from Definition 5.2.1 and the following equivalence

$$y - \lambda z \in \partial_{\frac{\eta^2\lambda}{2}} g^*(z) \iff z \in \partial_{\frac{\varepsilon^2}{2\lambda}} g(y - \lambda z)$$

(see Theorem 2.4.4, item (iv), in [Zăl02].) Combining (5.9) with Proposition 5.2.3, we are able to establish a link between the approximations of proximal points with respect to g^* and g.

Corollay 5.2.5. *Let $g : \mathcal{H} \to \overline{\mathbb{R}}$ be proper, convex and l.s.c., $y \in \mathcal{H}$ and $t = \operatorname{prox}_{g^*/\lambda}(y/\lambda)$. Suppose* dom g^* *be bounded (in norm) and g^* be locally Lipschitz continuous in t, meaning that there exists $\delta > 0$ such that g^* is M^*-Lipschitz continuous on $B_\delta(t) \cap \operatorname{dom} g^*$ for some $M^* \geq 0$. For any $\varepsilon > 0$, if $0 < \sigma \leq \delta$ with $\sigma(\lambda \operatorname{diam}(\operatorname{dom} g^*) + \|y - \lambda t\| + M^*) \leq \varepsilon^2/(2\lambda)$, then*

$$\|z - t\| \leq \sigma \implies y - \lambda z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y)$$

for every $z \in \operatorname{dom} g^*$.

Proof. The condition on σ, given in the statement, is equivalent to

$$\sigma(\operatorname{diam}(\operatorname{dom} g^*) + \|y/\lambda - t\| + M^*/\lambda) \leq \eta^2/2$$

with $\eta = \varepsilon/\lambda$. Therefore we can apply Proposition 5.2.3 to the function g^* and the point $t = \operatorname{prox}_{g^*/\lambda}(y/\lambda)$, obtaining that for $z \in \operatorname{dom} g^*$ with $\|z - t\| \leq \sigma$ it holds $z \approxeq_\eta \operatorname{prox}_{g^*/\lambda}(y/\lambda)$. Then, the inexact Moreau decomposition formula (5.9) gives $y - \lambda z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y)$ ☐

Remark 5.2.6. *The hypothesis* dom g^* *be bounded in Corollary 5.2.5 implies that g is Lipschitz continuous on* dom g*. Indeed, for a proper, convex function $g : \mathcal{H} \to \overline{\mathbb{R}}$, we have*

$$\operatorname{dom} g^* = \bigcup_{x\in\mathcal{H}} \partial_\varepsilon g(x)$$

for every $\varepsilon > 0$. Therefore, if dom g^* *is bounded in norm, say by $M \geq 0$, it is easy to see that*

$$|g(x_1) - g(x_2)| \leq M\|x_1 - x_2\| + \varepsilon$$

for every $x_1, x_2 \in \operatorname{dom} g$ and $\varepsilon > 0$. Since ε is arbitrary, this shows that g is in fact M-Lipschitz on the whole dom g*.*

In case g is positively homogeneous, namely $g(\alpha x) = \alpha g(x)$ for $\alpha \geq 0$, λg is positively homogeneous too and $(\lambda g)^* = \delta_{\partial(\lambda g)(0)} = \delta_{\lambda K}$ with $K := \partial g(0)$. The inexact Moreau decomposition (5.9) applied to λg gives

$$z \approxeq_\varepsilon P_{\lambda K}(y) \iff y - z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y) \tag{5.10}$$

meaning that we can approximate the proximity operator of λg by means of an approximation of the projection onto the closed and convex set λK. Thus, we can specialize Corollary 5.2.5, obtaining the following result.

Corollay 5.2.7. *Suppose $g : \mathcal{H} \to \overline{\mathbb{R}}$ be proper, convex, l.s.c. and positively homogeneous and $K = \partial g(0)$ be bounded. If $\sigma > 0$ and $\sigma(\lambda \operatorname{diam}(K) + \|y - P_{\lambda K}(y)\|) \leq \varepsilon^2/2$, then*

$$\|z - P_{\lambda K}(y)\| \leq \sigma \implies y - z \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y)$$

for $z \in \lambda K$.

5.3 Nesterov's estimate sequences

In [Nes04], Nesterov illustrates a flexible mechanism to produce minimizing sequences for an optimization problem. The idea is to generate recursively a sequence of simple functions that approximate φ in the sense introduced below. In this section we briefly describe this method and review the general results obtained in [SV12a] for constructing quadratic estimate sequences when φ is convex. We do not provide proofs, referring to the mentioned works for details.

5.3.1 General framework

We start by providing the definition and motivation of estimate sequences.

Definition 5.3.1. *A pair of sequences $(\phi_k)_{k\in\mathbb{N}}$, $\phi_k : \mathcal{H} \to \mathbb{R}$ and $(\beta_k)_{k\in\mathbb{N}}$, $\beta_k \geq 0$ is called an* estimate sequence *of a proper function $\varphi : \mathcal{H} \to \overline{\mathbb{R}}$ iff*

$$\forall x \in \mathcal{H}, \forall k \in \mathbb{N} : \ \phi_k(x) - \varphi(x) \leq \beta_k(\phi_0(x) - \varphi(x)) \quad \textit{and} \quad \beta_k \to 0. \tag{5.11}$$

The next statement represents the main result about estimate sequences and explains how to use them to build minimizing sequences and get corresponding convergence rates.

Theorem 5.3.2. *Let $((\phi_k)_{k\in\mathbb{N}}, (\beta_k)_{k\in\mathbb{N}})$ be an estimate sequence of φ and denote by ϕ_{k*} the infimum of ϕ_k. If, for some sequences $(x_k)_{k\in\mathbb{N}}$, $x_k \in \mathcal{H}$ and $(\delta_k)_{k\in\mathbb{N}}, \delta_k \geq 0$, we have*

$$\varphi(x_k) \leq \phi_{k*} + \delta_k, \tag{5.12}$$

then for any $x \in \operatorname{dom}\varphi$

$$\varphi(x_k) \leq \beta_k(\phi_0(x) - \varphi(x)) + \delta_k + \varphi(x). \tag{5.13}$$

Thus, if $\delta_k \to 0$ (being also $\beta_k \to 0$), $(x_k)_{k\in\mathbb{N}}$ is a minimizing sequence for φ, that is

$$\lim_{k\to\infty} \varphi(x_k) = \varphi_*.$$

If in addition the infimum φ_* is attained at some point $x_* \in \mathcal{H}$, then the following rate of convergence holds true

$$\varphi(x_k) - \varphi_* \leq \beta_k(\phi_0(x_*) - \varphi_*) + \delta_k.$$

We point out that the previous theorem provides convergence of the sequence $(\varphi(x_k))_{k\in\mathbb{N}}$ to the infimum of φ without assuming any existence of a minimizer for φ, neither the boundedness from below. However, the hypothesis of attainability of the infimum is required if an estimate of the convergence rate is needed.

Remark 5.3.3. *A common way to define estimate sequences is via recursive inequalities. More precisely one can show that, if $(\phi_k)_{k\in\mathbb{N}}$ satisfies*

$$\boxed{\phi_{k+1}(x) - \varphi(x) \leq (1-\alpha_k)(\phi_k(x) - \varphi(x)),} \tag{5.14}$$

with $0 \leq \alpha_k < 1$, then $((\phi_k)_{k\in\mathbb{N}}, (\beta_k)_{k\in\mathbb{N}})$ is an estimate sequence of φ with

$$\beta_k = \prod_{i=0}^{k-1}(1-\alpha_i) \tag{5.15}$$

provided that $\sum_{i=0}^{+\infty} \alpha_i = +\infty$. See [SV12a] for details.

5.3.2 Construction of an estimate sequence

In this section, we review a general procedure, introduced in [SV12a], for generating an estimate sequence of a proper, l.s.c. and convex function $\varphi : \mathcal{H} \to \overline{\mathbb{R}}$. We recall that an estimate sequence of φ is a sequence of (simple) functions ϕ_k and a numerical sequence β_k. Furthermore, in order to apply Theorem 5.3.2, we also need a third sequence of points x_k.

First of all, we deal with the generation of the sequence of functions $(\phi_k)_{k\in\mathbb{N}}$. Denote by $\mathcal{F}(\mathcal{H},\mathbb{R})$ the space of functions from $\mathcal{H}$ to $\mathbb{R}$. Given φ, we define an updating rule for functions $\phi \in \mathcal{F}(\mathcal{H},\mathbb{R})$, depending on the choice of four parameters $(z,\eta,\xi,\alpha) \in \operatorname{dom}\varphi \times \mathbb{R}_+ \times \mathcal{H} \times [0,1)$, as

$$U(z,\eta,\xi,\alpha) : \mathcal{F}(\mathcal{H},\mathbb{R}) \to \mathcal{F}(\mathcal{H},\mathbb{R})$$
$$U(z,\eta,\xi,\alpha)(\phi)(x) = (1-\alpha)\phi(x) + \alpha(\varphi(z) + \langle x - z, \xi\rangle - \eta)\ .$$

Hereafter, for convenience, we will often denote the update of ϕ simply by $\hat{\phi}$, that is

$$\hat{\phi} := U(z,\eta,\xi,\alpha)(\phi)$$

hiding the dependence on the parameters. The same hat notation will also be used for other quantities: in all cases it will stand for an update of the corresponding variable. With a proper choice of parameters, the iteration of the operator $U(z,\eta,\xi,\alpha)$ will allow us to generate estimate sequences for φ. Indeed, it is easy to see that if $\xi \in \partial_\eta\varphi(z)$, then the following inequalities hold

$$\begin{aligned}\hat{\phi}(x) - \varphi(x) &= (1-\alpha)(\phi(x) - \varphi(x)) + \alpha(\varphi(z) + \langle x - z, \xi\rangle - \eta - \varphi(x)) \\ &\leq (1-\alpha)(\phi(x) - \varphi(x))\ ,\end{aligned}$$

obtaining the recursive inequality of estimate sequences (5.14).

Summarizing, given $((z_k,\eta_k,\xi_k,\alpha_k))_{k\in\mathbb{N}}$, $(z_k,\eta_k,\xi_k,\alpha_k) \in \operatorname{dom}\varphi \times \mathbb{R}_+ \times \mathcal{H} \times [0,1)$ with $\xi_{k+1} \in \partial_{\eta_k}\varphi(z_{k+1})$, $\sum_{k\in\mathbb{N}}\alpha_k = +\infty$, and an arbitrary function $\phi : \mathcal{H} \to \mathbb{R}$, the sequence defined by setting

$$\begin{cases}\phi_0 = \phi \\ \phi_{k+1} = U(z_{k+1},\eta_k,\xi_{k+1},\alpha_k)\phi_k\ ,\end{cases} \tag{5.16}$$

satisfies the assumptions of Remark 5.3.3, and therefore the pair $((\phi_k)_{k\in\mathbb{N}}, (\beta_k)_{k\in\mathbb{N}})$, with β_k given by (5.15), is an estimate sequence of φ.

We now describe in detail the update when the starting ϕ is a quadratic function written in canonical form, namely

$$\phi(x) = \phi_* + \frac{A}{2}\|x-\nu\|^2, \quad \text{with } \phi_* \in \mathbb{R},\ A > 0,\ \nu \in \mathcal{H},$$

where clearly $\phi_* = \inf\phi$. Then, for an arbitrary choice of the parameters, the update $\hat{\phi}$ of ϕ introduced above is still a quadratic function, that can be written in canonical form as

$$\hat{\phi}(x) = \hat{\phi}_* + \frac{\hat{A}}{2}\|x-\hat{\nu}\|^2$$

with

$$
\begin{cases}
\hat{\phi}_* = (1-\alpha)\phi_* + \alpha\varphi(z) + \alpha\langle \nu - z, \xi\rangle - \dfrac{\alpha^2}{2(1-\alpha)A}\|\xi^2\| - \alpha\eta \\
\hat{A} = (1-\alpha)A \\
\hat{\nu} = \nu - \dfrac{\alpha}{(1-\alpha)A}\xi.
\end{cases}
\tag{5.17}
$$

This means that the subset of quadratic functions is closed with respect to the action of the operator $U(z, \eta, \xi, \alpha)$, which therefore induces a transformation on the relevant parameters defining their canonical form, depending of course on (z, η, ξ, α).

Next, we treat the problem of generating a sequence $(x_k)_{k\in\mathbb{N}}$ satisfying inequality (5.12). We first recall two lemmas, whose proofs are provided in [SV12a], that will be crucial in the whole subsequent analysis.

Lemma 5.3.4. *Let $x, \nu \in \mathcal{H}$, $A > 0$ and $\phi = \phi_* + A/2\|\cdot - \nu\|^2$ be such that $\varphi(x) \le \phi_* + \delta$ for some $\delta \ge 0$. If $z, \xi \in \mathcal{H}$, $\eta \ge 0$ are given with $\xi \in \partial_\eta\varphi(z)$, defining $\hat{\phi} = U(z, \eta, \xi, \alpha)(\phi)$, with $\alpha \in [0, 1)$ and setting $y = (1-\alpha)x + \alpha\nu$, we get*

$$
(1-\alpha)\delta + \eta + \hat{\phi}_* \ge \varphi(z) + \frac{\lambda}{2}\left(2 - \frac{\alpha^2}{(1-\alpha)A\lambda}\right)\|\xi\|^2 + \langle y - (\lambda\xi + z), \xi\rangle \tag{5.18}
$$

for every $\lambda > 0$.

Given $x \in \mathcal{H}$ satisfying $\varphi(x) \le \phi_* + \delta$ for some $\delta \ge 0$, the inequality stated in the previous lemma suggests different possibilities to choose an update of x, say $\hat{x}$, which satisfies the analogous condition $\varphi(\hat{x}) \le \hat{\phi}_* + \hat{\delta}$ for a suitable choice of $\hat{\delta}$. In particular, we want $\hat{x}$ to make the scalar product in the right side of the inequality (5.18) equal to zero and α to satisfy $2 - \alpha^2/((1-\alpha)A\lambda) \ge 0$.

Recalling that $\beta_k := \prod_{i=0}^{k-1}(1-\alpha_i)$, the next lemma shows the connection between the choice of α_k and the asymptotic behavior of β_k, which should tend to zero. The relevance of these two lemmas will be further clarified in the following section.

Lemma 5.3.5. *Given the numerical sequence $(\lambda_k)_{k\in\mathbb{N}}$, $\lambda_k > 0$ and $A > 0$, $a, b > 0$, $a \le b$, define $(A_k)_{k\in\mathbb{N}}$ and $(\alpha_k)_{k\in\mathbb{N}}$ such that $A_0 = A$ and for $k \in \mathbb{N}$*

$$
\begin{aligned}
&\alpha_k \in [0,1), \ \text{with } a \le \frac{\alpha_k^2}{(1-\alpha_k)A_k\lambda_k} \le b \\
&A_{k+1} = (1-\alpha_k)A_k.
\end{aligned}
\tag{5.19}
$$

Then $\beta_k := \prod_{i=0}^{k-1}(1-\alpha_i)$ satisfies

$$
\frac{1}{(1 + \sqrt{bA}\sum_{j=0}^{k-1}\sqrt{\lambda_j})^2} \le \beta_k \le \frac{1}{(1 + (\sqrt{aA}/2)\sum_{j=0}^{k-1}\sqrt{\lambda_j})^2} \tag{5.20}
$$

In particular, $\beta_k \sim 1/(\sum_{j=0}^{k-1}\sqrt{\lambda_j})^2$ *and* $\beta_k \to 0$ *if and only if* $\sum_{k=0}^{\infty}\sqrt{\lambda_k} = +\infty$. *Moreover, if* $\lambda_k \geq \lambda > 0$ *for every* $k \in \mathbb{N}$, *then* $\beta_k = O(1/k^2)$.

Remark 5.3.6. *We note that the function*

$$\alpha \in [0,1[\to \frac{\alpha^2}{(1-\alpha)A_k\lambda_k} \in \mathbb{R}_+$$

is strictly increasing, it tends towards 0 *for* $\alpha \to 0$ *and towards* $+\infty$ *for* $\alpha \to 1$. *Therefore the inequality* (5.19) *is always solvable.*

5.4 Derivation of the general algorithm

In this section, we show how the mechanism of estimate sequences can be used to generate an inexact version of accelerated forward-backward algorithms. A general theorem of convergence will also be provided.

We shall assume both the hypotheses H1) and H2), given in the introduction, be satisfied. The following lemma generalizes a well-known result [BT09b] and will enable us to build an appropriate estimate sequence.

Lemma 5.4.1. *For any* $x, y \in \mathcal{H}$, $z \in \operatorname{dom} g$, $\varepsilon \geq 0$ *and* $\zeta \in \partial_\varepsilon g(z)$ *it holds*

$$\varphi(x) \geq \varphi(z) + \langle x - z, \nabla f(y) + \zeta\rangle - \frac{L}{2}\|z - y\|^2 - \varepsilon. \tag{5.21}$$

In other words,

$$\nabla f(y) + \zeta \in \partial_\eta \varphi(z), \quad \text{with } \eta = \frac{L}{2}\|z-y\|^2 + \varepsilon \tag{5.22}$$

Proof. Fix $y, z \in \mathcal{H}$, since ∇f is L-Lipschitz continuous we get (see [Pol87])

$$f(y) \geq f(z) - \langle z - y, \nabla f(y)\rangle - \frac{L}{2}\|z-y\|^2 \,. \tag{5.23}$$

On the other hand, being f convex, we have $f(x) \geq f(y) + \langle x - y, \nabla f(y)\rangle$, which combined with (5.23) gives

$$f(x) \geq f(z) + \langle x - z, \nabla f(y)\rangle - \frac{L}{2}\|z-y\|^2 \,. \tag{5.24}$$

Since g is convex and $\zeta \in \partial_\varepsilon g(z)$, we have

$$g(x) \geq g(z) + \langle x - z, \zeta\rangle - \varepsilon \,. \tag{5.25}$$

Summing (5.24) and (5.25) we get

$$\varphi(x) \geq \varphi(z) + \langle x - z, \nabla f(y) + \zeta \rangle - \frac{L}{2}\|z - y\|^2 - \varepsilon \,. \tag{5.26}$$

Combining the previous Lemma 5.4.1 with Lemma 5.3.4, we derive the following result.

Lemma 5.4.2. *Let $x, \nu \in \mathcal{H}$, $A > 0$ and $\phi = \phi_* + A/2\|\cdot - \nu\|^2$ be such that $\varphi(x) \leq \phi_* + \delta$ for some $\delta \geq 0$. If $z, \zeta \in \mathcal{H}$, $\varepsilon \geq 0, \lambda > 0$ are given with $\zeta \in \partial_{\varepsilon^2/(2\lambda)} g(z)$, defining $\hat{\phi} = U(z, \eta, \nabla f(y) + \zeta, \alpha)\phi$, with $\alpha \in [0, 1)$ and setting $y = (1-\alpha)x + \alpha\nu$ and $\eta = L/2\|y - z\|^2 + \varepsilon^2/(2\lambda)$, we get*

$$\begin{aligned}(1-\alpha)\delta + \frac{\varepsilon^2}{2\lambda} + \hat{\phi}_* \geq \varphi(z) &+ \frac{\lambda}{2}\left(2 - \frac{\alpha^2}{(1-\alpha)A\lambda}\right)\|\nabla f(y) + \zeta\|^2 \\ &+ \langle y - (\lambda(\nabla f(y) + \zeta) + z), \nabla f(y) + \zeta \rangle - \frac{L}{2}\|y - z\|^2\end{aligned}$$

The next result shows how to choose ζ in order to derive an iterative procedure.

Theorem 5.4.3. *Fix $\lambda > 0$, $\varepsilon > 0$. Let $x, \nu \in \mathcal{H}$, $A > 0$ and $\phi = \phi_* + A/2\|\cdot - \nu\|^2$ be such that $\varphi(x) \leq \phi_* + \delta$ for some $\delta \geq 0$. If $\alpha^2/((1-\alpha)A\lambda) \leq 2 - \lambda L$, choosing*

$$\begin{aligned}
&y = (1-\alpha)x + \alpha\nu \\
&\hat{x} \approxeq_\varepsilon \operatorname{prox}_{\lambda g}(y - \lambda \nabla f(y)) \\
&\zeta = \frac{y - \hat{x}}{\lambda} - \nabla f(y) \quad (\in \partial_{\frac{\varepsilon^2}{2\lambda}} g(\hat{x})) \\
&\hat{\phi} = U(\hat{x}, \eta, \nabla f(y) + \zeta, \alpha)\phi, \quad \textit{with } \eta = \frac{L}{2}\|y - \hat{x}\|^2 + \frac{\varepsilon^2}{2\lambda} \\
&\hat{A} = (1-\alpha)A \\
&\hat{\nu} = \nu - \frac{\alpha}{\hat{A}}(\nabla f(y) + \zeta) \\
&\hat{\delta} = (1-\alpha)\delta + \frac{\varepsilon^2}{2\lambda},
\end{aligned}$$

we have $\hat{\delta} + \hat{\phi}_* \geq \varphi(\hat{x}) + \dfrac{c}{2\lambda}\|y - \hat{x}\|^2 \geq \varphi(\hat{x})$ with $c = 2 - \lambda L - \alpha^2/(\hat{A}\lambda) \geq 0$.

Proof. Applying Lemma 5.4.2, with $z = \hat{x}$ and ζ defined above, taking into account that $y - (\lambda(\nabla f(y) + \zeta) + \hat{x}) = 0$, we get

$$(1-\alpha)\delta + \frac{\varepsilon^2}{2\lambda} + \hat{\phi}_* \geq \varphi(\hat{x}) + \frac{1}{2\lambda}\left(2 - \lambda L - \frac{\alpha^2}{(1-\alpha)A\lambda}\right)\|y - \hat{x}\|^2.$$

If we choose λ and α such that $\alpha^2/(1-\alpha)A\lambda \leq 2-\lambda L$ we immediately obtain the statement of the theorem. $\square$

We are now ready to define a general accelerated and inexact forward-backward splitting algorithm (aiFOBOS) and to prove its convergence rate. (For the genesis of the name FOBOS see [DS09]). For fixed numbers $A > 0, a \in \ ]0,2]$ and a sequence of errors $(\varepsilon_k)_{k\in\mathbb{N}}$ with $\varepsilon_k \geq 0$, we set $A_0 = A, \delta_0 = 0$ and $x_0 = \nu_0 \in \operatorname{dom}\varphi$ and for every $k \in \mathbb{N}$ we recursively define

$$
\left|
\begin{aligned}
\lambda_k &\in \ ]0,(2-a)/L] \\
\alpha_k &\in [0,1) \quad \text{such that} \quad a \leq \frac{\alpha_k^2}{(1-\alpha_k)A_k\lambda_k} \leq 2-\lambda_k L \\
y_k &= (1-\alpha_k)x_k + \alpha_k\nu_k \\
x_{k+1} &\approxeq_{\varepsilon_k} \operatorname{prox}_{\lambda_k g}(y_k - \lambda_k \nabla f(y_k)) \\
A_{k+1} &= (1-\alpha_k)A_k \\
\nu_{k+1} &= \nu_k - \frac{\alpha_k}{(1-\alpha_k)A_k\lambda_k}(y_k - x_{k+1}) \\
\delta_{k+1} &= (1-\alpha_k)\delta_k + \frac{\varepsilon_k^2}{2\lambda_k}.
\end{aligned}
\right.
\tag{aiFOBOS}
$$

Then, by setting $\xi_{k+1} = (y_k - x_{k+1})/\lambda_k$, we get two sequences $(x_k)_{k\in\mathbb{N}}$ and $(\xi_k)_{k\in\mathbb{N}}$ such that $\xi_{k+1} \in \partial_{\eta_k}\varphi(x_{k+1})$, where $\eta_k = \frac{L}{2}\|y_k - x_{k+1}\|^2 + \varepsilon_k^2/(2\lambda_k)$. Therefore, the sequence of functions $(\phi_k)_{k\in\mathbb{N}}$ defined as $\phi_{k+1} = U(x_{k+1}, \eta_k, \xi_{k+1}, \alpha_k)\phi_k$ is an estimate sequence of φ provided that $\beta_k = \prod_{i=0}^{k-1}(1-\alpha_i) \to 0$. The last condition holds true due to Lemma 5.3.5 with $b = 2$ if $\lambda_k \geq \lambda > 0$ — actually in this case $\beta_k \sim 1/k^2$.

Moreover, starting from $\phi_0 = \varphi(x_0) + A_0/2\|\cdot - \nu_0\|^2$, we have $\delta_0 + \phi_0^* \geq \varphi(x_0)$ and, by induction, applying Theorem 5.4.3, also $\delta_k + \phi_k^* \geq \varphi(x_k)$ for every $k \geq 1$. If $\delta_k \to 0$, the sequence $(x_k)_{k\in\mathbb{N}}$ is a minimizing sequence for φ. The previous bounds obtained on β_k allow us to impose explicit conditions on the error sequence ε_k in order to get a convergent forward-backward splitting algorithm.

Remark 5.4.4. *To be more precise, Theorem 5.4.3 implies*

$$\delta_{k+1} + \phi_{k+1}^* \geq \varphi(x_{k+1}) + \frac{c_k}{2\lambda_k}\|y_k - x_{k+1}\|^2 \quad \textit{with } c_k = 2 - \lambda_k L - \frac{\alpha_k^2}{(1-\alpha_k)A_k\lambda_k}$$

From this inequality, along the lines of the proof of Theorem 1 in [SV12a], it follows that

$$\frac{c_{k-1}}{2\lambda_{k-1}}\|y_{k-1} - x_k\|^2 + \varphi(x_k) \leq \beta_k(\phi_0(x) - \varphi(x)) + \varphi(x) + \delta_k$$

for any $x \in \operatorname{dom}\varphi$. Again, if x_* is a minimizer of φ

$$\frac{c_{k-1}}{2\lambda_{k-1}}\|y_{k-1}-x_k\|^2+(\varphi(x_k)-\varphi_*)\leq \beta_k(\phi_0(x_*)-\varphi_*)+\delta_k$$

The last result shows that, if $c_k \geq c > 0$ (e.g. if $2-\lambda_k L - a \geq c > 0$), being λ_k bounded from above, then $\|y_{k-1}-x_k\| \to 0$.

Concerning the structure of the error term δ_k, it is easy to prove (see Lemma 3.3 in [Gϋ92]) that the solution of the last difference equation in (aiFOBOS) is given by

$$\delta_k = \frac{\beta_k}{2}\sum_{i=0}^{k-1}\frac{\varepsilon_i^2}{\lambda_i\beta_{i+1}}. \tag{5.27}$$

The following theorem is the main result of the chapter.

Theorem 5.4.5. *Consider the inexact accelerated forward-backward algorithm (aiFOBOS) for a bounded sequence $\lambda_k \in [\lambda,(2-a)/L]$, and fixed $\lambda \in\ ]0,2/L[$ and $a \in\ ]0,2-\lambda L[$. Then, if $\varepsilon_k = O(1/k^q)$ with $q > 1/2$, the sequence $(x_k)_{k\in\mathbb{N}}$ is minimizing for φ and if the infimum of φ is attained the following bounds on the rate of convergence holds true*

$$\varphi(x_k)-\varphi_* = \begin{cases} O\left(1/k^2\right) & \text{if } q > 3/2 \\ O\left(1/k^2\right)+O\left(\log k/k^2\right) & \text{if } q = 3/2 \\ O\left(1/k^2\right)+O\left(1/k^{2q-1}\right) & \text{if } q < 3/2. \end{cases}$$

Proof. Since $\lambda_k \in [\lambda,(2-a)/L]$, relying on the inequalities (5.20) with $b=2$, it is straightforward to prove that $\beta_k \sim 1/k^2$. Thus we get

$$\frac{1}{\lambda_i\beta_{i+1}} \leq \frac{c}{\sqrt{\lambda}}(i+1)^2$$

for a properly chosen constant $c > 0$. Hence the error δ_k can be majorized as follows

$$\begin{aligned}\delta_k &= \frac{\beta_k}{2}\sum_{i=0}^{k-1}\frac{\varepsilon_i^2}{\lambda_i\beta_{i+1}}.\\ &\leq \frac{c}{2(k+1)^2}\sum_{i=0}^{k-1}\varepsilon_i^2(i+1)^2.\end{aligned}$$

If $\varepsilon_k = O(1/(k+1)^q)$, the last inequality implies

$$\delta_k \le \frac{\tilde{c}}{(k+1)^2} \sum_{i=0}^{k-1} \frac{1}{(i+1)^{2(q-1)}}.$$

The sequence $\sum_{i=0}^{k-1} 1/(i+1)^{2(q-1)}$ is convergent if $q > 3/2$, it is an $O(\log k)$ if $q = 3/2$ and an $O((k+1)^{3-2q})$ if $q < 3/2$. $\square$

5.5 Backtracking stepsize rule

As other forward-backward splitting schemes, the above procedure requires the explicit knowledge of the Lipschitz constant of ∇f. Often in practice, especially for large scale problems, computing L might be too demanding. For this reason, procedures allowing the use of a forward-backward splitting algorithm while avoiding the computation of L have been proposed [Nes09, BT09b]. In this section, we describe how the so called *backtracking procedure* can be applied in our context as well, when L is not known. The key idea is the fact that the statement of Lemma 5.4.1 still holds if $y \in \mathcal{H}$, $z \in \operatorname{dom} g$ and $M > 0$ satisfy the inequality

$$f(y) \ge f(z) - \langle z - y, \nabla f(y) \rangle - \frac{M}{2} \|z - y\|^2. \tag{5.28}$$

Then, a straightforward generalization of Theorem 5.4.3 yields the key inequality $\hat{\delta} + \hat{\phi}_* \ge \varphi(\hat{x})$, for $y, \hat{x}$ satisfying (5.28). These two facts allow us to add a subroutine to aiFOBOS, denoted BT, without affecting its convergence rate. More precisely, the direct choice of λ_k and α_k and the computation of y_k and x_{k+1} in aiFOBOS is substituted at each step by means of the following function:

$$(M_k, \lambda_k, \alpha_k, y_k, x_{k+1}) = BT(M_{k-1}, \varepsilon_k, x_k, \nu_k),$$

where M_{k-1} is the current guess for L. Let $\gamma > 1$, for arbitrary M, ε, x, ν, we define $BT(M, \varepsilon, x, \nu)$ by iteratively constructing the finite sequence $((\tilde{M}_i, \tilde{\lambda}_i, \tilde{\alpha}_i, \tilde{y}_i, \tilde{x}_{i+1}))_{i=0}^{m}$, for $i \ge 0$ as

$$\left[\begin{array}{l}
\tilde{M}_i = \gamma^i M \\[2ex]
\tilde{\lambda}_i \in \left]0, (2-a)/\tilde{M}_i\right] \\[2ex]
\tilde{\alpha}_i \in [0,1) \quad \text{such that} \quad a \le \dfrac{\tilde{\alpha}_i^2}{(1-\tilde{\alpha}_i) A \tilde{\lambda}_i} \le 2 - \tilde{\lambda}_i \tilde{M}_i \\[2ex]
\tilde{y}_i = (1-\tilde{\alpha}_i) x + \tilde{\alpha}_i \nu \\[2ex]
\tilde{x}_{i+1} \approxeq_\varepsilon \operatorname{prox}_{\tilde{\lambda}_i g}(\tilde{y}_i - \tilde{\lambda}_i \nabla f(\tilde{y}_i))
\end{array}\right.$$

We then let $BT(M, \varepsilon, x, \nu) = (\tilde{M}_m, \tilde{\lambda}_m, \tilde{\alpha}_m, \tilde{y}_m, \tilde{x}_{m+1})$, where m is defined as

$$m := \min\{i \in \mathbb{N} \, : \, f(\tilde{y}_i) \geq f(\tilde{x}_{i+1}) - \langle \tilde{x}_{i+1} - \tilde{y}_i, \nabla f(\tilde{y}_i) \rangle - \frac{\tilde{M}_i}{2} \|\tilde{x}_{i+1} - \tilde{y}_i\|^2\}.$$

Note that m is finite, since $\lim_i \tilde{M}_i = +\infty$ (being $\gamma > 1$) and the condition (5.28) is satisfied by any point when $M \geq L$.

5.6 Recovering FISTA

Here we show that the proposed general algorithm can be rewritten in equivalent forms, which include the well-known FISTA [BT09b]. This implies that the framework of estimate sequences can be used to derive FISTA, as it is the case for other popular accelerated schemes, such as NESTA [BBC09] and the ones proposed by Nesterov in [Nes09].

We prove that the sequence ν_k in aiFOBOS can be replaced with y_k, achieving a first alternative form of the algorithm. To this purpose, choose two sequences $(a_k)_{k \in \mathbb{N}}$, $a_k \in [a, 2[$, with $0 < a < 2$ and $(\lambda_k)_{k \in \mathbb{N}}$, $0 < \lambda_k \leq (2 - a_k)/L$. Then we have $0 < \lambda_k L + a_k \leq 2$ and $a \leq a_k$. Now, let $A_0 = A$ and for each $k \in \mathbb{N}$ define recursively

$$\begin{aligned} \alpha_k &= \frac{\sqrt{(a_k A_k \lambda_k)^2 + 4(a_k A_k \lambda_k)} - a_k A_k \lambda_k}{2} \\ A_{k+1} &= (1 - \alpha_k) A_k \, . \end{aligned}$$

Then we have $\alpha_k \in [0, 1[$ and

$$\frac{\alpha_k^2}{(1 - \alpha_k) A_k \lambda_k} = a_k \in [a, 2[\, . \tag{5.29}$$

The updating rule for ν can be written as

$$\nu_{k+1} = \nu_k - \frac{a_k}{\alpha_k}(y_k - x_{k+1}) \, .$$

Now from $y_k = (1 - \alpha_k) x_k + \alpha_k \nu_k$, we get $\nu_k = \alpha_k^{-1}(y_k - (1 - \alpha_k) x_k)$ and we can substitute it into the formula for ν_{k+1} obtaining $\nu_{k+1} = \nu_k - a_k \alpha_k^{-1}(y_k - x_{k+1}) = \alpha_k^{-1}((1 - a_k) y_k + a_k x_{k+1} - (1 - \alpha_k) x_k)$. If we substitute ν_{k+1} back again into the formula for y_{k+1} we finally obtain

$$\begin{aligned}
y_{k+1} &= (1-\alpha_{k+1})x_{k+1} + \alpha_{k+1}\nu_{k+1} \\
&= (1-\alpha_{k+1})x_{k+1} + \frac{\alpha_{k+1}}{\alpha_k}((1-a_k)y_k + a_k x_{k+1} - (1-\alpha_k)x_k) \\
&= x_{k+1} + \alpha_{k+1}\Big(\frac{a_k}{\alpha_k} - 1\Big)x_{k+1} - \alpha_{k+1}\Big(\frac{1}{\alpha_k} - 1\Big)x_k + (1-a_k)\frac{\alpha_{k+1}}{\alpha_k}y_k \\
&= x_{k+1} + \alpha_{k+1}\Big(\frac{1}{\alpha_k} - 1\Big)(x_{k+1} - x_k) + (1-a_k)\frac{\alpha_{k+1}}{\alpha_k}(y_k - x_{k+1})\ .
\end{aligned}$$

Thus, the algorithm has the following final form

$$\left|\begin{aligned}
\alpha_k &= \frac{\sqrt{(A_k a_k \lambda_k)^2 + 4A_k a_k \lambda_k} - A_k a_k \lambda_k}{2} \\
x_{k+1} &\approxeq_{\varepsilon_k} \operatorname{prox}_{\lambda_k g}(y_k - \lambda_k \nabla f(y_k)) \\
y_{k+1} &= x_{k+1} + \alpha_{k+1}\Big(\frac{1}{\alpha_k} - 1\Big)(x_{k+1} - x_k) + (1-a_k)\frac{\alpha_{k+1}}{\alpha_k}(y_k - x_{k+1}) \\
A_{k+1} &= (1-\alpha_k)A_k\ ,
\end{aligned}\right.$$

which depends on an extra arbitrary numerical sequence $(a_k)_{k\in\mathbb{N}}$ with $0 < a \le a_k < 2$.

We can formulate the algorithm in yet another, simpler form, replacing the two numerical sequences $(\alpha_k)_{k\in\mathbb{N}}$ and $(A_k)_{k\in\mathbb{N}}$ with a new one. By defining $t_k = 1/\alpha_k$ the update of y_k becomes

$$y_{k+1} = x_{k+1} + \frac{t_k - 1}{t_{k+1}}(x_{k+1} - x_k) + (1-a_k)\frac{t_k}{t_{k+1}}(y_k - x_{k+1})$$

and t_{k+1} can be computed recursively. Indeed, being $\alpha_k^2 = a_k A_{k+1}\lambda_k$ and taking into account (5.29) for $k+1$, we have

$$\begin{aligned}
\alpha_{k+1}^2 &= a_{k+1}(1-\alpha_{k+1})A_{k+1}\lambda_{k+1} \\
&= (1-\alpha_{k+1})\alpha_k^2 \frac{a_{k+1}}{a_k}\frac{\lambda_{k+1}}{\lambda_k}\ .
\end{aligned}$$

Substituting $t_k = 1/\alpha_k$ in the last equation, we get the equation

$$t_{k+1}^2 - t_{k+1} - \frac{\lambda_k}{\lambda_{k+1}}\frac{a_k}{a_{k+1}}t_k^2 = 0$$

which can be solved in the unknown t_{k+1}. Therefore, a third form of the algorithm reads as follows

$$\left| \begin{array}{l} t_{k+1} = \dfrac{1+\sqrt{1+4(a_k\lambda_k)t_k^2/(a_{k+1}\lambda_{k+1})}}{2} \\ x_{k+1} \approxeq_{\varepsilon_k} \operatorname{prox}_{\lambda_k g}(y_k - \lambda_k \nabla f(y_k)) \\ y_{k+1} = x_{k+1} + \dfrac{t_k - 1}{t_{k+1}}(x_{k+1} - x_k) + (1-a_k)\dfrac{t_k}{t_{k+1}}(y_k - x_{k+1})\ . \end{array} \right. \tag{5.30}$$

Regarding the initialization, we highlight that we are free to choose any $t_0 > 1$ as well as $x_0 = y_0 \in \mathcal{H}$. Indeed $\alpha_0 = 1/t_0 \in\ ]0,1[$ and $\alpha_0^2/((1-\alpha_0)A_0\lambda_0) = a_0$ holds if we choose $A_0 = A = \alpha_0^2/((1-\alpha_0)a_0\lambda_0)$.

Remark 5.6.1. *Actually, we are also allowed to choose $t_0 = 1$ in the initialization step because, as one can easily check, with this choice we get $t_1 > 1$ and if $a_0 = 1$, $y_1 = x_1$. Therefore the sequences continue as if they started from (t_1, x_1, y_1).*

The last form of the algorithm, together with Remark 5.6.1, shows that we can recover FISTA [BT09b, Tse10] by choosing $a_k = 1$ and $\lambda_k = \lambda \leq 1/L$, starting with $t_0 = 1$. Moreover, for $f = 0$ and $a_k = 2$, we also obtain the proximal point algorithm given in the appendix of [G$\ddot{9}$2].

As a final remark, we empirically observed (without reporting here the results) that in our simple experiments of Section 5.8, the choice of the parameters a_k, if indipendent from k, in practice does not influence the empirical speed of convergence.

5.7 Applications

In this section, we want to show that the error concept we introduced in Section 5.2 is well suited to deal with a general class of problems of type $(\mathcal{P})$. In particular, we consider functions g of the form

$$\boxed{g(x) = \omega(Bx),} \tag{5.31}$$

where $B : \mathcal{H} \to \mathcal{G}$ is a linear and bounded operator between Hilbert spaces, and $\omega : \mathcal{G} \to \overline{\mathbb{R}}$ is a proper, l.s.c. convex function (e.g. a seminorm). These functions often arise as regularization terms in ill-posed inverse problems [CL97, Bre09a, BKP10, RT05, RT06, SGG$^+$09, ZRY08, CDV10]. We will show that, in case ω be positively homogeneous, most iterative methods used to compute the proximity operator of g yield admissible approximations in the sense of Definition 5.2.1.

To that purpose, we first note that

$$\lambda B^*(\operatorname{dom}\,\omega^*) \subseteq \lambda\,\operatorname{dom}\,g^* = \operatorname{dom}\,(\lambda g)^*. \tag{5.32}$$

Therefore if $(v_n)_{n\in\mathbb{N}}$ is a sequence with $v_n \in \mathrm{dom}\,\omega^*$, then $\lambda B^* v_n \in \mathrm{dom}\,(\lambda g)^*$ for every $n \in \mathbb{N}$. The inclusion (5.32) is easy to prove, since if $v \in \mathrm{dom}\,\omega^*$, then

$$\begin{aligned} g^*(B^*v) &= \sup_{x\in\mathcal{H}}(\langle x, L^*v\rangle - \omega(Bx)) = \sup_{x\in\mathcal{H}}(\langle Bx, v\rangle - \omega(Bx)) \\ &\le \sup_{u\in\mathcal{G}}(\langle u, v\rangle - \omega(u)) = \omega^*(v) < +\infty \end{aligned}$$

If ω is also positively homogeneous (being as a result a sublinear functional), then $\omega^* = \delta_S$ with $S := \partial\omega(0) \subseteq \mathcal{G}$. Moreover $(\lambda g)^* = \delta_{\lambda K}$ with $K := \partial g(0) = B^*(S)$, thus the inclusion (5.32) becomes an equality. Then, if S is bounded, K is bounded too and we can apply the Corollary 5.2.7. We can summarize the result in the following proposition.

Proposition 5.7.1. *If in* (5.31)*, ω is positively homogeneous and $S := \partial\omega(0)$ is bounded, then for any sequence $(v_n)_{n\in\mathbb{N}}$ with $v_n \in S$ and $\lambda B^* v_n \to P_{\lambda K}(y)$ it holds $y - \lambda B^* v_n \approxeq_\varepsilon$ $\mathrm{prox}_{\lambda g}(y)$ for sufficiently large n.*

We note that a simple case in which S is bounded is when ω is continuous in the Hilbert space $\mathcal{H}$, that is $\omega(x) \le c\|x\|$ for every $x \in \mathcal{H}$.

We also remark that one can actually define a sequence according to Proposition 5.7.1. Indeed relying on the Fenchel-Moreau-Rockafellar duality theory [Zăl02], one can show that

$$\mathrm{prox}_{\lambda g}(y) = y - \lambda B^*\bar{v}, \qquad B^*\bar{v} = \mathrm{prox}_{g^*/\lambda}(y/\lambda)$$

where $\bar{v}$ is the solution of the dual problem

$$\min_{v\in\mathcal{G}} \frac{1}{2}\|B^*v - y/\lambda\|^2 + \frac{1}{\lambda}\omega^*(v)\ . \tag{5.33}$$

When ω is positively homogeneous, (5.33) is a constrained quadratic programming problem, and thus can be solved using different algorithms, such as for instance interior point methods [NW06] or projected Newton methods [Pol87], as well as forward-backward splitting algorithms [CDV10]. If these algorithms produce a feasible minimizing sequence v_n, such that B^*v_n strongly converges, then Proposition 5.7.1 applies.

In the following, for solving (5.33), we focus on the forward-backward splitting algorithm, and we define $(v_n)_{n\in\mathbb{N}}$ by setting (see Algorithm 3.5 in [CDV10])

$$\left|\begin{array}{l} v_0 \in \mathcal{G},\ \beta \in \left]0, \min\{1, \|B\|^{-2}\}\right[\quad \text{(initialization)} \\ \gamma_n \in [\beta, 2\|B\|^{-2} - \beta] \\ \mu_n \in [\beta, 1] \\ v_{n+1} = (1-\mu_n)v_n + \mu_n P_S(v_n - \gamma_n B(B^*v_n - y/\lambda)) \end{array}\right. \tag{5.34}$$

which enjoys the convergence properties:

$$v_n \rightharpoonup \bar{v}, \qquad \|B^* v_n - B^* \bar{v}\| \to 0.$$

Thus $y - \lambda B^* v_n \to \operatorname{prox}_{\lambda g}(y)$. We note that, since S convex, if the initialization of algorithm (5.34) takes $v_0 \in S$, then $v_n \in S$ for every $n \in \mathbb{N}$ and if S is bounded, the sequence so generated is compliant with the hypotheses required by Proposition 5.7.1.

A case of non admissible approximations of the proximal point We conclude this section by considering a simple function g and a common algorithm computing its proximity operator that generates approximations which could not be admissible in the sense of Definition 5.2.1.

Let $\mathcal{H} = \mathbb{R}^d$ and $g = \delta_C$ be the indicator function of the set $C = \{x \in \mathcal{H} \mid \|Bx\|_1 \leq r\}$, thus $\operatorname{prox}_g(y)$ is simply $P_C(y)$ the projection onto C. The function $g = \delta_C$ is of type (5.31) with $\omega = \delta_D$, $D = B_{r,1}$, where $B_{r,1}$ is the ball of radius r in $\mathbb{R}^d$ with respect to the norm $\|\cdot\|_1$. We solve the associated dual problem (5.33) again using the general algorithm provided in [CDV10], which in this case corresponds to algorithm (5.34), with the last line replaced by

$$v_{n+1} = \operatorname{prox}_{\gamma_n \omega^*}(v_n - \gamma_n B(B^* v_n - y)) \,, \tag{5.35}$$

where $\operatorname{prox}_{\gamma_n \omega^*} = I - P_{\gamma_n D}$ and we know $B^* v_n \to B^* \overline{v} = \operatorname{prox}_{g^*}(y)$. It is easy to prove that $\omega^* = r\|\cdot\|_\infty$, therefore dom $\omega^* = \mathcal{H}$. From the inclusion (5.32), it follows that in this case dom g^* is unbounded — this is because the range of B^* is obviously unbounded if $B^* \neq 0$. For that reason, we *cannot* apply the general result in Corollary 5.2.5 to this case and conclude that $y - B^* v_n \approxeq_\varepsilon \operatorname{prox}_g(y)$ for sufficiently large n. In fact we do not even know whether $y - B^* v_n \in$ dom g. As a result, we can say that the approximations obtained as $y - B^* v_n$, even for large n, might be unfeasible with respect to the constraint C. In Section 5.8.3, we verified this behavior numerically.

5.8 Numerical Experiments

In this section, we present a series of simple experiments designed to illustrate the behavior predicted by the theoretical results given in the previous sections.

In all the following cases, we consider the regularized least-squares functional

$$\varphi(x) := \|Ax - y\|^2_{\mathcal{Y}} + g(x) \,, \tag{5.36}$$

where $\mathcal{H}, \mathcal{Y}$ are Euclidean spaces, $x \in \mathcal{H}$, $y \in \mathcal{Y}$, $A : \mathcal{H} \to \mathcal{Y}$ is a linear operator and $g : \mathcal{H} \to \overline{\mathbb{R}}$ is of the type considered in the previous section, i.e. $g = \omega \circ B$, for specific choices of ω and B.

We minimized φ using aiFOBOS in the equivalent form (5.30), with $\lambda_k = 1/L$, where $L = 2\|A^*A\|$ and $a_k = 1$. As already noted at the end of Section 5.6, we empirically observed that if $a_k = a$, the choice of a, if admissible, does not seem to influence the speed of convergence of the algorithm. At each iteration, we employed Algorithm (5.34) to approximate the proximity operator of g up to a precision ε_k, which is measured on the difference of two successive iterates. In particular, we let $\varepsilon_k = 1/k^q$, with q, hereafter referred as *accuracy rate*, chosen between 0.1 and 1.7, and we compared the empirical convergence rate of $\varphi(x_k) - \varphi_*$ to the theoretical one provided in Theorem 5.4.5.

This study is independent of the algorithm chosen to produce an admissible approximation of the proximal points, although this choice does determine the time complexity of aiFOBOS. In fact, we only provide the convergence rate versus the number of external iterations k and, for our purposes, it is sufficient to restrict our analysis to a single algorithm, while we leave a more comprehensive comparison to future work.

Our experiments show that the empirical convergence rate of $\varphi(x_k) - \varphi_*$ is indeed affected by the accuracy rate q: to smaller values of q correspond slower convergence rates. On the one hand, in certain cases, when the accuracy rates are higher than 0.8, we obtained empirical convergence rates faster than the theoretically "optimal" $1/k^2$ (see [NY83, Nes04] for a precise definition of optimal convergence rate). On the other hand, when the errors in the computation of the proximity operator do not decay fast enough, the convergence rates are much deteriorated and the algorithm can even not converge to the infimum. However, in no tests, we observe a sharp distinction between accuracy rates smaller than 1/2, for which theoretically aiFOBOS might not converge and accuracy rates greater than 1/2, which guarantee convergence. In other words, we were not able to find any worst case in which the lower bounds on the convergence rates predicted by Theorem 5.4.5 occurs. In this respect, the Total Variation experiment of Section 5.8.2 provides the best result, since we obtained convergent sequences only for accuracy rates greater then or equal to 0.4.

Furthermore, we conducted a numerical experiment where the approximations of the proximal points are not admissible. In spite of that, in this case too, we obtained convergent sequences even for accuracy rates lower then 1/2. The issue of convergence with approximations of type different than the one considered here is still open and will require further work.

These simple experiments suggest that the use of accelerated methods in the presence of large errors is a delicate issue, as also pointed out in [CP10].

5.8.1 Fused Lasso

The Fused Lasso [TSR$^+$05] is a regularization technique for linear models that penalizes strong variations of the coefficients of the model and is designed for problems with variables

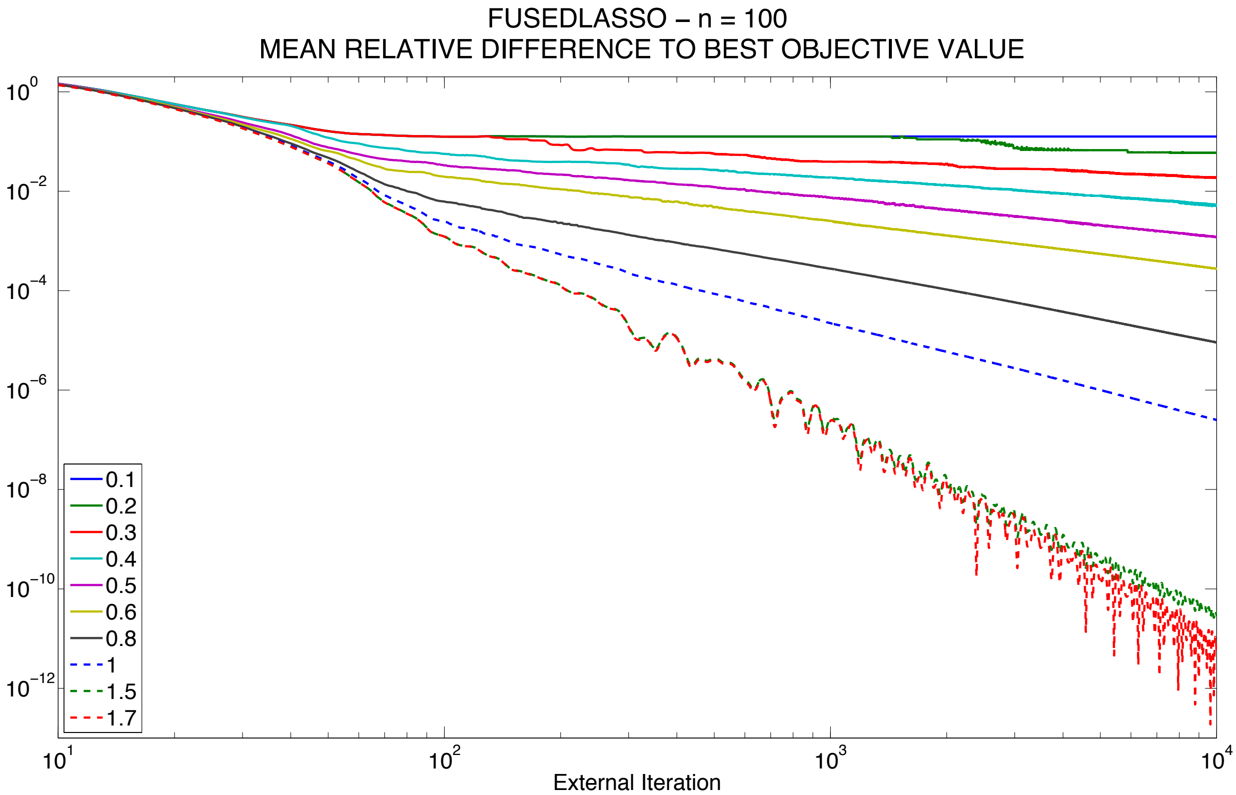

Figure 5.2: Relative objective value paths $(\varphi(x_k) - \varphi_*)/\varphi_*$ obtained for the Fused Lasso problem with aiFOBOS and different accuracy rates q in the computation of the proximity operator with Algorithm (5.34).

that can be ordered in some meaningful way.

In this case, $\mathcal{H} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}^m$, A is a $m \times p$ measurement matrix and y is a vector of outputs. The regularization term is $g = \lambda \|B \cdot\|_1$, where $B \in \mathbb{R}^{(p-1)\times p}$, with $(Bx)_i = x_i - x_{i+1}$. Note that g satisfies the hypothesis of Proposition 5.7.1 with $\omega = \lambda \| \cdot \|_1$, therefore Algorithm (5.34) produces admissible approximations of the proximity operator of g. We chose $p = 100$ and $m = 20$. The entries of the matrix A were sampled independently from a Gaussian distribution of zero mean and unit variance. The outputs y were obtained as $y = A\tilde{x}$, where $\tilde{x} \in \mathbb{R}^p$ contains 10 components equal to 1 in the positions 5 to 14 and 10 components equal to -1 in the positions 86 to 95. The remaining components of $\tilde{x}$ are equal to zero. Finally, Gaussian noise was added to y in order to yield a Signal-To-Noise Ratio of 10. We also set $\lambda = 0.1$.

We run aiFOBOS up to 10.000 iterations for 10 different samplings of the measurement matrix A and, consequently, of the outputs y. In Figure 5.2, we report the mean values of $(\varphi(x_k) - \varphi_*)/\varphi_*$, where φ_* is the minimum objective value found by any method. The values

Table 5.1: Fused Lasso. Lower Bounds on the Convergence Rates (LBCR) and Estimated Convergence Rates (ECR) for $\varphi(x_k) - \varphi_*$ generated by aiFOBOS when the proximity operator is computed with an approximation $\varepsilon_k = 1/k^q$. The former are computed according to Theorem 5.4.5. The latter are estimated from the linear parts of the objective value paths in Figure 5.2.

Accuracy rate q	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1	1.5	1.7
LBCR	0	0	0	0	0	0.2	0.6	1	2	2
ECR	0	0.29	0.37	0.53	0.77	0.94	1.4	2	3.9	4.4

are averaged over the 10 samplings of the data. We observed that the standard deviations over the ten repetitions were small and, for clarity, we decided to not show them in the plot. Note that both the x-axis and the y-axis are in log scale to better illustrate the effect of computing the proximity operator with different accuracies.

According to our theoretical analysis, when the accuracy rate q is below $1/2$, aiFOBOS might not converge to the optimal solution. From Figure 5.2, it appears that even when the rate is as low as 0.3, aiFOBOS yields a converging sequence, albeit very slow. However, note that for the rate 0.1, 0.2 and also 0.3, the objective value path presents a very flat region starting at around the $100th$ iteration. Hence, common stopping criteria for iterative algorithms that compute the (relative) difference between $\varphi(x_k)$ and some previous iterates, would stop the iterations early, far from an optimal solution.

For most rates of accuracy q, the objective value path in the log-log scale shows a linear part between 100 and 10.000 iterations, allowing for an empirical estimation of the convergence rates. In Table 5.1, we report the estimated convergence rates alongside the lower bounds on the convergence rates given in the theoretical analysis. It is interesting to observe that the estimated rates are always better than the ones predicted by the theoretical analysis.

5.8.2 Deblurring with total variation

Regularization with the Total Variation [ROF92b, Cha04, BT09a] is a widely used technique for deblurring and denoising images, that preserves sharp edges.

In this problem, $\mathcal{H} = \mathcal{Y} = \mathbb{R}^{N\times N}$ is the space of (discrete 2D) images on the grid $[1, N]^2$, A is a linear map representing some blurring operator [BT09a] and y is the observed noisy and blurred datum. The (discrete) *total variation* regularizer is defined as

$$g = \omega \circ \nabla \qquad g(x) = \lambda \sum_{i,j=1}^{N} \|(\nabla x)_{i,j}\|_2$$

where $\nabla : \mathcal{H} \to \mathcal{H}^2$ is the (discrete) gradient operator (see [Cha04] for the precise defi-

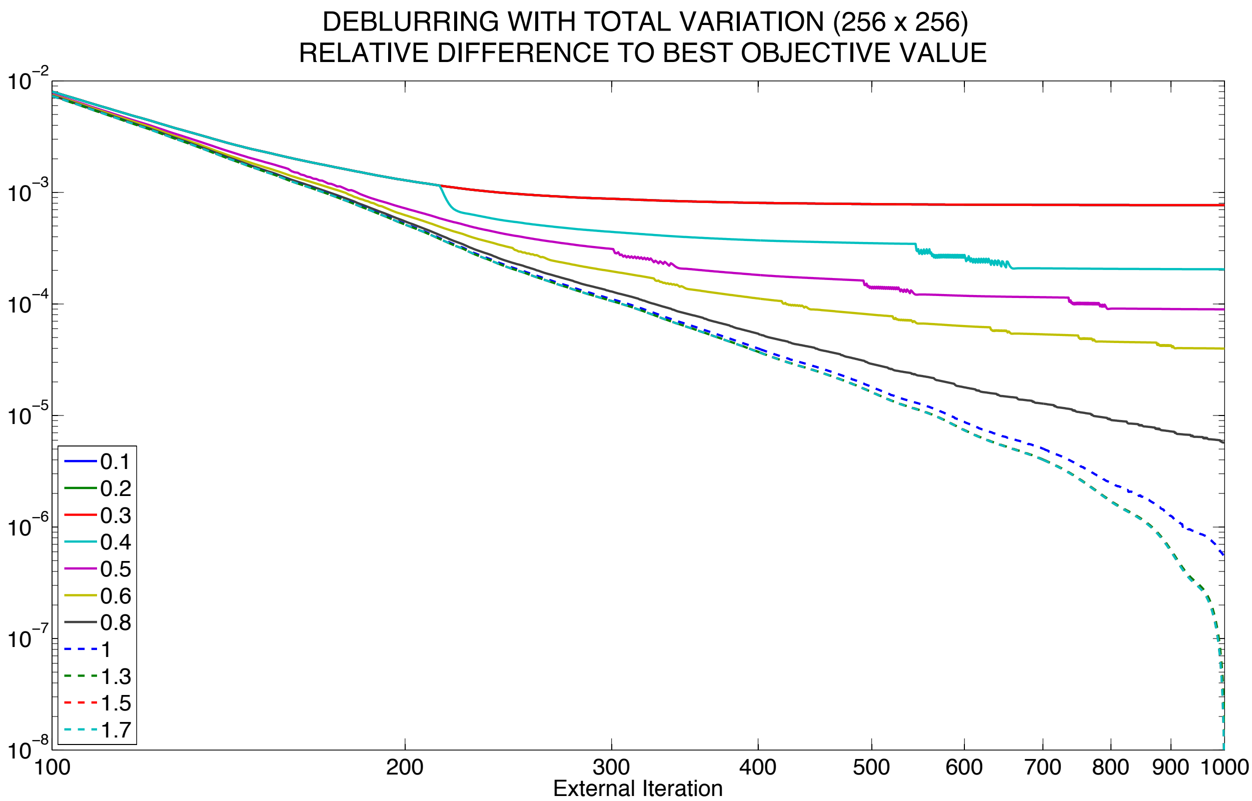

Figure 5.3: Relative objective value paths $(\varphi(x_k) - \varphi_*)/\varphi_*$ obtained for Total Variation regularization with aiFOBOS and different accuracy rates q in the computation of the proximity operator with Algorithm (5.34).

nition) and $\omega : \mathcal{H}^2 \to \mathbb{R}$, $\omega(\mathbf{p}) = \lambda \sum_{i,j=1}^{N} \|\mathbf{p}_{i,j}\|_2$. Note that also in this case, g satisfies the hypothesis of Proposition 5.7.1 with $B = \nabla$, therefore Algorithm (5.34) produces admissible approximations of the proximity operator of g.

We followed the same experimental setup as in [BT09a]. We considered the 256×256 Lena test image, blurred by a 9×9 gaussian blur with standard deviation 4, followed by additive normal noise with zero mean and standard deviation 10^{-3}. The regularization parameter λ was set to 10^{-4}.

We run aiFOBOS up to 1.000 iterations and we report in Fig. 5.3, for all the accuracy rates q, the relative differences $(\varphi(x_k) - \varphi_*)/\varphi_*$, where φ_* is the best objective value found. Note that both axes are in logarithmic scale and that the curves for $q = 1.3,\ 1.5$ and 1.7 coincide with one another, and the same happens for $q = 0.1,\ 0.2$ and 0.3. In Table 5.2, we report the convergence rates estimated from the linear parts of the objective value paths of Figure 5.3, alongside the lower bounds on convergence rates estimated from the theoretical analysis. For this problem, only accuracy rates $q \geq 0.4$ seem to provide convergent sequences,

Table 5.2: Deblurring with Total Variation. Lower Bound on the Convergence Rates (LBCR) and Estimated Convergence Rates (ECR) for aiFOBOS when the proximity operator is computed with an approximation $\varepsilon_k = 1/k^q$. The former are computed according to Theorem 5.4.5. The latter are estimated from the linear parts of the objective value paths in Figure 5.3.

Accuracy rate q	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1	1.3	1.5	1.7
LBCR	0	0	0	0	0	0.2	0.6	1	1.6	2	2
ECR	0.09	0.09	0.09	0.85	0.97	1.3	2.7	3.7	3.9	3.9	3.9

suggesting that the discriminatory rate of 0.5 between non-convergent and convergent sequences of Theorem 5.4.5 could indeed be close to the optimal one.

5.8.3 A case of non admissible approximations

We consider the least-squares problem (5.36), where $\mathcal{H} = \mathbb{R}^p$, $g = \delta_C$ is the indicator function of the set $C = \{x \in \mathcal{H} \,|\, \|Bx\|_1 \leq r\}$, where B is the successive differences operator used for the Fused Lasso problem. We have that $\mathrm{prox}_g(y)$ is simply $P_C(y)$, the projection onto C. We studied this case, for a general linear operator B, at the end of Section 5.7 and we argued that, using the general algorithm provided in [CDV10], we do not obtain admissible approximations of the proximity operator.

To show the effect of non admissible approximations of the proximal points, we consider the same experimental set up as for the Fused Lasso case, where we replaced the regularization term with δ_C and we set $r = 3$. We run aiFOBOS up to 10.000 iterations and computed the proximity operator up to different levels of accuracy as in the previous experiments. At each iteration of aiFOBOS, we also compute the value of the constraint $\|Bx_k\|_1$.

In Figure 5.4-left, we report the objective value $\|Ax_k - y\|^2_{\mathcal{Y}}$ and in Figure 5.4-right, the value of $\|Bx_k\|_1$. We observe that the iterates fall off of the domain of g and appear indeed as not feasible for the constraint C, therefore they are not of the kind considered in the Definition 5.2.1: they approach the proximal point, but from the exterior of the domain of C. Nonetheless, it is interesting to observe that for accuracy rates $q > 0.2$, the algorithm seems to converge to a feasible solution. Furthermore, by increasing the accuracy rate q, we obtain not only faster convergence to an optimal solution, but also faster convergence to a feasible point.

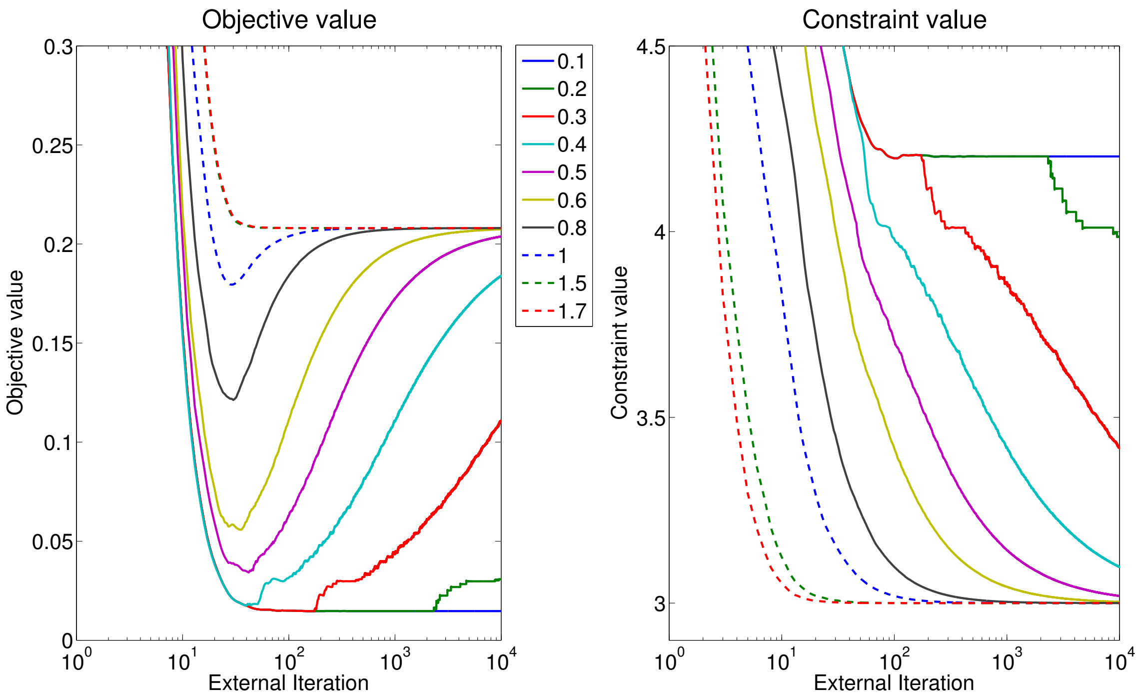

Figure 5.4: Non admissible approximations: on the left the objective value $\|Ax_k - y\|_{\mathcal{Y}}^2$ obtained applying aiFOBOS and algorithm (5.35) for computing the proximity operator for different accuracy rates q. On the right the corresponding values of $\|Bx_k\|_1$.

Chapter 6

Forward-backward Algorithms for Non-convex Problems

In this chapter we address the issue of minimizing composite functions, where the data term is non-convex smooth and the penalty term is convex non-smooth. We consider again a forward-backward splitting algorithm, but in its basic form (non accelereted). Convergence has been studied in [BK09] in Hilbert spaces for general (non-convex) functionals and in [Bre09b] in Banach spaces but only for convex functions. We merge the two studies and analyze the algorithm under both non-convex and Banach space hypotheses. Convergence properties are proved following the same machinery devised in the cited papers. We show finally the applicability of the algorithm at the image registration problem regularized with total variation.

Section 1 contains the analysis of the algorithm's convergence. In Section 2 we show that the proposed algorithm can indeed tackle the problem of total variation based image registration.

6.1 A general algorithm for local minima

Let be given a Frechét differentiable functional $f : U \to \mathbb{R}$ defined over a strictly convex Banach space U. We soppose its derivative be *Hölder continuous* with exponent $q - 1$ for some $q \in (1, 2]$, that is

$$\|f'(u_1) - f'(u_2)\|_{U^*} \leq L\|u_1 - u_2\|_U^{q-1},\ \forall u_1, u_2 \in U, \tag{6.1}$$

We want to solve the minimum problem

$$\boxed{\min_{u \in U} f(u) + g(u)} \tag{6.2}$$

where $g : U \to \overline{\mathbb{R}}$ is a proper, convex, lower semicontinuous and coercive functional in the *strong*[1] topology of U — clearly the functional g, being convex, is also l.s.c. in the weak topology of U.

We point out that, being the functional $f + g$ non-convex, whatever algorithm we choose we can obtain at most convergence to local minima (or stationary points).

The first order condition for a *local minimum* $u_* \in U$ of $f + g$ reads as follows

$$-f'(u_*) \in \partial g(u_*) \tag{6.3}$$

where ∂g is the subdifferential of g in the sense of convex analysis [Zăl02]. To solve problem (6.2), we shall apply a forward-backward splitting algorithm [CW05]. We recall, in case U is a Hilbert space, the algorithm is based on the iteration of the operator $G_\tau : U \to U$ defined as follows

$$\begin{aligned} G_\tau(u) &= \operatorname{prox}_{\tau g}(u - \tau \nabla f(u)) \\ &= \operatorname*{argmin}_{v \in U} \left\{ \frac{\|v - u + \tau \nabla f(u)\|^2}{2} + \tau g(v) \right\} \end{aligned}$$

for a given parameter $\tau > 0$. Then, the *forward-backward splitting algorithm* is

$$u_{n+1} = G_{\tau_n}(u_n)$$

for a sequence $(\tau_n)_{n \in \mathbb{N}}$ of positive numbers such that $0 < \tau_n \leq 2/L$, where L is a Hölder constant for the derivative ∇f given in (6.1).

The above operator can be written equivalently as

$$G_\tau(u) = \operatorname*{argmin}_{v \in U} \left\{ \frac{\|v - u\|^2}{2} + \tau(\langle \nabla f(u), v \rangle + g(v)) \right\}$$

This last formulation allows to be generalized to the case of U Banach space as follows

$$G_\tau(u) = \operatorname*{argmin}_{v \in U} \left\{ \frac{\|v - u\|_U^q}{q} + \tau(\langle f'(u), v \rangle + g(v)) \right\} \tag{6.4}$$

In a moment we will show that the definition is well-posed. The significance of operator (6.4) stands in the fact that its fixed points are exactly the stationary points (6.3) of the functional $f + g$ as the following result shows

[1]This hypothesis will make a difference and actually will reduce the complication of being in infinite dimensional spaces.

Proposition 6.1.1. *Let be given $u_* \in U$ and $\tau > 0$. Then*

$$-f'(u_*) \in \partial g(u_*) \iff u_* = G_\tau(u_*)$$

Proof. From the definition of $G_\tau(u)$ in (6.4), it follows

$$\begin{aligned} v = G_\tau(u) &\iff 0 \in j_p(v-u) + \tau f'(u) + \tau \partial g(v) \\ &\iff -\tau f'(u) \in j_p(v-u) + \tau \partial g(v) \end{aligned}$$

Therefore, noticing that $j_q(0) = 0$, it holds

$$\begin{aligned} u_* = G_\tau(u_*) &\iff -\tau f'(u_*) \in \tau \partial g(u_*) \\ &\iff -f'(u_*) \in \partial g(u_*) \end{aligned}$$

which completes the proof. □

Thus, we are lead to the following iterative procedure that is a generalization of the classical forward-backward splitting algorithm to Banach spaces and for non-convex functions f (*Banach Forward-Backward Algorithm*)

$$u_{n+1} = \operatorname*{argmin}_{u \in U} \left\{ \frac{\|u - u_n\|^q}{q} + \tau_n(\langle f'(u_n), u\rangle + g(u)) \right\} \tag{BFBA}$$

for suitable numbers $\tau_n > 0$. Convergence properties of this algorithm have been studied in [Bre09b] for the case of f being convex and in [BK09] for general f, but in the framework of Hilbert spaces. We are going to combine both arguments given in those articles to cope with our more general framework. We will provide proofs for completeness.

We shall begin with a simple lemma (see see [Bre09b])

Lemma 6.1.2. *If $f : U \to \mathbb{R}$ is a Gâteaux derivative functional with $(q-1)$-Holder continuous derivative satisfying* (6.1)*, then it holds*

$$|f(v) - f(u) - \langle f'(u), v - u\rangle| \le \frac{L}{q}\|v - u\|_U^q$$

for all $u, v \in U$.

Proof. By Lagrange theorem

$$f(v) - f(u) = \int_0^1 \langle f'(u + t(v-u)), v - u\rangle \,\mathrm{d}t$$

and hence,

$$\begin{aligned}
|f(v) - f(u) - \langle f'(u), v - u\rangle| &= \left| \int_0^1 \langle f'(u + t(v-u)) - f'(u), v - u\rangle \, \mathrm{d}t \right| \\
&\leq \int_0^1 \|f'(u + t(v-u)) - f'(u)\|_{U^*} \|v - u\|_U \, \mathrm{d}t \\
&\leq \int_0^1 Lt^{q-1} \|v - u\|_U^q \, \mathrm{d}t \\
&= \frac{L}{q} \|v - u\|_U^q \, . \qquad \square
\end{aligned}$$

We now prove that the operator G_τ is well-defined. More generally the operator $P_\tau : U \times U^* \to U$ such that

$$P_\tau(u, w) = \operatorname*{argmin}_{v \in U} \left\{ \frac{\|v - u\|_U^q}{q} + \tau(\langle w, v\rangle + g(v)) \right\}$$

is well-defined. Indeed, it is enough to prove that the function, $\|\cdot - u\|_U^q/q + \tau\langle w, \cdot\rangle + g$ is weakly lower semicontinuous and coercive (being the space U strictly convex, the function $\|\cdot\|_U^p$ is also strictly convex and this gives the uniqueness of the minimum). As regards coerciveness, recall that g is bounded from below by an affine linear functional, thus, for $q > 1$ and $\|v\| \geq \|u\|$ we have

$$\begin{aligned}
\frac{\|v - u\|_U^q}{q} + \tau(\langle w, v\rangle + g(v)) &\geq \frac{(\|v\| - \|u\|)^q}{q} - c\|v\| - b \\
&\geq \frac{\|v\|^q}{q} - c\|v\| - b
\end{aligned}$$

for suitable constants $c, b \in \mathbb{R}$. Since $q > 1$, it follows

$$\lim_{\|v\| \to +\infty} \frac{\|v - u\|_U^q}{q} + \tau(\langle w, v\rangle + g(v)) = +\infty$$

We now show some descent properties for the forward-backward algorithm. Let u_n the current iterate and $w_n \in U^*$ and define $u_{n+1} = P_{\tau_n}(u_n, w_n)$

Lemma 6.1.3. *Set $d_n = u_{n+1} - u_n$ (the n-th step). Then it holds*

$$g(u_{n+1}) - g(u_n) + \langle w_n, u_{n+1} - u_n\rangle \leq -\frac{\|d_n\|_U^q}{\tau_n}.$$

Moreover if $w_n = f'(u_n)$, then

$$(f + g)'(u_n, d_n) \leq -\frac{\|d_n\|_U^q}{\tau_n}.$$

meaning that the direction d_n is a descent direction for $f + g$.

Proof. Since $u_{n+1} \in P_{\tau_n}(u_n, w_n)$, the first order condition gives

$$-\frac{j_q(u_{n+1} - u_n)}{\tau_n} - w_n \in \partial g(u_{n+1})$$

Thus,

$$g(x_n) \geq g(u_{n+1}) - \langle \frac{j_q(u_{n+1} - u_n)}{\tau_n} + w_n, u_n - u_{n+1} \rangle$$

and hence

$$g(u_{n+1}) - g(u_n) + \langle w_n, u_{n+1} - u_n \rangle \leq -\frac{\|d_n\|_U^q}{\tau_n}.$$

where $\langle j_p(u_{n+1} - u_n), u_{n+1} - u_n \rangle = \|u_{n+1} - u_n\|_U^p$ has been used. If $w_n = f'(u_n)$, then, since the incremental ratio of a convex function is increasing, we have for $0 < t \leq 1$

$$\begin{aligned} \frac{g(u_n + td_n) - g(u_n)}{t} &\leq g(u_n + d_n) - g(u_n) \\ &\leq \langle -f'(u_n), d_n \rangle - \frac{\|d_n\|_U^q}{\tau_n}. \end{aligned}$$

Hence for $t \to 0$

$$g'(u_n, d_n) \leq \langle -f'(u_n), d_n \rangle - \frac{\|d_n\|_U^q}{\tau_n}.$$

that is

$$(f + g)'(u_n, d_n) \leq -\frac{\|d_n\|_U^q}{\tau_n}.$$

□

From Lemma 6.1.2, we get

$$f(u_{n+1}) - f(u_n) - \langle f'(u_n), u_{n+1} - u_n \rangle \leq \frac{L}{q} \|u_{n+1} - u_n\|_U^q$$

and if we sum with the inequality obtained in Lemma 6.1.3, then we get

$$\boxed{(f + g)(u_{n+1}) - (f + g)(u_n) \leq -\Big(\frac{1}{\tau_n} - \frac{L}{q}\Big) \|d_n\|_U^q} \tag{6.5}$$

If we choose $\tau_n \leq q/L$, then *the values of the functional $f + g$ decreases at the next iteration* and the whole sequence $((f + g)(u_n))_{n\in\mathbb{N}}$ is a convergent sequence, since it is decreasing and bounded from below. Furthermore

$$\Big(\frac{1}{\tau_n} - \frac{L}{q}\Big) \|d_n\|_U^q \leq (f + g)(u_n) - (f + g)(u_{n+1})$$

and the right term tends to zero. Thus, if we assume $\tau_n \leq \overline{\tau} < q/L$, then

$$\|u_{n+1} - u_n\|_U \to 0$$

The functional $\Psi : \mathbb{R}_{++} \times U^* \times U \to \mathbb{R}$ defined as

$$\Psi(\tau, w, u) = \tau\langle w, u\rangle + \tau g(u) - \min_{v \in U} \left[\frac{\|v - u\|_U^q}{q} + \tau\langle w, v\rangle + \tau g(v) \right]$$

satisfies $\Psi(\tau, w, u) \geq 0$ for all $u \in U$, $w \in U^*$, $\tau > 0$, and $\Psi(\tau, w, u) = 0$ if and only if $u \in P_\tau(u, w)$. Thus we have

$$u \in G_\tau(u) \iff \Psi(\tau, f'(u), u) = 0 \tag{6.6}$$

Evidently the functional Ψ can be rewritten as follows

$$\Psi(\tau, w, u) = \sup_{v \in \operatorname{dom} g} \left[\tau\langle w, u - v\rangle + \tau(g(u) - g(v)) - \frac{\|v - u\|_U^q}{q} \right]$$

showing that it is, in fact, the upper envelop of a family of lower semicontinuous functions in the variables (τ, w, u) and hence a lower semicontinuous function. Now, if we set $u_{n+1} = P_{\tau_n}(u_n, w_n)$, $d_n = u_{n+1} - u_n$ and simply computes $\Psi(\tau_n, w_n, u_n)$, we get

$$\frac{\Psi(\tau_n, w_n, u_n)}{\tau_n} = -\langle w_n, d_n\rangle + g(u_n) - g(u_{n+1}) - \frac{\|d_n\|_U^q}{\tau_n q}$$

Next, from Lemma 6.1.2

$$0 \leq f(u_n) - f(u_{n+1}) + \langle f'(u_n), d_n\rangle + \frac{L}{q}\|d_n\|_U^q$$

and summing the two equations we obtain

$$\frac{\Psi(\tau_n, w_n, u_n)}{\tau_n} \leq (f + g)(u_n) - (f + g)(u_{n+1}) - \frac{1}{q}\left(\frac{1}{\tau_n} - L\right)\|d_n\|_U^q$$

Therfore, if we assume $0 < \tau_n \leq 1/L$, then

$$\Psi(\tau_n, w_n, u_n) \leq \tau_n \left[(f + g)(u_n) - (f + g)(u_{n+1})\right]$$

and the right term tends to zero. In the end we proved

$$0 \leq \Psi(\tau_n, f'(u_n), u_n) \to 0 \tag{6.7}$$

The descent property, being $(f + g)$ (strongly) coercive, implies that $(u_n)_{n\in\mathbb{N}}$ is relatively compact in the strong topology of U. Therefore there exists a subsequence $(u_{k_n})_{n\in\mathbb{N}}$ converging strongly to some $u_* \in U$. At this point it is not clear whether u_* should be a fixed point of the map G_τ for some $\tau > 0$. This fact is proved in the following theorem.

Theorem 6.1.4. *Suppose $\tau_n \in [\underline{\tau}, \overline{\tau}]$, with $\underline{\tau} > 0$ and $\overline{\tau} \leq 1/L$. Suppose the sequnce $(u_n)_{n\in\mathbb{N}}$, defined according* (BFBA)*, has a strong cluster point u_*. Then u_* is a fixed point of G_{τ_*} for some $\tau_* \in [\underline{\tau}, \overline{\tau}]$ and thus a local minimum of the functional $f+g$ (more precisely it satisfy the necessary condition* (6.3)*).*

Proof. Let $(u_{k_n})_{n\in\mathbb{N}}$ be a subsequence convergent to a point, say $u_* \in U$. Since the corresponding sequence of step-sizes τ_{k_n} are contained in a compact set, we can assume without loss of generality that $\tau_{k_n} \to \tau_* \in [\underline{\tau}, \overline{\tau}]$. Then we have

$$(\tau_{k_n}, f'(u_{k_n}), u_{k_n}) \to (\tau_*, f'(u_*), u_*)$$

Since Ψ is lower semicontinuous and it holds (6.7), we have

$$0 \leq \Psi(\tau_*, f'(u_*), u_*) \leq \liminf_{n\to\infty} \Psi(\tau_{k_n}, f'(u_{k_n}), u_{k_n}) = 0$$

Thus $\Psi(\tau_*, f'(u_*), u_*) = 0$ and, for (6.6), we have $u_* \in G_{\tau_*}(u_*)$. □

Summarizing this section, we proved that for the sequence defined iteratively according to (BFBA), all its cluster points (in the strong topology) are local solutions of problem 6.2.

6.2 Total variation based image registration

We study the minimization of the Tikhonov functional

$$\boxed{\mathscr{T}_\lambda : L^p(\Omega, \mathbb{R}^d) \to \overline{\mathbb{R}}, \quad \mathscr{T}_\lambda(\mathbf{u}) = \|I(\mathbf{u}) - I_0\|_q^q + \lambda J(\mathbf{u})} \tag{6.8}$$

for $1 \leq p < d/(d-1)$, $1 \leq q < +\infty$ and J being the total variation as defined at the end of section 4.3.3.2 (it equals $+\infty$ outside the space $U_{\Omega_0}(\Omega, \mathbb{R}^d)$). We will check the hypotheses required for the convergence of (BFBA).

First of all, we recall that, in section 4.3.3.2 we showed that (with the above assumptions on the exponent p and for any $q \geq 1$), the total variation is l.s.c. and coercive in the strong topology of $L^p(\Omega, \mathbb{R}^d)$ (clearly it is also convex). Hence, the only thing that remains to check is the Hölder continuity of the matching term. We address this issue in the remaining part of the section.

We shall study the functional

$$f : L^p(\Omega, \mathbb{R}^d) \to \mathbb{R}, \quad f(\mathbf{u}) = \|I(\mathbf{u}) - I_0\|_q^q \tag{6.9}$$

We suppose $p \geq q > 1$. Indeed in that case, according to theorem 4.2.3, one can make the warping operator (4.1) Gâteaux differentiable, as soon as the image $I : \mathbb{R}^d \to \mathbb{R}$ is taken differentiable with bounded (partial) derivatives, and it holds

$$I'(\mathbf{u})[\mathbf{v}] = \nabla I(\mathbf{u}) \cdot \mathbf{v}$$

Furthermore the norm $\|\cdot\|_q^q : L^q(\Omega) \to \mathbb{R}$ is differentiable too, if $q > 1$, and it is

$$\nabla \|\cdot\|_q^q(I) = q|I|^{q-2}I = qj_q(I) \in L^{q'}(\Omega)$$

where $1/q' + 1/q = 1$ and $j_q : L^q(\Omega) \to L^{q'}(\Omega)$ is the duality map. Therefore f is Gâteaux differentiable and

$$f'(\mathbf{u})[\mathbf{v}] = q \int_\Omega |I(\mathbf{u}) - I_0|^{q-2}(I(\mathbf{u}) - I_0)\nabla I(\mathbf{u}) \cdot \mathbf{v} \, \mathrm{d}x$$

thus

$$\boxed{\nabla f(\mathbf{u}) = q|I(\mathbf{u}) - I_0|^{q-2}(I(\mathbf{u}) - I_0)\nabla I(\mathbf{u}) \in L^{p'}(\Omega, \mathbb{R}^d)}$$

If we make the extra hypothesis that ∇I is continuous, that is $I \in \mathscr{C}^1(\mathbb{R}^d)$, then one can show that ∇f is continuous, therfore f is Frechét differentiable (just notice that $t \in \mathbb{R} \to |t|^{q-1}t/|t| \in \mathbb{R}$ is continuous everywhere).

In case $q \leq 2$,[2] the duality map $j_q : L^q(\Omega) \to L^{q'}(\Omega)$ can be proved to be Hölder continuous with exponent $q - 1$. More precisely it holds

$$|j_q(I_1)(\mathbf{x}) - j_q(I_2)(\mathbf{x})| \leq 2|I_1(\mathbf{x}) - I_2(\mathbf{x})|^{q-1} \tag{6.10}$$

We will show that $\nabla f : L^p(\Omega, \mathbb{R}^d) \to L^{p'}(\Omega, \mathbb{R}^d)$ is Hölder continuous of exponent $q - 1$ too. Indeed

$$\nabla f(\mathbf{u}) = qj_q(I(\mathbf{u}) - I_0)\nabla I(\mathbf{u})$$

where $j_q(I(\mathbf{u}) - I_0) \in L^{q'}(\Omega) \subseteq L^{p'}(\Omega)$ ($p \geq q \implies p' \leq q'$). Then, if $\mathbf{u}_1, \mathbf{u}_1 \in L^p(\Omega, \mathbb{R}^n)$ it is

$$\begin{aligned}
\nabla f(\mathbf{u}_1) - \nabla f(\mathbf{u}_2) &= q[j_q(I(\mathbf{u}_1) - I_0)\nabla I(\mathbf{u}_1) - j_q(I(\mathbf{u}_2) - I_0)\nabla I(\mathbf{u}_2)] \\
&= q[j_q(I(\mathbf{u}_1) - I_0) - j_q(I(\mathbf{u}_2) - I_0)]\nabla I(\mathbf{u}_1) \\
&\qquad + qj_q(I(\mathbf{u}_2) - I_0)\,(\nabla I(\mathbf{u}_1) - \nabla I(\mathbf{u}_2))
\end{aligned}$$

[2]Since we need to assume $1 \leq p < d/(d-1) \leq 2$ for getting the coercivity of the total variation in $L^p(\Omega, \mathbb{R}^d)$, we have in fact necessarily $q < 2$.

and hence, if the gradient of the image ∇I is supposed Hölder continuous of exponent (at least) $q-1(\leq 1)$ and taking into account (6.10), we have

$$\begin{aligned}|\nabla f(\mathbf{u}_1)-\nabla f(\mathbf{u}_2)| &\leq 2q\mathrm{Lip}(I)^{q-1}|\mathbf{u}_1-\mathbf{u}_2|^{q-1}\|\nabla I\|_\infty \\ &\quad + q(\|I\|_\infty+\|I_0\|_\infty)^{q-1}[\nabla I]_{0,q-1}|\mathbf{u}_1-\mathbf{u}_2|^{q-1} \\ &= q\big\{2\mathrm{Lip}(I)^q+(\|I\|_\infty+\|I_0\|_\infty)^{q-1}[\nabla I]_{0,q-1}\big\}|\mathbf{u}_1-\mathbf{u}_2|^{q-1}\end{aligned}$$

From which it follows

$$\|\nabla f(\mathbf{u}_1)-\nabla f(\mathbf{u}_2)\|_{q'} \leq C\|\mathbf{u}_1-\mathbf{u}_2\|_q^{q-1}$$

where $C=2q\big\{\mathrm{Lip}(I)^q+(\|I\|_\infty+\|I_0\|_\infty)^{q-1}[\nabla I]_{0,q-1}\big\}$, and hence

$$\|\nabla f(\mathbf{u}_1)-\nabla f(\mathbf{u}_2)\|_{p'} \leq C|\Omega|^{\frac{1}{q}-\frac{1}{p}}\|\mathbf{u}_1-\mathbf{u}_2\|_q^{q-1}$$

We thus have shown that the problem of minimizing the Tikhonov functional associated to the total variation based image registration can indeed be tackle by algorithm (BFBA). However we underline that, since the algorithm provides local (convergence), it must be embedded into a linear scale-space framework for focusing the solution from a coarse to a fine scale in order to avoid to get stuck into local minima and reach perhaps global minima [WII99, AWS00].

Chapter 7

A Proximal Gauss-Newton Method

In this last chapter an extension of the Gauss-Newton algorithm is proposed to find local minimizers of penalized nonlinear least squares problems, under generalized Lipschitz assumptions. Convergence results of local type are obtained, as well as an estimate of the radius of the convergence ball. Some applications for solving constrained nonlinear equations are discussed and the numerical performance of the method is assessed on some significant test problems.

The chapter is organized as follows: Section 7.1 presents the problem and provides and outline of the contributions. An analysis of the state-of-the art literature on related problems is contained in Section 7.2. Then, in Section 7.3 we review some basic concepts that will be used: generalized Lipschitz conditions, generalized inverses and proximity operators. In Section 7.4 the minimization problem is precisely stated and some necessary conditions satisfied by local minimizers are presented. The main result of the paper, Theorem 7.5.2, is discussed in Section 7.5 and proved in Section 7.6. Section 7.7 gives an application to the problem of constrained nonlinear equations and, finally, in Section 7.8 numerical tests are set up and analyzed.

7.1 Problem setting and main contribution

Given Hilbert spaces U and V, a Fréchet differentiable nonlinear operator $F : U \to V$, and a convex lower semicontinuous penalty functional $g : U \to \mathbb{R} \cup \{+\infty\}$, we consider the optimization problem

$$\boxed{\min_{u \in U} \frac{1}{2}\|F(u) - v\|^2 + g(u) := \varphi(u).} \tag{$\mathcal{P}$}$$

Problem ($\mathcal{P}$) is in general a nonconvex and nonsmooth problem, having on the other hand a particular structure: it is in fact the sum of a nonconvex, smooth term and a convex and possibly nonsmooth one. The aim of the chapter is to find a convergent algorithm towards a local minimizer of φ, assuming that it exists. Motivated by several applications [EHN96b, SGG⁺09, FP90], problem ($\mathcal{P}$) is receiving an increasing attention. In particular, for $g = 0$, ($\mathcal{P}$) is a classical nonlinear least squares problem [DS96, Xu09]. This kind of problems can be solved by general optimization methods, but typically is solved by more efficient ad hoc methods. In many cases they achieve better than linear convergence, sometimes even quadratic, even though they do not need computation of second derivatives. Among the various approaches, one of the most popular is the *Gauss-Newton method*, introduced in [BI65]:

$$u_{n+1} = u_n - [F'(u_n)^* F'(u_n)]^{-1} F'(u_n)^* (F(u_n) - v). \tag{7.1}$$

Under suitable assumptions, such a procedure is convergent to a stationary point of $x \mapsto \frac{1}{2}\|F(u) - v\|^2$, namely to a point $\bar{u}$ such that $F'(\bar{u})^*(F(\bar{u}) - v) = 0$. Moreover, one can easily show that the point u_{n+1} defined in (7.1) is the minimizer of the "linearized" functional:

$$u \mapsto \frac{1}{2}\|F(u_n) + F'(u_n)(u - u_n) - v\|^2. \tag{7.2}$$

There is a wide literature devoted to the study of convergence results for the Gauss-Newton method under different perspectives. In particular we can distinguish two main streams of research: the papers devoted to a local analysis, and the ones devoted to semilocal results. The first class of studies [DS96, AH09, AH10, LZJ04] assume the existence of a local minimizer, and they actually determine a region of attraction around that point, meaning that if the starting point is chosen inside that region the iterative process is guaranteed to converge towards the minimizer. On the contrary, the semilocal results — also known as Kantorovich type theorems — do not assume the existence of a local minimizer, they just establish sufficient conditions on the starting point in order to make the iterative procedure convergent towards a point that is proved to be a local minimizer [Arg05, FS09, Häu86, LHW10].

Here we propose a generalization of the Gauss-Newton algorithm to the case in which $g \neq 0$, that reads as follows:

$$u_{n+1} = \operatorname{prox}_g^{H(u_n)}\left(u_n - [F'(u_n)^* F'(u_n)]^{-1} F'(u_n)^* (F(u_n) - v)\right), \tag{7.3}$$

where $\operatorname{prox}_g^{H(u_n)}$ is the proximity operator associated to g (see [Mor62, Mor63, Mor65]), with respect to the metric defined by the operator $H(u_n) := F'(u_n)^* F'(u_n)$. The algorithmic framework in (7.3) is determined following the same line of (7.2), i.e. linearizing the operator F at the point u_n, and computing the minimizer of the corresponding "linearized" functional

$$u \mapsto \frac{1}{2}\|F(u_n) + F'(u_n)(u - u_n) - v\|^2 + g(u)$$

This approach is the common way to deal with generalizations of the Gauss-Newton method, as we better explain in the next section. The convergence results we obtain are of local type, and they are comparable to those obtained for the classical Gauss-Newton method. In particular, we get linear convergence in the general case, and quadratic convergence for zero residual problems. Furthermore, we are able to give an estimate of the radius of the convergence ball around a local minimizer. It should be noted that the computation of the proximity operator is in general not straightforward and it may require an iterative algorithm itself, since in general a closed form is not available. On the other hand, we could have denoted u_{n+1} simply as the minimizer of the generalized version of (7.2). The formulation in terms of proximity operators allows to use the well developed theory on this kind of operators, and in our opinion enlightens the connections and the differences with other first order methods that have recently been proposed to solve problem $(\mathcal{P})$ (see the next section for further details).

7.2 Comparison with related work

We review the available algorithms to solve this problem, enlightening the connections and the differences with our approach.

Convex composite optimization. Problem $(\mathcal{P})$ can be cast, in principle, as a composite optimization problem of the form

$$\min_{u\in U} h(c(u)), \tag{7.4}$$

by setting $h : V \times U \to \mathbb{R} \cup \{+\infty\}$ and $c : U \to V \times U$ as follows:

$$h(s,u) = \frac{1}{2}\|s\|^2 + g(u), \qquad c(u) = (F(u) - v, u). \tag{7.5}$$

Problem (7.4) has been deeply studied in [BF95, LW08, LN07, LW02, Wom85, WF86] from different point of views, mainly in the case $U = \mathbb{R}^n$ and $V = \mathbb{R}^m$, but the hypotheses significantly differ, as well as the obtained results. More specifically, in [LW08], the assumptions are too general to capture the features of problem $(\mathcal{P})$, and allow only to get convergence results much weaker than the ones obtained in Theorem 7.5.2. Regarding all the remaining papers, as a matter of fact, the following special case of *inclusion problem* is treated

$$c(u) \in C, \qquad C = \operatorname{argmin} h. \tag{7.6}$$

In particular, the existence of an x such that $c(u) \in \operatorname{argmin} h$ is always assumed. That hypothesis is of course reasonable if we think of h as a kind of norm, but if we take it as in (7.5), then $C = \{(s,v) \,:\, s = 0, u \in \operatorname{argmin} g\}$ and we are lead to the condition

$$\exists\, u \in U, \quad F(u) = v \text{ and } u \in \operatorname{argmin} g$$

which is too demanding for our original problem $(\mathcal{P})$.

Nonlinear inverse problems with regularization. Here the problem is to solve the nonlinear equation

$$F(u) = v \tag{7.7}$$

in the ill-posed case. Typically a solution is found by introducing a regularization term weighted with a positive parameter. There are two possible approaches. The first one employs *iterative methods* which deal directly with problem (7.7), see [BB09]. In this case an iterative process is set up by minimizing at each step a simplified regularized problem (generally linear) having the structure of $(\mathcal{P})$ — with a weight for g varying at each iteration. Within this class of methods, one popular choice is the *iteratively regularized Gauss-Newton method*, see [BNS97, Jin08, KH10, Lan10]. Anyway, we remark that, despite the name, that algorithm is different from any kind of Gauss-Newton optimization method above, since it is not designed to "optimize" any objective functional φ, but, in fact, it directly looks for an exact solution of the equation (7.7).

An alternative approach is the classical *Tikhonov method* [EHN96b] replacing (7.7) by the minimization of the associated Tikhonov functional. A problem of the same type of $(\mathcal{P})$ arises, with g weighted by a properly chosen parameter. Up to our knowledge, besides our method, the papers by Ramlau and Teschke, e.g. [RT05, RT06], are the only ones providing algorithms for the minimization of such type of functionals. In addition, the scheme they propose is different from ours and in general it converges only weakly. On the other hand, our algorithm assumes the derivative $F'(u)$ to be injective with closed range — a hypothesis not suitable for handling the ill-posed case.

7.3 Preliminaries and notations

We start with some notations. In the whole chapter U and V denote a Hilbert space and Ω is a nonempty open subset of U. $F : \Omega \subseteq U \to V$ is an operator, in general nonlinear, and F' denotes its derivative (Fréchet or Gâteaux). $\mathbb{L}(U, V)$ is the space of bounded linear operators from U to V. If $A \in \mathbb{L}(U, V)$, $R(A)$ and $N(A)$ shall denote respectively its range and kernel and A^* its adjoint.

7.3.1 Generalized Lipschitz conditions

Convergence results for the Gauss-Newton algorithm are typically obtained requiring Lipschitz continuity of the operator F' [DS96]. In [Wan99, Wan00], Wang introduced some weaker notions of Lipschitz continuity in the context of Newton's method. Recently, also convergence of the Gauss-Newton method has been proved under such generalized Lipschitz conditions, see e.g. [LZJ04, AH09, AH10]. In this section we recall the definitions and review some basic properties of generalized Lipschitz continuous functions.

First of all recall that a set $\Lambda \subset U$ is called *star shaped* with respect to some of its points $u_* \in \Lambda$ if the segment $[u_*, u]$ is contained in Λ for every $u \in \Lambda$.

Definition 7.3.1. *Let $f : \Omega \subseteq U \to V$ and $\Lambda \subseteq \Omega$ be a starshaped set with respect to $u_* \in \Lambda$. Fix $R \in (0, +\infty]$ such that $\sup_{u\in\Lambda} \|u - u_*\| \leq R$ and let $L : [0, R) \to \mathbb{R}$ be a positive and continuous function. The mapping f is said to satisfy the* radius Lipschitz condition *of center u_* with L average on Λ if*

$$\|f(u) - f(u_* + t(u - u_*))\| \leq \int_{t\|u-u_*\|}^{\|u-u_*\|} L(s)\,\mathrm{d}s \tag{7.8}$$

for all $t \in [0, 1]$ and $u \in \Lambda$.

Note that denoting by $\Gamma : [0, R) \to \mathbb{R}$ a primitive function of L, e.g. $\Gamma(r) = \int_0^r L(s)\,\mathrm{d}s$, inequality (7.8) can be written as

$$\|f(u) - f(u_* + t(u - u_*))\| \leq \Gamma(\|u - u_*\|) - \Gamma(t\|u - u_*\|).$$

By definition Γ is absolutely continuous and differentiable, with $\Gamma'(r) = L(r)$. Since $L \geq 0$, Γ is monotonically increasing. Assuming L to be increasing, we get that Γ is convex.

Definition 7.3.2. *Assume the hypotheses of Definition 7.3.1. We say that $f : \Omega \subseteq U \to V$ satisfies the* center Lipschitz condition *of center u_* with L average on Λ if it verifies*

$$\|f(u) - f(u_*)\| \leq \int_0^{\|u-u_*\|} L(s)\,\mathrm{d}s \tag{7.9}$$

for every $u \in \Lambda$.

The original definitions of Wang [Wan99] do not require the continuity of the function L but just an integrability assumption. Our choice simplifies the proofs, but we remark that this requirement is not essential. Indeed, the proofs can be modified to handle also the more general case of Wang, at the cost of slight technical complications. In addition, the most well-known examples of Lipschitz averages are continuous.

Remark 7.3.3. *If f is Lipschitz continuous on a convex set Λ with constant L then it satisfies the radius and center Lipschitz condition of center u_* with average constantly equal* *to L on Λ, for every $u_* \in \Lambda$. Vice versa, in the definitions above, if we take L constant we obtain two intermediate concepts of Lipschitz continuity, called radius and center Lipschitz continuity, which are still in general weaker than the classical notion, being centered at a specific point.*

Note also that the center Lipschitz condition is weaker than the corresponding radius one.

Let $F : \Omega \subseteq U \to V$ be a a Fréchet differentiable operator. It is well-known, see e.g. [Pol87], that if F' is Lipschitz continuous with constant L then the following inequality holds for every $u, u_* \in \Omega$:

$$\|F(u_*) - F(u) - F'(u)(u_* - u)\| \leq \frac{L}{2}\|u_* - u\|^2. \tag{7.10}$$

We are going to show that under the weaker Lipschitz conditions introduced above it is still possible to prove two estimates which are similar to (7.10). To this aim we need the following three propositions. In the first one we prove two key inequalities, and in the subsequent ones we rewrite them in a form more similar to (7.10). The subsequent result is contained implicitly in several recent papers providing local results about Gauss-Newton method, see e.g. [LW02, LZJ04].

Proposition 7.3.4. *Let $F : \Omega \subseteq U \to V$ be a Gâteaux differentiable operator. Then:*

(i) if F' satisfies the radius Lipschitz condition of center u_* with L average on $U \subseteq \Omega$ (with L and Λ as in Definition 7.3.1), then for all $u \in \Lambda$

$$\|F(u_*) - F(u) - F'(u)(u_* - u)\| \leq \int_0^{\|u-u_*\|} L(s)s\, \mathrm{d}s. \tag{7.11}$$

(ii) if F' satisfies the center Lipschitz condition with L average at u_* on $\Lambda \subseteq \Omega$ (with L and U as in Definition 7.3.2), then for all $u \in \Lambda$

$$\|F(u_*) - F(u) - F'(u)(u_* - u)\| \leq \int_0^{\|u-u_*\|} (2\|u - u_*\| - s)L(s)\, \mathrm{d}s. \tag{7.12}$$

Proof. Let $u \in \Lambda$ and define $\phi : [0, 1] \to V$ by setting $\phi(t) = F(u_* + t(u - u_*))$. Clearly ϕ is differentiable and $\phi'(t) = F'(u_* + t(u - u_*))(u - u_*)$. Then

$$F(u) - F(u_*) = \phi(1) - \phi(0) = \int_0^1 F'(u_* + t(u - u_*))(u - u_*)\, \mathrm{d}t.$$

Therefore

$$F(u_*) - F(u) - F'(u)(u_* - u) = \int_0^1 \left(F'(u_* + t(u - u_*)) - F'(u)\right)(u_* - u)\, \mathrm{d}t$$

and hence

$$\|F(u_*) - F(u) - F'(u)(u_* - u)\| \leq \int_0^1 \|F'(u_* + t(u - u_*)) - F'(u)\| \|u - u_*\| \,\mathrm{d}t.$$

Let us first prove (i). By (7.8), we get

$$\int_0^1 \|F'(u_* + t(u - u_*)) - F'(u)\| \|u - u_*\| \,\mathrm{d}t \leq \|u - u_*\| \int_0^1 \int_{t\|u-u_*\|}^{\|u-u_*\|} L(s) \,\mathrm{d}s \,\mathrm{d}t. \qquad (7.13)$$

Note that in general, setting $\Gamma(\rho) = \int_0^\rho L(s)\,\mathrm{d}s$, it follows

$$\begin{aligned}
\int_0^1 \left(\int_{t\rho}^{\rho} L(s)\,\mathrm{d}s \right) \rho \,\mathrm{d}t &= \int_0^1 \left(\int_0^{\rho} L(s)\,\mathrm{d}s - \int_0^{t\rho} L(s)\,\mathrm{d}s \right) \rho \,\mathrm{d}t \\
&= \rho\, \Gamma(\rho) - \int_0^1 \Gamma(t\rho)\rho \,\mathrm{d}t \\
&= [s\, \Gamma(s)]_0^\rho - \int_0^\rho \Gamma(s)\,\mathrm{d}s \\
&= \int_0^\rho s\, \Gamma'(s)\,\mathrm{d}s \\
&= \int_0^\rho L(s) s \,\mathrm{d}s \qquad (7.14)
\end{aligned}$$

where we used the change of variables $s = t\rho$ and an integration by parts. Writing the equality obtained in (7.14) for $\rho = \|u - u_*\|$, (7.13) becomes

$$\|F(u_*) - F(u) - F'(u)(u_* - u)\| \leq \int_0^{\|u-u_*\|} L(s) s \,\mathrm{d}s,$$

so that (i) is proved.
To show that (ii) holds, observe that the center Lipschitz condition (7.9) implies

$$\begin{aligned}
\|F'(u_* + t(u - u_*)) - F'(u)\| &\leq \|F'(u_* + t(u - u_*)) - F'(u_*)\| + \|F'(u_*) - F'(u)\| \\
&\leq \int_0^{t\|u-u_*\|} L(s)\,\mathrm{d}s + \int_0^{\|u-u_*\|} L(s)\,\mathrm{d}s
\end{aligned}$$

Reasoning as in the previous case and using the same notations it follows

$$\begin{aligned}\|F(u_*) - F(u) - F'(u)[u_* - x]\| &\le \int_0^1 \Gamma(t\rho)\rho \,\mathrm{d}t + \Gamma(\rho)\rho \\ &= \int_0^\rho \Gamma(s)\,\mathrm{d}s + \Gamma(\rho)\rho \\ &= \int_0^\rho \Gamma(s)\,\mathrm{d}s + \big[(2\rho - s)\Gamma(s)\big]_0^\rho \\ &= \int_0^\rho (2\rho - s)\Gamma'(s)\,\mathrm{d}s \\ &= \int_0^{\|u-u_*\|} (2\|u-u_*\| - s)L(s)\,\mathrm{d}s. \qquad \square\end{aligned}$$

The following Propositions are a direct consequence of Lemma 2.2 in [LW03], and have already been stated in a slightly different form in [LZJ04]. We include the proofs for the sake of completeness.

Proposition 7.3.5. *Given $L : [0,R) \to \mathbb{R}$ a continuous, positive and increasing function, the function γ_λ defined by setting*

$$\gamma_\lambda : [0,R) \to \mathbb{R}, \qquad \gamma_\lambda(r) = \begin{cases} \dfrac{1}{r^{1+\lambda}} \displaystyle\int_0^r s^\lambda L(s)\,\mathrm{d}s & \text{if } r \in (0,R) \\[2ex] \dfrac{L(0)}{1+\lambda} & \text{if } r = 0, \end{cases} \tag{7.15}$$

is well-defined, continuous, positive and increasing for all $\lambda \ge 0$. Moreover γ_λ is constant and equal to $L/(1+\lambda)$ if L is constant, and it is strictly increasing if L is strictly increasing. Finally the following inequality holds for every $r \in [0,R)$

$$(1+\lambda)\gamma_\lambda(r) \le L(r). \tag{7.16}$$

Proof. Clearly γ_λ is differentiable on $(0,R)$ since it is a product of differentiable functions and by definition

$$r^{1+\lambda}\gamma_\lambda(r) = \int_0^r s^\lambda L(s)\,\mathrm{d}s. \tag{7.17}$$

Differentiating both members of (7.17), it follows

$$(1+\lambda)r^\lambda\gamma_\lambda(r) + r^{1+\lambda}\gamma_\lambda'(r) = r^\lambda L(r),$$

therefore

$$r\gamma_\lambda'(r) = L(r) - (1+\lambda)\gamma_\lambda(r), \tag{7.18}$$

Thus, if we prove (7.16) we also get that $\gamma_\lambda(r)$ is increasing. To this aim, taking into account that L is increasing, we have

$$r^{1+\lambda}\gamma_\lambda(r) = \int_0^r u^\lambda L(s)\,\mathrm{d}s \le \int_0^r u^\lambda L(r)\,\mathrm{d}s = \frac{r^{1+\lambda}}{1+\lambda}L(r) \tag{7.19}$$

from which (7.16) follows. Note that if L is strictly increasing the inequality in (7.19) is strict, therefore in this case, recalling (7.18), $\gamma_\lambda'(r) > 0$ on $(0,R)$. On the other hand, if L is constant the inequality in (7.19) is indeed an equality and $\gamma_\lambda'(r) = 0$ by (7.18) implying that γ_λ is constant on $(0,R)$. The continuity of γ_λ at 0 follows by L'Hospital's rule. In fact, using that L is continuous at 0:

$$\lim_{r\to 0}\gamma_\lambda(r) = \lim_{r\to 0}\frac{\int_0^r u^\lambda L(s)\,\mathrm{d}s}{r^{1+\lambda}} = \lim_{r\to 0}\frac{r^\lambda L(r)}{(1+\lambda)r^\lambda} = \frac{L(0)}{1+\lambda}. \qquad \square$$

Using the function γ_0 introduced in Proposition 7.3.5 the center Lipschitz condition with L average can be written in the following form, resembling the classical definition of Lipschitz continuity

$$\|f(u) - f(u_*)\| \le \gamma_0(\|u-u_*\|)\|u-u_*\|.$$

Proposition 7.3.6. *Under the assumptions of Proposition 7.3.5, the function*

$$\gamma^c : [0,R) \to \mathbb{R}, \qquad \gamma^c(r) = \begin{cases} \dfrac{1}{r^2}\displaystyle\int_0^r (2r-s)L(s)\,\mathrm{d}s & \text{if } r\in(0,R) \\[2ex] \dfrac{3L(0)}{2} & \text{if } r = 0, \end{cases} \tag{7.20}$$

is well-defined, continuous, positive and increasing.

Proof. The definition of γ^c immediately implies

$$r^2\gamma^c(r) = \int_0^r (2r-s)L(s)\,\mathrm{d}s = 2r\int_0^r L(s)\,\mathrm{d}s - \int_0^r sL(s)\,\mathrm{d}s \tag{7.21}$$

and differentiating both members of (7.21)

$$2r\gamma^c(r) + r^2(\gamma^c)'(r) = 2\int_0^r L(s)\,\mathrm{d}s + rL(r)$$

Dividing by r, and using the notations of Proposition 7.3.5, we obtain

$$r(\gamma^c)'(r) = 2(\gamma_0(r) - \gamma^c(r)) + L(r).$$

Therefore, in order to prove that γ^c is increasing we just need to show that

$$2\gamma^c(r) \le 2\gamma_0(r) + L(r). \tag{7.22}$$

In fact, using the definitions of the functions γ^c and γ_0 and the monotonicity of L we have:

$$\begin{aligned}2r^2\gamma^c(r) &= 2\int_0^r rL(s)\,\mathrm{d}s + 2\int_0^r (r-s)L(s)\,\mathrm{d}s\\ &\le 2r^2\gamma_0(r) + 2L(r)\int_0^r (r-s)\,\mathrm{d}s\\ &= 2r^2\gamma_0(r) + r^2L(r),\end{aligned}$$

that clearly implies (7.22). The continuity of γ^c at 0 can be deduced as follows

$$\lim_{r\to 0}\gamma^c(r) = \lim_{r\to 0} 2\gamma_0(r) - \gamma_1(r) = 2L(0) - \frac{L(0)}{2} = \frac{3}{2}L(0).$$

relying on the continuity of γ_0 and γ_1 proved in Proposition 7.3.5. $\square$

Remark 7.3.7. *Using the functions γ_0, γ_1 and γ^c introduced in* (7.15) *and in* (7.20)*, the inequality* (7.9) *written for F' becomes*

$$\|F'(u) - F'(u_*)\| \le \gamma_0(\|u-u_*\|)\|u-u_*\|.$$

The inequalities (7.11) *and* (7.12) *can be written respectively as*

$$\|F(u_*) - F(u) - F'(u)(u_*-u)\| \le \gamma_1(\|u-u_*\|)\|u-u_*\|^2 \tag{7.23}$$

and

$$\|F(u_*) - F(u) - F'(u)(u_*-u)\| \le \gamma^c(\|u-u_*\|)\|u-u_*\|^2, \tag{7.24}$$

that generalize the inequality (7.10)*.*

If F' is radius Lipschitz continuous of center u_* with L average, it is also center Lipschitz continuous at u_* with the same average L. Thus both inequalities (7.23) *and* (7.24) *hold true, but the first one gives a tighter bound. Indeed, using equation* (7.21) *and the fact that $\gamma_1(r) \le \gamma_0(r)$, it is straightforward to see that $\gamma_1(r) \le \gamma^c(r)$.*

Note moreover that the functions $r\gamma_0(r), r^2\gamma_1(r)$ and $r^2\gamma^c(r)$ are always strictly increasing and if L is a constant function equal to L, then

$$\gamma_0(r) = L, \qquad \gamma_1(r) = \frac{L}{2}, \qquad \gamma^c(r) = \frac{3}{2}L.$$

Remark 7.3.8. *It is worth noting that, even though only a Gâteaux differentiability has been required, the previous inequalities together with the hypothesis on the function L implies Fréchet differentiability at u_*.*

7.3.2 Generalized inverses

In this section we collect some well-known results regarding the *Moore-Penrose generalized inverse* (also known as *pseudoinverse*) $A^\dagger$ of a linear operator A. They will be useful in the rest of the chapter. For the definition and a comprehensive analysis of the properties of the Moore-Penrose inverse we refer the reader to [Gro77].

Assume that $A \in \mathbb{L}(U, V)$ has a closed range. The pseudoinverse of A is the linear operator $A^\dagger \in \mathbb{L}(V, U)$ defined by means of the four "Moore-Penrose equations"

$$AA^\dagger A = A, \quad A^\dagger AA^\dagger = A^\dagger, \quad (AA^\dagger)^* = AA^\dagger, \quad (A^\dagger A)^* = A^\dagger A. \tag{7.25}$$

Denoting by $P_{N(A)}$ and $P_{R(A)}$ the orthogonal projectors onto the kernel and the range of A respectively, from the definition it is clear that

$$A^\dagger A = I - P_{N(A)}, \qquad AA^\dagger = P_{R(A)}. \tag{7.26}$$

In case A is injective, $N(A) = \{0\}$ and $A^\dagger A = I$, that is $A^\dagger$ is a left inverse of A. Furthermore, for each $A \in \mathbb{L}(U, V)$ the following statements are equivalent:

- A is injective and the range of A is closed;
- $A^* A$ is invertible in $\mathbb{L}(U, U)$.

and if one of those equivalent conditions is true then $A^\dagger = (A^*A)^{-1}A^*$ and $\|A^\dagger\|^2 = \|(A^*A)^{-1}\|$.

The following lemma gives a perturbation bound for the Moore-Penrose pseudoinverse, see [Ste69, Wed73].

Lemma 7.3.9. *Let $A, B \in \mathbb{L}(U, V)$ with A injective and $R(A)$ closed. If $\|(B - A)A^\dagger\| < 1$, then B is injective, $R(B)$ is closed and*

$$\|B^\dagger\| \leq \frac{\|A^\dagger\|}{1 - \|(B - A)A^\dagger\|}.$$

Moreover

$$\|B^\dagger - A^\dagger\| \leq \sqrt{2}\|A^\dagger\|\|B^\dagger\|\|B - A\|,$$

and therefore

$$\|B^\dagger - A^\dagger\| \leq \sqrt{2}\frac{\|A^\dagger\|^2\|B - A\|}{1 - \|A^\dagger\|\|B - A\|}.$$

7.3.3 The proximity operator

This section consists of an introduction on proximity operators, which were first introduced by Moreau in [Mor62], and further investigated in [Mor63, Mor65] as a generalization of the notion of convex projection operator. Let $H : U \to U$ be a continuous, positive and selfadjoint operator, bounded from below, and therefore invertible. Then we can define a new scalar product on U by setting $\langle u, z\rangle_H = \langle u, Hz\rangle$. The corresponding induced norm $\|\cdot\|_H$ is equivalent to the given norm on U, since the following inequalities hold true

$$\frac{1}{\|H^{-1}\|}\|u\|^2 \le \|u\|_H^2 \le \|H\|\|u\|^2. \tag{7.27}$$

The *Moreau-Yosida approximation* of a convex and lower semicontinuous function $g : U \to \mathbb{R}\cup\{+\infty\}$ with respect to the scalar product induced by H is the function $M_g : U \to \mathbb{R}$ defined by setting

$$M_g(z) = \inf_{u\in U}\left\{g(u) + \frac{1}{2}\|u - z\|_H^2\right\}. \tag{7.28}$$

For every $z \in U$, the infimum in equation (7.28) is attained at a unique point, denoted $\operatorname{prox}_g^H(z)$. In this way, an operator

$$\operatorname{prox}_g^H : U \to U$$

is defined, which is called the *proximity operator* associated to g w.r.t. H. In case $H = I$ is the identity, the proximity operator is denoted simply by prox_g. Writing the first order optimality conditions for (7.28), we get

$$p = \operatorname{prox}_g^H(z) \iff 0 \in \partial g(p) + H(p - z) \iff Hz \in (\partial g + H)(p), \tag{7.29}$$

which gives

$$\operatorname{prox}_g^H(z) = (H + \partial g)^{-1}(Hz).$$

We remark that the map $(H + \partial g)^{-1}$ (in principle multi-valued) is single-valued, since we know that the minimum is attained at a unique point.

Lemma 7.3.10. *The proximity operator* $\operatorname{prox}_g^H : U \to U$ *is Lipschitz with constant* $\sqrt{\|H\|\|H^{-1}\|}$ *with respect to* $\|\cdot\|$, *namely*

$$\|\operatorname{prox}_g^H(z_1) - \operatorname{prox}_g^H(z_2)\| \le \sqrt{\|H\|\|H^{-1}\|}\|z_1 - z_2\|. \tag{7.30}$$

Proof. Being the proximity operator firmly nonexpansive with respect to the scalar product induced by H (see e.g. Lemma 2.4 in [CW05]) we have

$$\|\operatorname{prox}_g^H(z_1) - \operatorname{prox}_g^H(z_2)\|_H \le \|z_1 - z_2\|_H.$$

Using the inequalities in (7.27) relating $\|\cdot\|$ and $\|\cdot\|_H$ we get the desired result. □

It is also possible to show that in some cases the computation of the proximity operator with respect to the scalar product induced by H can be brought back to the computation of the proximity operator with respect to the original norm. In particular, the following proposition holds.

Proposition 7.3.11. *Let $A \in \mathbb{L}(U, V)$. Let us suppose A to be injective with closed range. Set $H = A^*A$ and assume $g : U \to \mathbb{R} \cup \{+\infty\}$ a proper, convex and lower semicontinuous functional. Then*

$$\operatorname{prox}_g^H = A^\dagger \operatorname{prox}_{g \circ A^\dagger} A$$

Proof. Being A injective, H is positive and invertible, thus

$$\operatorname{prox}_g^H : U \to U \qquad \operatorname{prox}_g^H(u) = \operatorname{argmin}_{z \in U} \left\{ g(z) + \frac{1}{2}\|z - u\|_H^2 \right\}$$

where

$$\|z - x\|_H^2 = \langle A^*A(z - u), z - x\rangle = \langle A(z - u), A(z - u)\rangle = \|A(z - u)\|^2.$$

Therefore

$$\operatorname{prox}_g^H(u) = \operatorname{argmin}_{z \in U} \left\{ g(z) + \frac{1}{2}\|A(z - u)\|^2 \right\}. \tag{7.31}$$

On the other hand, since $g \circ A^\dagger : V \to \mathbb{R} \cup \{+\infty\}$ is convex and lower semicontinuous the corresponding proximity operator with respect to $\|\cdot\|$ is well-defined and

$$\operatorname{prox}_{g \circ A^\dagger} : V \to V \qquad \operatorname{prox}_{g \circ A^\dagger}(v) = \operatorname{argmin}_{t \in V} \left\{ g(A^\dagger t) + \frac{1}{2}\|t - v\|^2 \right\}$$

If we set $\overline{u} = \operatorname{prox}_g^H(u)$, by (7.31) we obtain

$$g(\overline{u}) + \frac{1}{2}\|A\overline{u} - Au\|^2 \le g(z) + \frac{1}{2}\|Az - Au\|^2 \quad \forall z \in U.$$

Moreover, by setting $\overline{v} = A\overline{u}$, taking $t \in V$, with $t = t_1 + t_2$ such that $t_1 \in R(A)$ and $t_2 \in R(A)^\perp$ and $z = A^\dagger t \in U$, we have

$$\begin{aligned}
g(A^\dagger t) + \frac{1}{2}\|t - Au\|^2 &= g(A^\dagger t) + \frac{1}{2}\|t_1 + t_2 - Au\|^2 \\
&= g(A^\dagger t) + \frac{1}{2}\|P_{R(A)}t - Au\|^2 + \frac{1}{2}\|t_2\|^2 \\
&\ge g(A^\dagger t) + \frac{1}{2}\|AA^\dagger t - Au\|^2 \\
&= g(z) + \frac{1}{2}\|Az - Au\|^2 \\
&\ge g(\overline{u}) + \frac{1}{2}\|A\overline{u} - Au\|^2 \\
&= g(A^\dagger \overline{v}) + \frac{1}{2}\|\overline{v} - Au\|^2.
\end{aligned}$$

We finally get

$$\overline{v} = \operatorname{argmin}_{t\in V} \left\{ g(A^\dagger t) + \frac{1}{2}\|t - Au\|^2 \right\} = \operatorname{prox}_{g\circ A^\dagger}(Au)$$

and thus using (7.26)

$$\operatorname{prox}_g^H(u) = \overline{u} = A^\dagger A\overline{u} = A^\dagger \overline{v} = A^\dagger \operatorname{prox}_{g\circ A^\dagger}(Au). \qquad \square$$

Since in the sequel the proximity operators will be computed with respect to a variable norm $\|\cdot\|_H$, we are interested in the behavior of the proximity operator when H varies.

Lemma 7.3.12. *Let H_1 and H_2 be two continuous positive selfadjoint operators on U, both bounded from below. It holds*

$$\|\operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\| \leq \|H_1^{-1}\|\|(H_1 - H_2)(z - \operatorname{prox}_g^{H_2}(z))\|. \tag{7.32}$$

Proof. By (7.29) it follows

$$H_i(z - \operatorname{prox}_g^{H_i}(z)) \in \partial g(\operatorname{prox}_g^{H_i}(z)), \quad i = 1, 2.$$

Then, by definition of subdifferential the following inequalities hold true

$$\begin{aligned} g(\operatorname{prox}_g^{H_2}(z)) \geq & g(\operatorname{prox}_g^{H_1}(z)) \\ & + \langle H_1(z - \operatorname{prox}_g^{H_1}(z)), \operatorname{prox}_g^{H_2}(z) - \operatorname{prox}_g^{H_1}(z)\rangle \end{aligned}$$

$$\begin{aligned} g(\operatorname{prox}_g^{H_1}(z)) \geq & g(\operatorname{prox}_g^{H_2}(z)) \\ & + \langle H_2(z - \operatorname{prox}_g^{H_2}(z)), \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle. \end{aligned}$$

Summing them, we obtain

$$0 \geq \langle H_2(z - \operatorname{prox}_g^{H_2}(z)) - H_1(z - \operatorname{prox}_g^{H_1}(z)), \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle,$$

and equivalently

$$\begin{aligned} &\langle H_1 \operatorname{prox}_g^{H_1}(z) - H_2 \operatorname{prox}_g^{H_2}(z), \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle \leq \\ &\qquad\qquad \langle (H_1 - H_2)z, \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle. \end{aligned}$$

Adding and subtracting the same term, the previous inequality can also be written as

$$\begin{aligned} &\langle H_1(\operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)), \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle \leq \\ &\qquad\qquad \langle (H_1 - H_2)(z - \operatorname{prox}_g^{H_2}(z), \operatorname{prox}_g^{H_1}(z) - \operatorname{prox}_g^{H_2}(z)\rangle, \end{aligned}$$

from which (7.32) follows. $\square$

Note that in the previous lemma H_1 and H_2 play a symmetric role, so that they can be interchanged.

Remark 7.3.13. *Combining* (7.30) *and* (7.32)*, we get:*

$$\begin{aligned}\|\mathrm{prox}_g^{H_1}(z_1) - \mathrm{prox}_g^{H_2}(z_2)\| &\leq \|\mathrm{prox}_g^{H_1}(z_1) - \mathrm{prox}_g^{H_1}(z_2)\| + \|\mathrm{prox}_g^{H_1}(z_2) - \mathrm{prox}_g^{H_2}(z_2)\| \\ &\leq \left(\|H_1\|\|H_1^{-1}\|\right)^{1/2}\|z_1 - z_2\| \qquad (7.33) \\ &\qquad + \|H_1^{-1}\|\|(H_1 - H_2)(z_2 - \mathrm{prox}_g^{H_2}(z_2))\|,\end{aligned}$$

for every $z_1, z_2 \in U$ and H_1, H_2 continuous and positive selfadjoint operators on U, bounded from below.

7.4 Setting the minimization problem

In this section we collect some basic properties of the solutions of problem $(\mathcal{P})$. The following will be standing hypotheses throughout the chapter.

$$(SH) \qquad \begin{cases} F : \Omega \subseteq U \to V \text{ is Gâteaux differentiable} \\ \\ g : U \to \mathbb{R} \cup \{+\infty\} \text{ is proper, lower semicontinuous and convex.} \end{cases}$$

Recall that g proper means the *effective domain* $\mathrm{dom}(g) := \{u \in U \ : \ g(u) < +\infty\}$ is nonempty.

Without loss of generality, we shall assume $v = 0$ in the problem $(\mathcal{P})$, since the general case can be recovered just by replacing F with $F - v$. Thus, hereafter, the following optimization problem will be considered

$$\boxed{\min_{u \in U} \frac{1}{2}\|F(u)\|^2 + g(u) := \varphi_0(u).} \qquad (\mathcal{P}_0)$$

The functional φ_0 is in general nonconvex and searching for global minimizers turns out to be a challenging task. Therefore, the focus of this chapter is on local minimizers of φ_0, whose existence shall be assumed from now on. Generally speaking, Gauss-Newton methods are of a local character, and allow to find a local minimizer. As it is well-known a *local minimizer* u_* of φ_0 is a point such that $u_* \in \mathrm{dom}(g) \cap \Omega$ and there exists a neighborhood U of u_* such that $\varphi_0(u_*) \leq \varphi_0(u)$ for all $x \in U$.

By the way, hypotheses (SH) are not enough to guarantee the existence of a global minimizer of the problem $(\mathcal{P}_0)$. Such existence can be proved relying on the Weierstrass theorem as soon as we impose F to be weak to weak continuous and φ_0 (weakly) coercive, namely $\lim_{\|u\| \to +\infty} \varphi_0(u) = +\infty$.

We start by providing first order conditions for local minimizers.

Proposition 7.4.1. *Suppose* (SH) *are satisfied and let* $u_* \in \Omega$ *be a local minimizer of* φ_0. *Then the following* stationary condition *holds*

$$-F'(u_*)^* F(u_*) \in \partial g(u_*).$$

Moreover, if $F'(u_*)$ *is injective and* $R(F'(u_*))$ *is closed, then* u_* *satisfies the* fixed point equation

$$u_* = \operatorname{prox}_g^{H(u_*)}(u_* - F'(u_*)^\dagger F(u_*)),$$

with $H(u_*) := F'(u_*)^* F'(u_*)$.

Proof. Suppose that u_* is a local minimizer of φ_0. Denoting by $\varphi_0'(u_*, d)$ the directional derivative of φ_0 at u_* in the direction $d \in U$, which exists thanks to (SH), the first order optimality conditions for u_* implies

$$\varphi_0'(u_*, d) \geq 0 \qquad \forall d \in U. \tag{7.34}$$

As a consequence of the differentiability of F and the convexity of g (7.34) can be rewritten as

$$\langle -F'(u_*)^* F(u_*), d\rangle \leq g'(u, d) \qquad \forall d \in U,$$

and consequently, by Proposition 3.1.6 in [BL00], also as

$$-F'(u_*)^* F(u_*) \in \partial g(u_*), \tag{7.35}$$

which is the stationary condition of the thesis. To prove that u_* satisfies the fixed point equation note that adding $H(u_*)u_*$ to both members of (7.35) we have

$$H(u_*)u_* - F'(u_*)^* F(u_*) \in (H(u_*) + \partial g)(u_*).$$

Since $H(u_*)$ is invertible, then the previous equation can be also rewritten as

$$H(u_*)(u_* - H(u_*)^{-1} F'(u_*)^* F(u_*)) \in (H(u_*) + \partial g)(u_*).$$

Recalling equation (7.29) and the properties enjoyed by the pseudoinverse we obtain the second assertion. $\square$

7.5 The algorithm - convergence analysis

In this section we state the main result of the chapter, consisting in the study of the convergence of a generalized Gauss-Newton method for solving problem $(\mathcal{P}_0)$. The flavor is similar to the most recent results concerning the standard Gauss-Newton method, proved in [LZJ04]. We start describing some basic properties of the proposed algorithmic framework.

$$\left|\begin{array}{l} u_0 \in \mathrm{dom}(g) \\ u_{n+1} = \mathrm{argmin}_{u\in U} \dfrac{1}{2}\|F(u_n) + F'(u_n)(u-u_n)\|^2 + g(u). \end{array}\right. \tag{7.36}$$

Note that since the quantity inside the norm has been linearized, this problem can be solved explicitly, for instance using first order methods for the minimization of nonsmooth convex functions, such as bundle methods or forward-backward methods (see [HUL93, CW05]). Writing down the first order optimality conditions we will get a similar formula to the one in Proposition 7.4.1 for a minimizer u_*.

Proposition 7.5.1. *Let us suppose $F'(u_n)$ to be injective with closed range and set $H(u_n) = F'(u_n)^*F'(u_n)$. Then, the formula* (7.36) *defining u_{n+1} is equivalent to*

$$u_{n+1} = \mathrm{prox}_g^{H(u_n)}(u_n - F'(u_n)^\dagger F(u_n)). \tag{7.37}$$

Proof. Thanks to the assumptions made on $F'(u_n)$ the operator $H(u_n)$ is invertible. Writing the first order necessary conditions, which are satisfied by u_{n+1} we obtain

$$\begin{aligned} & 0 \in F'(u_n)^*[F(u_n) + F'(u_n)(u_{n+1}-u_n)] + \partial g(u_{n+1}) \\ \iff & F'(u_n)^*F'(u_n)u_n - F'(u_n)^*F(u_n) \in (F'(u_n)^*F'(u_n) + \partial g)(u_{n+1}) \\ \iff & u_{n+1} = (F'(u_n)^*F'(u_n) + \partial g)^{-1}(F'(u_n)^*F'(u_n)u_n - F'(u_n)^*F(u_n)) \\ \iff & u_{n+1} = (F'(u_n)^*F'(u_n) + \partial g)^{-1}F'(u_n)^*F'(u_n)\left(u_n - F'(u_n)^\dagger F(u_n)\right) \\ \iff & u_{n+1} = \mathrm{prox}_g^{H(u_n)}\left(u_n - F'(u_n)^\dagger F(u_n)\right) \end{aligned}$$

□

In the next theorem we provide a local convergence analysis of the proximal Gauss-Newton method, under the generalized Lipschitz conditions on F' introduced in Section 7.3.1. The proof is postponed to Section 7.6.

Theorem 7.5.2. *Suppose that (SH) are satisfied. Let $\Lambda \subseteq \Omega$ be an open starshaped set with respect to u_*, where $u_* \in \mathrm{dom}(g) \cap \Lambda$ is a local minimizer of φ_0. Moreover assume*

1. *$F'(u_*)$ is injective with closed range;*
2. *$F' : \Omega \subseteq U \to \mathbb{L}(U, V)$ is center Lipschitz continuous of center u_* with L average on Λ (L as in the definition 7.3.2 and increasing);*
3. *$[(1+\sqrt{2})\kappa + 1]\alpha\beta^2 L(0) < 1$, where $\alpha = \|F(u_*)\|, \beta = \|F'(u_*)^\dagger\|$, $\kappa = \|F'(u_*)^\dagger\|\|F'(u_*)\|$, the conditioning number of $F'(u_*)$.*

Define $\bar{R}$ and $q : [0, \bar{R}) \to \mathbb{R}_+$ by setting $\bar{R} = \sup\{r \in (0, R) \,:\, \gamma_0(r)r < 1/\beta\}$ and

$$q(r) = \frac{\beta}{1-\beta\gamma_0(r)r}\left\{\frac{\beta\gamma_0(r)\gamma^c(r)r^2 + \kappa\gamma^c(r)r}{(1-\beta\gamma_0(r)r)} + \frac{(1+\sqrt{2})\alpha\beta^2\gamma_0(r)^2 r}{1-\beta\gamma_0(r)r} + \frac{[(1+\sqrt{2})\kappa+1]\alpha\beta\gamma_0(r)}{1-\beta\gamma_0(r)r}\right\}.$$

The function q is continuous and strictly increasing. If we define

$$\bar{r} = \sup\{r \in (0, \bar{R}] \,:\, q(r) < 1\}, \tag{7.38}$$

and we fix $r \in \mathbb{R}$, with $0 < r \leq \bar{r}$, such that $B_r(u_*) \subseteq U$, we get that the sequence

$$u_0 \in B_r(u_*), \qquad u_{n+1} = \mathrm{prox}_g^{H(u_n)}\big(u_n - F'(u_n)^\dagger F(u_n)\big)$$

with $H(u_n) := F'(u_n)^* F'(u_n)$, is well-defined, i.e. $u_n \in B_r(u_*)$ and $F'(u_n)$ is injective with closed range and it holds

$$\|u_n - u_*\| \leq q_0^n \|u_0 - u_*\|,$$

where $q_0 := q(\|u_0 - u_*\|) < 1$.
More precisely, the following inequality is true

$$\|u_{n+1} - u_*\| \leq C_2\|u_n - u_*\|^2 + C_1\|u_n - u_*\|,$$

for constants $C_1 \geq 0$ and $C_2 > 0$ defined as

$$\begin{aligned} C_1 &= \frac{[(1+\sqrt{2})\kappa+1]\alpha\beta^2\gamma_0(\rho_{u_0})}{(1-\beta\gamma_0(\rho_{u_0})\rho_{u_0})^2}; \\ C_2 &= \frac{\kappa\beta\gamma^c(\rho_{u_0}) + (1+\sqrt{2})\alpha\beta^3\gamma_0(\rho_{u_0})^2 + \beta^2\gamma_0(\rho_{u_0})\gamma^c(\rho_{u_0})\rho_{u_0}}{(1-\beta\gamma_0(\rho_{u_0})\rho_{u_0})^2}, \end{aligned}$$

with $\rho_{u_0} = \|u_0 - u_*\|$.

Since $\bar{r}$ is chosen as the biggest value ensuring $q(r) \leq 1$ (a sufficient condition making the Gauss-Newton sequence convergent), $\bar{r}$ can be thought as the radius of the basin of attraction around the local minimum point u_*, even though in general we can't prove the optimality of this value.

Remark 7.5.3. *An analogous theorem is true if we strengthen the assumption 2 requiring F' to satisfy the radius Lipschitz condition with L average. All the statements remain true also replacing γ^c with γ_1. In particular the expression of $q(r)$ becomes*

$$q(r) = \frac{\beta}{1-\beta\gamma_0(r)r}\left\{\frac{\beta\gamma_0(r)\gamma_1(r)r^2 + \kappa\gamma_1(r)r}{1-\beta\gamma_0(r)r} + \frac{(1+\sqrt{2})\alpha\beta^2\gamma_0(r)^2 r}{1-\beta\gamma_0(r)r} + \frac{[(1+\sqrt{2})\kappa+1]\alpha\beta\gamma_0(r)}{1-\beta\gamma_0(r)r}\right\}. \tag{7.39}$$

This expression allows to increase the radius of convergence. Indeed $\gamma_1(r) \leq \gamma^c(r)$ by Remark 7.3.7 and then $q(r)$ computed in (7.39) *is always smaller then the corresponding one in Theorem 7.5.2.*

Actually, under the radius Lipschitz condition with L average on F', along the same line of the results given in [AH09, AH11], one can further improve the radius of convergence using a different average L_0 tailored for the center Lipschitz condition. In fact, being the center Lipschitz condition weaker then the radius one, one can possibly find a smaller average $L_0 \leq L$ for which equation (7.9) *is satisfied. In this event, we can employ the function γ_0 defined starting from L_0, that is*

$$\gamma_0(r; L_0) = \frac{1}{r}\int_0^r L_0(s)\,\mathrm{d}s,$$

which is smaller than the corresponding $\gamma_0(\cdot; L)$. Replacing $\gamma_0(r; L)$ with $\gamma_0(r; L_0)$ in formula (7.39) *a larger radius of convergence can be obtained (see the proof in the next section).*

Remark 7.5.4. *The hypotheses we impose are in line with the state-of-art literature about classical Gauss-Newton method ($g = 0$), see [LZJ04]. It is worth noting that the expression of $\bar{r}$ is not affected by the choice of g. On the other hand, the presence of the function g reduces the radius of convergence of the Gauss-Newton method. Indeed, the expression for $\bar{r}$ obtained in* (7.38)*, which is valid also in the case $g = 0$ is always smaller than the maximum radius of convergence that can be derived from equation (3.4) in [LZJ04], namely*

$$r_0 = \sup\{r \in (0, \bar{R}) \,:\, q_0(r) < 1\},$$

with

$$q_0(r) = \frac{\beta}{1-\beta\gamma_0(r)r}\left\{\gamma^c(r)r + \sqrt{2}\beta\alpha\gamma_0(r)\right\}.$$

The reason is that the bound (7.30) *we use, is not sharp in case $g = 0$, and this causes an additional term in the expression of $q(r)$.*

Remark 7.5.5. *The classical Gauss-Newton method, under generalized Lipschitz conditions, is also studied without assuming the injectivity of $F'(u_*)$. This actually falls into the topic of singular systems of equations (see e.g. [XL08, LHW10, AH11]). However, in our setting, the injectivity assumption is needed to ensure that the operator $H(u_n)$ is positive definite — this allowing the proper definition of the proximal operator* $\mathrm{prox}_g^{H(u_n)}$.

Conditions ensuring quadratic convergence. As in the classical case, also with the additional term g, for zero residual problems quadratic convergence holds. In fact, from the expression of C_1, we see that $C_1 = 0$ if $\alpha = 0$, i.e. $F(u_*) = 0$.

7.5.1 The case of constant average L

In case the function L is constant, we can derive also an explicit expression for the maximum ray of convergence $\bar{r}$.

Corollay 7.5.6. *Let the assumptions of Theorem 7.5.2 be satisfied and moreover assume $F'(u_*)$ to be center Lipschitz continuous of center u_* with* constant *average L on Λ. Define $q : [0, 1/(\beta L)) \to \mathbb{R}_+$ as*

$$q(r) = \frac{\beta}{1-\beta L r}\left\{\frac{3(\beta L^2 r^2 + \kappa L r)}{2(1-\beta L r)} + \frac{(1+\sqrt{2})\alpha\beta^2 L^2 r}{1-\beta L r} + \frac{[(1+\sqrt{2})\kappa + 1]\alpha\beta L}{1-\beta L r}\right\}, \quad (7.40)$$

which is continuous and strictly increasing in its domain. If we define

$$\begin{aligned} h &= [(1+\sqrt{2})\kappa + 1]\alpha\beta^2 L \quad (<1), \\ \bar{r} &= \frac{1}{\beta L}\left[-\left(2 + \frac{3\kappa}{2} + (1+\sqrt{2})\alpha\beta^2 L\right) + \sqrt{\left(2 + \frac{3\kappa}{2} + (1+\sqrt{2})\alpha\beta^2 L\right)^2 + 2(1-h)}\right] \end{aligned}$$

and we fix $r \in \mathbb{R}$ with $0 < r \leq \bar{r}$ such that $B_r(u_*) \subseteq \Lambda$ the conclusions of Theorem 7.5.2 hold with

$$\begin{aligned} C_1 &= \frac{[(1+\sqrt{2})\kappa + 1]\alpha\beta^2 L}{(1-\beta L \rho_{u_0})^2}; \\ C_2 &= \beta\frac{3\kappa L + 2(1+\sqrt{2})\alpha\beta^2 L^2 + 3\beta L^2 \rho_{u_0}}{2(1-\beta L \rho_{u_0})^2}. \end{aligned}$$

Proof. Using the expressions of γ_0 and γ^c found in Remark 7.3.7, one can easily show that $\overline{R} = 1/(\beta L)$ and q can be written as in (7.40).

As before q is continuous and strictly increasing on the interval $[0, 1/(\beta L))$, and

$$q(0) = h < 1, \qquad \lim_{r \to 1/(\beta L)} q(r) = +\infty.$$

Therefore $\bar{r}$ defined in (7.38) is the unique solution in $(0, 1/(\beta L))$ of the equation $q(r) = 1$. We are going to find that point explicitly by solving the equation $q(r) = 1$. The latter is equivalent to the following quadratic equation

$$z^2 + (4 + 3\kappa + 2(1 + \sqrt{2})\alpha\beta^2 L)z - 2(1 - h) = 0,$$

with $z \in [0, 1)$, $z = \beta L r$. That equation has the two distinct solutions

$$z = -\left(2 + \frac{3}{2}\kappa + (1 + \sqrt{2})\alpha\beta^2 L\right) \pm \sqrt{\left(2 + \frac{3}{2}\kappa + 2(1 + \sqrt{2})\alpha\beta^2 L\right)^2 + 2(1 - h)}.$$

Of course, we discard the negative solution, and we keep the one with the plus sign, which can be easily checked to belong to $(0, 1)$. □

Along the same line, a similar result concerning the case of radius Lipschitz continuity can be proved.

Corollary 7.5.7. *Let the assumptions of Theorem 7.5.2 be satisfied and moreover assume $F'(u_*)$ to be radius Lipschitz continuous of center u_* with* constant *average L on Λ. Define $q : [0, 1/(\beta L)) \to \mathbb{R}_+$ as*

$$q(r) = \frac{\beta}{1 - \beta L r}\left\{\frac{\beta L^2 r^2 + \kappa L r}{2(1 - \beta L r)} + \frac{(1 + \sqrt{2})\alpha\beta^2 L^2 r}{1 - \beta L r} + \frac{[(1 + \sqrt{2})\kappa + 1]\alpha\beta L}{1 - \beta L r}\right\},$$

which is continuous and strictly increasing in its domain. If we define

$$h = [(1 + \sqrt{2})\kappa + 1]\alpha\beta^2 L (< 1),$$

$$\bar{r} = \frac{1}{\beta L}\left[\left(2 + \frac{\kappa}{2} + (1 + \sqrt{2})\alpha\beta^2 L\right) - \sqrt{\left(2 + \frac{\kappa}{2} + (1 + \sqrt{2})\alpha\beta^2 L\right)^2 - 2(1 - h)}\right]$$

and we fix $r \in \mathbb{R}$ with $0 < r \leq \bar{r}$ such that $B_r(u_*) \subseteq \Lambda$ the conclusions of Theorem 7.5.2 hold with

$$C_1 = \frac{[(1 + \sqrt{2})\kappa + 1]\alpha\beta^2 L}{(1 - \beta L \rho_{u_0})^2};$$

$$C_2 = \beta\frac{\kappa L + 2(1 + \sqrt{2})\alpha\beta^2 L^2 + \beta L^2 \rho_{u_0}}{2(1 - \beta L \rho_{u_0})^2}.$$

for $r < 1/(\beta L)$.

7.6 Proof of Theorem 7.5.2

We are going to state some auxiliary results for proving convergence of the algorithm discussed in the previous section. The following proposition will be one of the building blocks to show that convergence holds.

Proposition 7.6.1. *Let $G : D \subseteq U \to U$, be a mapping and $u_* \in D$ a fixed point of G. Let $\Lambda \subseteq D$ be an open starshaped set with respect to $u_* \in \Lambda$. Assume G to satisfy the inequality*

$$\|G(u) - G(u_*)\| \leq q(\|u - u_*\|)\|u - u_*\|, \qquad \textit{for all } x \in \Lambda \tag{7.41}$$

for a given increasing function $q : [0, \overline{R}) \to [0, +\infty)$, continuous at 0 and such that $q(0) < 1$. Define

$$\bar{r} = \sup\{r \in (0, \overline{R}) \, : \, q(r) < 1\}.$$

Then $\bar{r} > 0$ and given $r \in \mathbb{R}$ with $0 < r \leq \bar{r}$ and $B_r(u_*) \subseteq \Lambda$, it follows $G(B_r(u_*)) \subseteq B_r(u_*)$, thus, given $u_0 \in B_r(u_*)$ the sequence defined by setting $u_{n+1} = G(u_n)$ is well-defined. Moreover, denoting $q_0 = q(\|u_0 - u_*\|)$ it holds $q_0 < 1$ and

$$\|u_{n+1} - u_*\| \leq q_0^n \|u_0 - u_*\|.$$

Proof. First note that $\bar{r} = \sup\{r \in (0, \overline{R}) \, : \, q(r) < 1\} > 0$ being $q(0) < 1$ and q continuous at 0. Fix $r \in \mathbb{R}$, $0 < r \leq \bar{r}$ such that $B_r(u_*) \subseteq \Lambda$ and $x \in B_r(u_*)$. Then by definition of $\bar{r}$, $q(\|u - u_*\|) < 1$ and therefore (7.41) implies that

$$\|G(u) - u_*\| \leq \|u - u_*\| < r,$$

i.e. $G(u) \in B_r(u_*)$. Thus $G(B_r(u_*)) \subseteq B_r(u_*)$ and a sequence can be defined in $B_r(u_*)$ by choosing $u_0 \in B_r(u_*)$ and setting $u_{n+1} = G(u_n)$. Being $\|u_n - u_*\| < \bar{r}$, again from the definition of $\bar{r}$ we have $q(\|u_n - u_*\|) < 1$, and from (7.41) we get

$$\|u_{n+1} - u_*\| = \|G(u_n) - u_*\| \leq q(\|u_n - u_*\|)\|u_n - u_*\| < \|u_n - u_*\|.$$

This implies that $q(\|u_{n+1} - u_*\|) \leq q(\|u_n - u_*\|)$, since q is increasing. Therefore, denoting $q(\|u_0 - u_*\|) =: q_0$ we get $q(\|u_n - u_*\|) \leq q_0 < 1$ for all $n \in \mathbb{N}$ and

$$\|u_{n+1} - u_*\| \leq q(\|u_n - u_*\|)\|u_n - u_*\| \leq q_0\|u_n - u_*\| \leq \ldots \leq q_0^n \|u_0 - u_*\|. \qquad \square$$

We now introduce some notations, allowing for rewriting the conditions which have been described in Proposition 7.4.1 for a local minimizer of φ_0. Define G and $\tilde{G}$ by setting

$$G(u) = u - F'(u)^\dagger F(u) \qquad \text{and} \qquad \tilde{G}(u) = \operatorname{prox}_g^{H(u)}(G(u)), \tag{7.42}$$

where $H(u) = F'(u)^* F'(u)$. The domain of G and $\tilde{G}$ is the subset D of Ω defined as

$$D = \{u \in \Omega \,:\, F'(u) \text{ is injective and } R(F'(u)) \text{ is closed}\}. \tag{7.43}$$

If $u_* \in D$ is a local minimizer of $(\mathcal{P}_0)$ the fixed point equation of Proposition 7.4.1 can be restated by saying that u_* is a fixed point for $\tilde{G}$, namely

$$u_* = \tilde{G}(u_*). \tag{7.44}$$

Proposition 7.6.2. *Assume (SH) and let u_* be a local minimizer of φ_0 belonging to D. Suppose that $\Lambda \subseteq \Omega$ is open and starshaped with respect to u_*. Moreover assume*

i) $F' : \Omega \subseteq U \to \mathbb{L}(U, V)$ *is center Lipschitz continuous of center u_* with $L : [0, R) \to \mathbb{R}_+$ average on $\Lambda \subseteq \Omega$;*

ii) $\alpha = \|F(u_*)\|$, $\beta = \|F'(u_*)^\dagger\|$ *and* $\kappa = \|F'(u_*)^\dagger\|\|F'(u_*)\|$.

Then, defining $\bar{R}$ by setting

$$\bar{R} = \sup\{r \in (0, R) \,:\, \gamma_0(r)r < 1/\beta\}$$

it follows that for all $r \in \mathbb{R}$ with $0 < r \leq \bar{R}$ and $B_r(u_*) \subseteq \Lambda$, $\tilde{G}$ satisfies

$$\|\tilde{G}(u) - u_*\| \leq q(\|u - u_*\|)\|u - u_*\|,$$

for all $x \in B_r(u_*)$, where $q : [0, \bar{R}) \to \mathbb{R}_+$ is defined as

$$q(r) = \frac{\beta}{1 - \beta\gamma_0(r)r}\left\{\frac{\beta\gamma_0(r)\gamma^c(r)r^2 + \kappa\gamma^c(r)r}{(1 - \beta\gamma_0(r)r)} + \frac{(1+\sqrt{2})\alpha\beta^2\gamma_0(r)^2 r}{1 - \beta\gamma_0(r)r} + \frac{[(1+\sqrt{2})\kappa + 1]\alpha\beta\gamma_0(r)}{1 - \beta\gamma_0(r)r}\right\}$$

and it is continuous and strictly increasing.

Proof. Since u_* is a local minimizer of φ_0 and $u_* \in D$, with D defined as in (7.43), u_* is a fixed point of $\tilde{G}$ (see (7.44)), therefore

$$G(u_*) - \operatorname{prox}_g^{H(u_*)} G(u_*) = G(u_*) - u_* = -F'(u_*)^\dagger F(u_*). \tag{7.45}$$

Fix $r \in \mathbb{R}$, with $0 < r \leq \bar{R}$ such that $B_r(u_*) \subseteq \Lambda$ and take $x \in B_r(u_*)$. Adopting the notations of Proposition 7.3.5, as noted in Remark 7.3.7, from the center Lipschitz hypothesis we get

$$\|F'(u) - F'(u_*)\|\|F'(u_*)^\dagger\| \leq \gamma_0(\|u - u_*\|)\|u - u_*\|\beta.$$

Recalling that Remark 7.3.7 ensures that the function $\rho \mapsto \rho\gamma_0(\rho)$ is continuous, strictly increasing and takes value 0 in 0, we have that $\bar{R} > 0$ and

$$\|F'(u) - F'(u_*)\|\|F'(u_*)^\dagger\| < \beta\gamma_0(r)r \leq 1,$$

and thus applying Lemma 7.3.9, $F'(u)$ is injective, with closed range, and

$$\|F'(u)^\dagger\| \leq \frac{\beta}{1 - \beta\gamma_0(\rho_u)\rho_u}, \quad \text{where} \quad \rho_u = \|u - u_*\|. \tag{7.46}$$

Applying inequality (7.33) with $H_1 = H(u)$, $H_2 = H(u_*)$, $z_1 = G(u)$ and $z_2 = G(u_*)$, and taking into account (7.45) we get

$$\begin{aligned}
\|\tilde{G}(u) - u_*\| &= \|\mathrm{prox}_g^{H(u)}(G(u)) - \mathrm{prox}_g^{H(u_*)}(G(u_*))\| \\
&\leq \big(\|H(u)\|\|H(u)^{-1}\|\big)^{1/2}\|G(u) - G(u_*)\| \\
&\quad + \|H(u)^{-1}\|\big\|(H(u) - H(u_*))\big(G(u_*) - \mathrm{prox}_g^{H(u_*)}G(u_*)\big)\big\| \\
&= \big(\|H(u)\|\|H(u)^{-1}\|\big)^{1/2}\|G(u) - G(u_*)\| \\
&\quad + \|H(u)^{-1}\|\|(H(u) - H(u_*))F'(u_*)^\dagger F(u_*)\|.
\end{aligned} \tag{7.47}$$

Moreover

$$\begin{aligned}
\|H(u)\| &= \|F'(u)^*F'(u)\| = \|F'(u)\|^2 \\
\|H(u)^{-1}\| &= \|[F'(u)^*F'(u)]^{-1}\| = \|F'(u)^\dagger\|^2.
\end{aligned}$$

Recalling the properties of the Moore-Penrose generalized inverse in (7.26) and Lemma 7.3.9 we get

$$\begin{aligned}
(H(u) - H(u_*))F'(u_*)^\dagger &= (F'(u)^*F'(u) - F'(u_*)^*F'(u_*))F'(u_*)^\dagger \\
&= F'(u)^*F'(u)F'(u_*)^\dagger - F'(u_*)^*F'(u_*)F'(u_*)^\dagger \\
&= F'(u)^*F'(u)F'(u_*)^\dagger - F'(u)^*P_{R(F'(u_*))} \\
&\qquad + F'(u)^*P_{R(F'(u_*))} - F'(u_*)^*P_{R(F'(u_*))} \\
&= F'(u)^*(F'(u) - F'(u_*))F'(u_*)^\dagger \\
&\qquad + (F'(u) - F'(u_*))^*P_{R(F'(u_*)),}
\end{aligned}$$

therefore,

$$\|(H(u) - H(u_*))F'(u_*)^\dagger\| \leq \big(\|F'(u)\|\|F'(u_*)^\dagger\| + 1\big)\,\|F'(u) - F'(u_*)\|. \tag{7.48}$$

Hence, substituting in (7.47) the bound derived in (7.48) we obtain

$$\begin{aligned}\|\tilde{G}(u) - u_*\| \leq \|F'(u)\|\|F'(u)^\dagger\|\|G(u) - G(u_*)\| \\ + \|F'(u)^\dagger\|^2 \left(\|F'(u)\|\|F'(u_*)^\dagger\| + 1\right) \|F'(u) - F'(u_*)\|\|F(u_*)\|.\end{aligned} \tag{7.49}$$

On the other hand, thanks to the properties of the Moore-Penrose pseudoinverse reported in (7.26) and the injectivity of $F'(u)$

$$\begin{aligned}G(u) - G(u_*) &= u - u_* - F'(u)^\dagger F(u) + F'(u_*)^\dagger F(u_*) \\ &= F'(u)^\dagger[F'(u)(u - u_*) - F(u) + F(u_*)] \\ &\quad + (F'(u_*)^\dagger - F'(u)^\dagger)F(u_*)\end{aligned}$$

and thus, using Lemma 7.3.9

$$\begin{aligned}\|G(u) - G(u_*)\| &\leq \|F'(u)^\dagger\|\|F(u_*) - F(u) - F'(u)(u_* - u)\| \\ &\quad + \|F'(u_*)^\dagger - F'(u)^\dagger\|\|F(u_*)\| \\ &\leq \|F'(u)^\dagger\|\|F(u_*) - F(u) - F'(u)(u_* - u)\| \\ &\quad + \sqrt{2}\|F'(u)^\dagger\|\|F'(u_*)^\dagger\|\|F'(u) - F'(u_*)\|\|F(u_*)\| \\ &= \|F'(u)^\dagger\|\big\{\|F(u_*) - F(u) - F'(u)(u_* - u)\| \\ &\quad + \sqrt{2}\|F'(u_*)^\dagger\|\|F(u_*)\|\|F'(u) - F'(u_*)\|\big\} \end{aligned} \tag{7.50}$$

Substituting (7.50) in (7.49)

$$\begin{aligned}\|\tilde{G}(u) - u_*\| \leq \|F'(u)^\dagger\|^2 \Big\{ &\|F'(u)\|\big(\|F(u_*) - F(u) - F'(u)(u_* - u)\| \\ &+ (1 + \sqrt{2})\|F'(u_*)^\dagger\|\|F(u_*)\|\|F'(u) - F'(u_*)\|\big) \\ &+ \|F'(u) - F'(u_*)\|\|F(u_*)\|] \Big\}\end{aligned} \tag{7.51}$$

Taking into account Remark 7.3.7, we can rewrite inequality (7.51) as

$$\begin{aligned}&\|\tilde{G}(u) - u_*\| \\ &\leq \|F'(u)^\dagger\|^2 \left\{\|F'(u)\| \left[\gamma^c(\rho_u)\rho_u^2 + (1 + \sqrt{2})\|F'(u_*)^\dagger\|\|F(u_*)\|\gamma_0(\rho_u)\rho_u\right] \right. \\ &\quad \left. + \|F(u_*)\|\gamma_0(\rho_u)\rho_u\right\}\end{aligned}$$

To find a bound for the quantity $\|F'(u)\|$, recall that κ is the conditioning number of $F'(u_*)$, i.e. $\kappa := \|F'(u_*)^\dagger\|\|F'(u_*)\|$, and by the triangular inequality and Remark (7.3.7) we get $\|F'(u)\| \leq \|F'(u) - F'(u_*)\| + \|F'(u_*)\| \leq \gamma_0(\rho_u)\rho_u + \kappa/\beta$. Thus, recalling (7.46), we finally obtain

$$
\begin{aligned}
&\|\tilde{G}(u) - u_*\| \\
&\leq \frac{\beta^2}{(1-\beta\gamma_0(\rho_u)\rho_u)^2}\Big\{(\gamma_0(\rho_u)\rho_u + \kappa/\beta)\Big[\gamma^c(\rho_u)\rho_u^2 + (1+\sqrt{2})\beta\alpha\gamma_0(\rho_u)\rho_u\Big] \\
&\qquad\qquad + \alpha\gamma_0(\rho_u)\rho_u\Big\},
\end{aligned}
$$

or, equivalently

$$
\begin{aligned}
\|\tilde{G}(u) - u_*\| \leq \frac{\beta}{1-\beta\gamma_0(\rho_u)\rho_u}&\Bigg\{\frac{\beta\gamma_0(\rho_u)\gamma^c(\rho_u)\rho_u^2 + \kappa\gamma^c(\rho_u)\rho_u}{1-\beta\gamma_0(\rho_u)\rho_u} \\
&+\frac{(1+\sqrt{2})\alpha\beta^2\gamma_0(\rho_u)^2\rho_u}{1-\beta\gamma_0(\rho_u)\rho_u} + \frac{[(1+\sqrt{2})\kappa+1]\alpha\beta\gamma_0(\rho_u)}{1-\beta\gamma_0(\rho_u)\rho_u}\Bigg\}\rho_u \\
= q(\|u-u_*\|)\|u-u_*\|,&
\end{aligned}
$$

where we set

$$
\begin{aligned}
q(r) = \frac{\beta}{1-\beta\gamma_0(r)r}\Bigg\{&\frac{\beta\gamma_0(r)\gamma^c(r)r^2 + \kappa\gamma^c(r)r}{(1-\beta\gamma_0(r)r)} + \frac{(1+\sqrt{2})\alpha\beta^2\gamma_0(r)^2 r}{1-\beta\gamma_0(r)r} \\
&+ \frac{[(1+\sqrt{2})\kappa+1]\alpha\beta\gamma_0(r)}{1-\beta\gamma_0(r)r}\Bigg\}
\end{aligned}
$$

Finally, it is easy to prove that q is continuous and strictly increasing relying on Remark 7.3.7. □

Proof of Theorem 7.5.2. Let G and $\tilde{G}$ be defined as in (7.42) and define $\bar{R}$ and q as in Proposition 7.6.2. Now fix $r < \bar{r}$ such that $B_r(u_*) \subseteq U$. Then, thanks to hypothesis 3), it is possible to apply Proposition 7.6.1 and to get the first part of the thesis. Finally, relying on the structure of the function q shown in Proposition 7.6.2, and denoting $\rho_{u_0} = \|u - u_0\|$, the expression of the constants C_1, C_2 easily follows. □

7.7 Applications

Algorithm (7.37) is a two-steps algorithm, consisting of the classical Gauss-Newton step followed by a "g-projection" in a variable metric. In this section the general framework shall be specialized to solve constrained nonlinear systems of equations in the least squares sense. We remark that due to hypotheses of Theorem 7.5.2 we are dealing with regular problems in the sense of Bakushinskiĭ and Kokurin [BK04]. In the finite dimensional case this implies the number of equations to be greater than the number of unknowns. This subject has been studied in [BMM04, KMS97, Kan01, Ulb01] (see also references therein). Denoting by C a closed and convex subset of U, we consider the problem

$$\min_{u \in C} \|F(u)\|^2, \tag{7.52}$$

which can be cast in our framework by setting $g(u) = \iota_C(u)$, where ι_C denotes the indicator function of the set C, i.e. $\iota_C(u) = 0$ for $u \in C$ and $\iota_C(u) = +\infty$ otherwise. The proximity operator of ι_C with respect to $H(u_n) = F'(u_n)^* F'(u_n)$, turns out to be the projection onto C w.r.t. the metric defined by $H(u_n)$, and therefore algorithm (7.37) reads as follows

$$u_{n+1} = P_C^{H(u_n)}(u_n - F'(u_n)^\dagger F(u_n)). \tag{7.53}$$

Since in general a closed form of the projection operator is not available, a further algorithm is needed for solving the projection task, which adds an inner iteration to the main procedure. We choose the *forward-backward algorithm* [CW05]. Though there are many other methods for that purpose, we do not carry out any comparison among them, because this is beyond the scope of the present work. By definition of proximity operator, given $H = A^* A$, A injective with closed range, we have

$$\begin{aligned} P_C^H(z) &= \operatorname{prox}_{\iota_C}^H(z) \\ &= \operatorname{argmin}_w \left\{ \iota_C(w) + \frac{1}{2}\|w - z\|_H^2 \right\} \\ &= \operatorname{argmin}_w \left\{ \iota_C(w) + \frac{1}{2}\|Aw - Az\|^2 \right\}. \end{aligned}$$

If P_C denotes the projection onto the convex set C, now with respect to the original metric of the space U, the sequence defined by

$$\begin{aligned} w_0 &\in U \\ w_{k+1} &= P_C(w_k - \sigma H(w_k - z)), \end{aligned}$$

with $\sigma \leq 2/\|A\|^2$, is strongly convergent to the point $P_C^H(z)$ [RMS+10]. Eventually, the full algorithm is

$$\left[\begin{array}{l} u_0 \in C \\ z_n = u_n - F'(u_n)^\dagger F(u_n) \\ \quad \left[\begin{array}{l} w_{0,n} \in C, \quad \sigma_n \leq 1/2\|F'(u_n)\|^2 \\ w_{k+1,n} = P_C(w_{k,n} - \sigma_n F'(u_n)^* F'(u_n)(w_{k,n} - z_n)) \end{array}\right. \\ u_{n+1} = \lim_k w_{k,n}. \end{array}\right. \tag{7.54}$$

It is worth noting that the inner iteration is not required when z_n belongs to C. Indeed, in that case, the projection leaves z_n untouched and the full step of the algorithm (7.53) reduces to the classical Gauss-Newton step. Such situation asymptotically occurs when u_* is internal to C.

Algorithm (7.54) requires explicit evaluation of the projection P_C, which can be done for simple sets, like spheres, boxes, etc. Particularly relevant from the point of view of the applications — see [BMM04] and references therein — is the case of box constraints in $\mathbb{R}^n$. We point out that when P_C can be computed explicitly the algorithm generates a sequence of feasible points, no matter when the inner iteration is stopped. This feature can be useful in forcing the sequence of iterates to remain in regions where the function is well-behaved, avoiding the Gauss-Newton step to lead to sites where the derivative is ill-conditioned.

7.8 Numerical experiments

This section summarizes the results of the numerical experiments we carried out in order to verify the effectiveness of algorithm (7.54) for solving real-life constrained nonlinear least-squares problems. In particular, we consider the case of box constraints, namely

$$\min_{u\in\mathbb{R}^n} \|F(u) - v\|^2, \qquad a \leq u \leq b,$$

where a and b are in $\overline{\mathbb{R}}^n$, $a \leq b$ and $C = \prod_{i=1}^n [a_i, b_i]$, $F : \Omega \supseteq C \to \mathbb{R}^m$.

The aim of the tests is to illustrate the behavior of our algorithm on some representative examples and show that it can be successfully applied to real problems. The algorithm is implemented in MatLab, and the convergence tests

$$\|u_{n+1} - u_n\| < \epsilon, \quad \|w_{k+1,n} - w_{k,n}\| < \epsilon$$

are used with precision $\epsilon = 10^{-12}$.

We remark that the implementation of the algorithm (7.54) computes the projection only approximately, meaning that the internal iteration is stopped either because the required precision has been attained or because an a priori fixed maximum number of iterations has been reached. For this reason, the projection step depends on the algorithm selected to that aim and the forward-backward algorithm is just one choice among several possibilities. Furthermore, the number of evaluations of F and F' depends only on the number of outer iterations. Therefore we provide just the number of outer iterations needed to reach the target precision as a measure of our method's performance. Yet, the number of inner iterations does affect the number of outer iterations. In fact, in our experiments we observed that, even though the algorithm is quite robust with respect to errors in the computation of the projection, the number of outer iterations can increase if the required inner precision is not attained (inner iterations reach the maximum allowed).

The experiments are performed on some standard test problems reported in the appendix for the convenience of the reader. One group of them is taken from chapter 6 in [Fle87] and a second group comes from the extensive library NLE [SBC02], which is accessible through the web site: `www.polymath-software.com/library`. We considered only problems for which the solution (or a good estimate of it) is known in advance and for which the Gauss-Newton method is known to be effective — since our proposal in fact extends the classical one.

The problems we select in the first group are `Rosenbrock`, `Osborne1`, `Osborne2` and `Kowalik` [Fle87]. They are actually unconstrained problems, to which we added some box constraints set up in order to make the provided solution fall on the boundary of the box (faces, edges, vertices, etc.). Besides, on Rosenbrock's example we tried out our method also in case the global minimizer is kept outside the fixed box. Note that in all cases the regularity conditions (SH) as well as the first two conditions of Theorem 7.5.2 are easily verified. However, the third condition of Theorem 7.5.2 does not hold and the theorem does not apply. In fact, we verified that

$$h := [(1+\sqrt{2})\kappa + 1]\alpha\beta^2 L(0) > 1,$$

by bounding $L(0)$ from below, with the norm of the second derivative $\|F''(u_*)\|$, and explicitly computing the remaining quantities. This is not surprising since, for the problems at hand, also the weaker condition needed for the convergence of the (unconstrained) Gauss-Newton method [LZJ04]

$$\sqrt{2}\alpha\beta^2 L(0) < 1$$

is not verified. The experiments on this group of problems confirm that the presence of the proximal operator does not deteriorate the good numerical behavior of the Gauss-Newton method even in cases where the hypotheses ensuring convergence are not fulfilled — as discussed in [Fle87].

The remaining problems, `Twoeq6` and `Teneq1b`, come as truly constrained and are labeled as "higher difficulty level" in the NLE library. Unlike the first group, here the constrained minimizers of `Twoeq6` and `Teneq1b` lie in the interior of the feasible set and moreover the problems are zero residual ($\alpha = 0$). This implies that condition 3. of Theorem 7.5.2 is trivially satisfied, guaranteeing convergence of our method since the other hypotheses can be easily checked. Observe in addition that the given constraints define a convex set that is not closed. More specifically, in `Teneq1b` example, the feasible region is the positive orthant

Table 7.1: Results of numerical experiments on the test problems specified in the first column for the box constraints given by a and b with starting point u_0. The point u_* is the detected minimizer, which we show with five digits precision for conciseness.

Function	n	m	a	b	u_0	u_*	avg. n. iter.
`Rosenbrock`	2	2	$\begin{bmatrix}-3\\-2\end{bmatrix}$	$\begin{bmatrix}3\\0.8\end{bmatrix}$	20 random	$\begin{bmatrix}0.89475\\0.80000\end{bmatrix}$	7
`Kowalik`	4	11	$\begin{bmatrix}0.1928\\0.1916\\0.1234\\0.1362\end{bmatrix}$	$\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$	20 random	$\begin{bmatrix}0.19281\\0.19165\\0.12340\\0.13620\end{bmatrix}$	7
`Osborne1`	5	33	$\begin{bmatrix}0.3754\\1\\-2\\0.01287\\0\end{bmatrix}$	$\begin{bmatrix}1\\2\\0\\1\\1\end{bmatrix}$	20 random	$\begin{bmatrix}0.37546\\1.93569\\-1.46461\\0.01287\\0.02212\end{bmatrix}$	21
`Osborne2`	11	65	$\begin{bmatrix}1.31\\0.4314\\0.6336\\0.5\\0.5\\0.6\\1\\4\\2\\4.5689\\5\end{bmatrix}$	$\begin{bmatrix}1.4\\0.8\\1\\1\\1\\3\\5\\7\\2.5\\5\\6\end{bmatrix}$	20 random	$\begin{bmatrix}1.31000\\0.43157\\0.63367\\0.59941\\0.75423\\0.90423\\1.36573\\4.82393\\2.39867\\4.56890\\5.67535\end{bmatrix}$	17
`Twoeq6`	2	2	$\begin{bmatrix}0.0001\\0.0001\end{bmatrix}$	$\begin{bmatrix}0.9999\\+\infty\end{bmatrix}$	$\begin{bmatrix}0.9\\0.5\end{bmatrix}$ $\begin{bmatrix}0.6\\0.1\end{bmatrix}$	$\begin{bmatrix}0.75739\\0.02130\end{bmatrix}$	20
`Teneq1b`	10	10	$\begin{bmatrix}0.0001\\0.0001\\0.0001\\0.0001\\0\\0\\0\\0\\0\\0\end{bmatrix}$	$\begin{bmatrix}+\infty\\+\infty\\+\infty\\+\infty\\+\infty\\+\infty\\+\infty\\+\infty\\+\infty\\+\infty\end{bmatrix}$	$\begin{bmatrix}1\\1\\20\\1\\0\\0\\0\\0\\0\\1\end{bmatrix}$ $\begin{bmatrix}2\\5\\40\\1\\0\\0\\0\\0\\0\\5\end{bmatrix}$	$\begin{bmatrix}2.99763\\3.96642\\79.99969\\0.00236\\0.00060\\0.00136\\0.06457\\3.53081\\26.43154\\0.00449\end{bmatrix}$	10

of $\mathbb{R}^{10}$, excluding four coordinate hyperplanes where the first derivative is undefined. We overcome this difficulty by shrinking slightly the feasible region of a small amount δ

$$C_\delta = \Big\{(u_1, \ldots, u_{10}) \,:\, u_i \geq \delta \text{ for } i = 1, \ldots, 4, \quad u_i \geq 0 \text{ for } i \geq 5\Big\},$$

and solving the problem in the closed and convex set C_δ with $\delta = 0.0001$. The same trick has been used also for solving problem `Twoeq6` too.

The experimental protocol is different for the two test groups: in the former group, 20 points belonging to the box are randomly chosen as initial guesses and the average number of required iterations is provided; whereas in the latter one the algorithm is fed with two critical initializations reported in the NLE's problem description. The results are collected in Table 7.1.

In all tests the algorithm reached the solution up to the required precision, and we did not detect any significant variation in the number of iterations depending on the starting points. Along the path we checked the condition number of F', observing that it always keeps bounded from above, the problem thus remaining well-conditioned. In case of `Osborne2`, we saw that the classical Gauss-Newton method does not converge for some initializations, due to ill-conditioning of the derivative F'. We were able to correct this behavior by setting the constraints properly around the known minimizer.

7.8.1 List of test functions

In this section we provide the expressions of the test functions for reader's convenience. All the objective functions are sum of squares

$$\frac{1}{2}\|F(u)\|^2 \qquad F : \mathbb{R}^n \to \mathbb{R}^m$$

where $\|\cdot\|$ denotes the euclidean norm in $\mathbb{R}^m$. We denote by $F_k : \mathbb{R}^n \to \mathbb{R}$ the k-component of the function F for $k \in [1, m]$.

`Rosenbrock` $(n = m = 2)$. See [Fle87] p. 7, for instance.

$$F_1(u) = 10(u_2 - u_1^2) \qquad F_2(u) = 1 - u_1$$

`Kowalik` $(n = 4, m = 11)$. It is the *Enzyme* problem given in [KO69] p. 104.

$$F_k(u) = V_k - \frac{u_1(v_k^2 + u_2 v_k)}{v_k^2 + u_3 v_k + u_4}$$

where the vectors of the V_k's and v_k's are given in Table 7.2.

`Osborne1` $(n = 5, m = 33)$. It is the *Exponential Fitting* problem given in [Osb72] p. 185.

$$F_k(u) = v_k - (u_1 + u_2 \exp(-u_4 t_k) + u_3 \exp(u_5 t_k))$$

where the vectors of the t_k's and v_k's are given in Table 7.3.

`Osborne2` $(n = 11, m = 65)$. It is the *Fitting Gaussian plus an Exponential Background* problem given in [Osb72] p. 186.

$$\begin{aligned} F_k(u) = v_k - \{&u_1 \exp(-u_5 t_k) + u_2 \exp[-u_6(t_k - u_9)^2] + u_3 \exp[-u_7(t_k - u_{10})^2] \\ &+ u_4 \exp[-u_8(t_k - u_{11})^2]\} \end{aligned}$$

where the t_k's and v_k's are given in Table 7.4.

`Twoeq6` $(n = m = 2)$. It is the *Conversion in a chemical reactor* problem listed in the NLE library `http://www.polymath-software.com/library/problemlist.shtml`

$$F_1(u) = \frac{u_1}{1 - u_1} - 5 \log\left(\frac{0.4(1 - u_1)}{u_2}\right) + 4.45977 \qquad F_2(u) = u_2 - (0.4 - 0.5u_1)$$

`Teneq1b` $(n = m = 10)$ It is the *Chemical Equilibrium Problem - $R = 40$* problem listed in the NLE library `http://www.polymath-software.com/library/problemlist.shtml`

$$\begin{aligned} F_1(u) &= u_1 + u_4 - 3 \\ F_2(u) &= 2u_1 + u_2 + u_4 + u_7 + u_8 + u_9 + 2u_{10} - R \\ F_3(u) &= 2u_2 + 2u_5 + u_6 + u_7 - 8 \\ F_4(u) &= 2u_3 + u_5 - 4R \\ F_5(u) &= u_1 u_5 - 0.193 u_2 u_4 \\ F_6(u) &= u_6 * \sqrt{u_2} - 0.002597 \sqrt{u_2 u_4 \sum_{i=1}^{10} x_i} \\ F_7(u) &= u_7 \sqrt{u_4} - 0.003448 \sqrt{u_1 u_4 \sum_{i=1}^{10} x_i} \\ F_8(u) &= u_8 u_4 - 1.799 \cdot 10^{-5} u_2 \sum_{i=1}^{10} x_i \\ F_9(u) &= u_9 u_4 - 0.0002155 u_1 \sqrt{u_3 \sum_{i=1}^{10} x_i} \\ F_{10}(u) &= u_{10} u_4^2 - 3.846 \cdot 10^{-5} u_4^2 \sum_{i=1}^{10} x_i \end{aligned}$$

where the constant $R = 40$.

Table 7.2: Data for the enzyme problem `Kowalik`

k	1	2	3	4	5	6	7	8	9	10	11
V_k	.1957	.1947	.1735	.1600	.0844	.0627	.0456	.0342	.0323	.0235	.0246
v_k	0	10	20	30	40	50	60	70	80	90	100

Table 7.3: Data for the exponential fitting problem `Osborne1`

k	t_k	v_k	k	t_k	v_k	k	t_k	v_k	k	t_k	v_k
1	0	0.844	10	90	0.784	19	180	0.538	28	270	0.431
2	10	0.908	11	100	0.751	20	190	0.522	29	280	0.424
3	20	0.932	12	110	0.718	21	200	0.506	30	290	0.420
4	30	0.936	13	120	0.685	22	210	0.490	31	300	0.414
5	40	0.925	14	130	0.658	23	220	0.478	32	310	0.411
6	50	0.908	15	140	0.628	24	230	0.467	33	320	0.406
7	60	0.881	16	150	0.603	25	240	0.457			
8	70	0.850	17	160	0.580	26	250	0.448			
9	80	0.818	18	170	0.558	27	260	0.438			

Table 7.4: Data for the problem `Osborne2`

k	t_k	v_k	k	t_k	v_k	k	t_k	v_k	k	t_k	v_k
1	0.0	1.366	18	1.7	0.626	35	3.4	0.538	52	5.1	0.431
2	0.1	1.191	19	1.8	0.651	36	3.5	0.522	53	5.2	0.431
3	0.2	1.112	20	1.9	0.724	37	3.6	0.506	54	5.3	0.424
4	0.3	1.013	21	2.0	0.649	38	3.7	0.490	55	5.4	0.420
5	0.4	0.991	22	2.1	0.649	39	3.8	0.478	56	5.5	0.414
6	0.5	0.885	23	2.2	0.694	40	3.9	0.467	57	5.6	0.411
7	0.6	0.831	24	2.3	0.644	41	4.0	0.457	58	5.7	0.406
8	0.7	0.847	25	2.4	0.624	42	4.1	0.457	59	5.8	0.406
9	0.8	0.786	26	2.5	0.661	43	4.2	0.457	60	5.9	0.406
10	0.9	0.725	27	2.6	0.612	44	4.3	0.457	61	6.0	0.406
11	1.0	0.746	28	2.7	0.558	45	4.4	0.457	62	6.1	0.406
12	1.1	0.679	29	2.8	0.533	46	4.5	0.457	63	6.2	0.406
13	1.2	0.608	30	2.9	0.495	47	4.6	0.457	64	6.3	0.406
14	1.3	0.655	31	3.0	0.500	48	4.7	0.457	65	6.4	0.406
15	1.4	0.616	32	3.1	0.423	49	4.8	0.457			
16	1.5	0.606	33	3.2	0.395	50	4.9	0.457			
17	1.6	0.602	34	3.3	0.375	51	5.0	0.457			

Chapter 8

Conclusion and Future Work

In this thesis we discussed in great detail the problem of image registration in the framework of variational regularization methods. We made contributions both on the theoretical/modeling side and algorithmic side.

As regards the theoretical part, we presented an analysis of the well-posedness and convergence properties of variational image registration methods. Perturbations of both the two images involved in the registration process have been allowed and also general similarity criteria suitable for mono-modal as well as multi-modal case have been treated. Although we focused on the problem of image registration, we have developed a generalized Tikhonov regularization theory in abstract spaces which can find applications also for other ill-posed problems. We dealt with several significant regularization terms, among them p-norms, polyconvex hyperelastic potentials and total variation.

Concerning the algorithmic part, we analyzed first proximal splitting algorithms of forward-backward type for the minimization of composite functions where the data term is smooth and the penalty term is convex non-smooth. In the convex case we studied accelerated and inexact versions of the algorithm. We devised a specific notion of errors in the computation of the proximity operator and proved a theorem relating rate of convergence vs error's decay. We provided also — as illustration — numerical examples that check that behavior for simple but significant applied problems. In the non-convex case we showed convergence results in Banach space setting. We have enlightened that the algorithm is suitable for minimizing the Tikhonov functional of the problem of image registration based on total variation. Finally we showed that the local theory of convergence of the Gauss-Newton method can be extended to deal with the more general case of least squares problems with a convex penalty. The main theoretical result demonstrates that, under weak Lipschitz conditions on the derivative, convergence rates analogous to those existing for the standard case can be derived. An explicit formula for the radius of the convergence ball is also provided. A valuable application we propose concerns nonlinear equations with constraints. Our algorithm has been found effective and robust in solving such problems as shown in several numerical tests. Both the cases of solutions on the boundary of the feasible set as well as solutions in its interior have been treated successfully.

A future work for the image registration problem is the study of source conditions in order to get rate of convergence and studying criteria for selecting the regularization parameter. Also we feel that registration based on total variation deserves a deeper study and can play a crucial role for many applications in medicine. Finally, in analogy to what we did with the Proximal Gauss-Newton method, a new research direction that deserve to be investigated is a sort of “Proximal Levenberg-Marquardt” algorithm. Indeed such a modification could allow to cope also with irregular problems.

Appendix A

The study of Mutual Information

We give here proofs of theorems presented in Section 4.3.1.

A.1 Functions defined by integrals

We begin with an often useful, but very simple, extension of the Lebesgue's dominated convergence theorem.

Theorem A.1.1 (Extended Dominated Convergence Theorem).[1] *Let* $(\Omega, \mathfrak{A}, \mu)$ *be a measure space,* f_n, g_n *and* f, g *be extended real valued* $\mathfrak{A}$*-measurable functions. Suppose*

1. $f_n \to f$ μ*-a.e. on* Ω*;*
2. $g_n, g \in L^1_+(\Omega, \mathfrak{A}, \mu)$ *with* $g_n \to g$ μ*-a.e. on* Ω *and* $\limsup_{n\to\infty} \int_\Omega g_n \,\mathrm{d}\mu \leq \int_\Omega g \,\mathrm{d}\mu$*;*
3. $|f_n| \leq g_n$ μ*-a.e. on* Ω *for every* $n \in \mathbb{N}$*.*

Then $f, f_n \in L^1(\Omega, \mathfrak{A}, \mu)$ *and*

$$\lim_{n\to\infty} \|f_n - f\|_1 = 0$$

and so $\lim_{n\to+\infty} \int_\Omega f_n \,\mathrm{d}\mu = \int_\Omega f \,\mathrm{d}\mu$*.*

[1] This result is not widely known. It appears explicitely – for instance – in [MP86] Theorem 3.4 p. 152 and in [Yeh06], Prob. 9.17, actually with the stonger hypothesis $\lim_{n\to\infty} \int_\Omega g_n \,\mathrm{d}\mu = \int_\Omega g \,\mathrm{d}x$. See also [Roy88] Prop. 18, p. 270.

Proof. The third condition above as well as the fact that $f_n \to f$ and $g_n \to g$ imply $|f| \leq g$ μ-a.e. on Ω; thus the μ-integrability of f and f_n follow. Evidently $|f_n - f| \leq |f_n| + |f| \leq g_n + |f|$. Thus letting $h_n = g_n + |f|$, it holds $0 \leq h_n - |f_n - f|$ and $h_n - |f_n - f| \to (g + |f|)$. Due to Fatou's lemma, it is

$$\int_\Omega \liminf_{n\to\infty}(h_n - |f_n - f|)\,\mathrm{d}\mu \leq \liminf_{n\to\infty} \int_\Omega h_n - |f_n - f|\,\mathrm{d}\mu \tag{A.1}$$

Now let $\varepsilon > 0$. From $\limsup_{n\to\infty} \int_\Omega g_n\,\mathrm{d}\mu \leq \int_\Omega g\,\mathrm{d}\mu$ it follows that there exists $\nu \in \mathbb{N}$ such that

$$\int_\Omega g_n\,\mathrm{d}\mu \leq \int_\Omega g\,\mathrm{d}\mu + \varepsilon$$

Thus, we have

$$\int_\Omega h_n\,\mathrm{d}\mu \leq \int_\Omega g + |f|\,\mathrm{d}\mu + \varepsilon$$

and therefore the inequality (A.1) becomes

$$\begin{aligned}\int_\Omega g + |f|\,\mathrm{d}\mu &\leq \liminf_{n\to+\infty}\Big(\int_\Omega (g + |f|)\,\mathrm{d}\mu + \varepsilon - \int_\Omega |f_n - f|\,\mathrm{d}\mu\Big)\\ &= \int_\Omega g + |f|\,\mathrm{d}\mu + \varepsilon - \limsup_{n\to\infty} \int_\Omega |f_n - f|\,\mathrm{d}\mu\end{aligned}$$

from which it follows

$$\limsup_{n\to\infty} \int_\Omega |f_n - f|\,\mathrm{d}\mu \leq \varepsilon$$

Since ε is arbitrary we can conclude the proof. □

The above theorem allows to get more powerful theorems on the continuity and differentiability of functions defined by integrals.

Theorem A.1.2 (continuity under the integral sign). *Let U be a* first-countable *topological space and $(\Omega, \mathfrak{A}, \mu)$ be a measure space. Let be given $f, g : U \times \Omega \to \mathbb{R}$ and suppose*

(*i*) *for μ-a.e. $x \in \Omega$, $f(\cdot, x) : U \to \mathbb{R}$ is continuous;*

(*ii*) *for μ-a.e. $x \in \Omega$, $g(\cdot, x) : U \to \mathbb{R}$ is continuous, $g(t, \cdot) \in L^1_+(\Omega, \mathfrak{A}, \mu)$ for every $t \in U$ and the function*

$$t \in U \to \int_\Omega g(t, \cdot)\,\mathrm{d}\mu \in \mathbb{R}$$

is continuous;[2]

[2] Actually, from the previous theorem, it follows that upper semicontinuity suffices.

(*iii*) $|f(t,\cdot)| \leq g(t,\cdot)$ *μ a.e. on* Ω.

Then the function $F : U \to \mathbb{R}$, *defined by* $F(t) = \int_\Omega f(t,\cdot)\,\mathrm{d}\mu$, *is well-defined and continuous.*

Proof. Being U a topological space with a countable neighbourhood basis, it is enough to prove that for each $(t_n)_{n\in\mathbb{N}} \in U^{\mathbb{N}}$ with $t_n \to t$ it holds $F(t_n) \to F(t)$. Thus, let $t \in U$ and $(t_n)_{n\in\mathbb{N}}$ with $t_n \to t$. Clearly $f(t_n,\cdot), f(t,\cdot) \in L^1(\Omega,\mathfrak{A},\mu)$ and

$$f(t_n,\cdot) \to f(t,\cdot)\ \mu\text{-a.e. on } \Omega$$

Moreover, from (*ii*), it follows $g(t_n,\cdot), g(t,\cdot) \in L^1_+(\Omega,\mathfrak{A},\mu)$, $g(t_n,\cdot) \to g(t,\cdot)$ μ-a.e. on Ω, $|f(t_n,\cdot)| \leq g(t_n,\cdot)$ and

$$\lim_{n\to\infty} \int_\Omega g(t_n,\cdot)\,\mathrm{d}\mu = \int_\Omega g(t,\cdot)\,\mathrm{d}\mu$$

Applying the theorem A.1.1, we get $F(t_n) \to F(t)$. □

Theorem A.1.3 (differentiation under the integral sign). *Let* $U \subseteq \mathbb{R}$ *be an interval of the real line* $\mathbb{R}$ *and* $(\Omega,\mathfrak{A},\mu)$ *be a measure space. Let* $f : U \times \Omega \to \mathbb{R}$ *be a function such that for each* $t \in U$ *it holds* $f(t,\cdot) \in L^1(\Omega,\mathfrak{A},\mu)$. *Let us define the function* $F : U \to \mathbb{R}$ *by*

$$F(t) = \int_\Omega f(t,\cdot)\,\mathrm{d}\mu$$

and suppose that for each $x \in \Omega$, $f(\cdot,x)$ *is differentiable on* U *with derivative* $f'(t,x)$ *at the point* t *and that*

$$\int_a^b \left(\int_\Omega |f'(t,x)|\,\mathrm{d}\mu(x) \right) \mathrm{d}t < +\infty \tag{A.2}$$

for every $a,b \in U$, $a \leq b$. *Suppose moreover that for each* $t \in U : f'(t,\cdot) \in L^1(\Omega,\mathfrak{A},\mu)$. *Then the functions* F *is a.e. differentiable on* U *and it holds*

$$F'(t) = \int_\Omega f'(t,\cdot)\,\mathrm{d}\mu \tag{A.3}$$

In case the function

$$t \in U \to \int_\Omega f'(t,\cdot)\,\mathrm{d}\mu \tag{A.4}$$

is continuous, then F *is differentiable at* every *point of* U *and it holds* (A.3) *(thus* F *is of class* $\mathscr{C}^1$*). A sufficient condition for the function* (A.4) *to be continuous and, at the same time, to satisfy* (A.2) *is that there exists* $g : U \times \Omega \to \mathbb{R}$ *such that*

(*i*) $g(\cdot,x)$ *is continuous on* U *for μ-a.e.* $x \in \Omega$;

(*ii*) $g(t,\cdot) \in L^1_+(\Omega, \mathfrak{A}, \mu)$ *and the function* $t \in U \to \int_\Omega g(t,\cdot)\,\mathrm{d}\mu \in \mathbb{R}$ *is continuous;*

(*iii*) $|f'(t,\cdot)| \leq g(t,\cdot)$ *for every* $t \in U$.

Proof. Let us define $\varphi(t) = \int_\Omega f'(t,\cdot)\,\mathrm{d}\mu$. For each $x \in \Omega$, since $f'(\cdot,x)$ is the derivative of $f(\cdot,x)$, it holds

$$\int_a^b f'(t,x)\,\mathrm{d}t = f(b,x) - f(a,x)$$

Then, for every $a, b \in U, a \leq b$, due to (A.2), we can apply the Fubini's theorem and it is

$$\begin{aligned} F(b) - F(a) &= \int_\Omega f(b,x)\,\mathrm{d}\mu(x) - \int_\Omega f(a,x)\,\mathrm{d}\mu(x) \\ &= \int_\Omega \left(\int_a^b f'(t,x)\,\mathrm{d}t \right) \mathrm{d}\mu(x) \\ &= \int_a^b \left(\int_\Omega f'(t,x)\,\mathrm{d}\mu(x) \right) \mathrm{d}t \\ &= \int_a^b \varphi(t)\,\mathrm{d}t \end{aligned}$$

Thus F is an indefinite integral of φ: note that φ is locally integrable over U because for each $a, b \in U, a \leq b$

$$\int_a^b |\varphi(t)|\,\mathrm{d}t \leq \int_a^b \left(\int_\Omega |f'(t,x)|\,\mathrm{d}\mu(x) \right) \mathrm{d}t < +\infty$$

Therefore, due to Lebesgue's theorem, the function F is defferentiable a.e. on U (in particular at the Lebesgue points of φ) and in such points $F'(t) = \varphi(t)$. In case φ is continuous at t, then F is derivable at t and $F'(t) = \varphi(t)$. As regards the second part of the statement, it is enough to apply the theorem of continuity of the integral to the function

$$\varphi(t) = \int_\Omega f'(t,x)\,\mathrm{d}\mu(x)\,. \qquad \square$$

A.2 Entropy and Kullback-Leibler distance

We recall the notions of differential entropy and Kullback-Leibler distance. Their correct definitions are consequences of Jensen's inequality.

Theorem A.2.1 (Jensen's inequality). *Let $(\Omega, \mathfrak{A}, \mu)$ be a finite measure space (that is $\mu(\Omega) < +\infty$) with $\mu(\Omega) > 0$ and $\varphi : I \subseteq \mathbb{R} \to \mathbb{R}$ a convex function defined on an interval I. If $f : \Omega \to \mathbb{R}$ is μ-integrable, $f(\Omega) \subseteq I$, then $\mu(\Omega)^{-1} \int_\Omega f \,\mathrm{d}\mu \in I$ and the integral $\int_\Omega \varphi \circ f \,\mathrm{d}\mu$ is well-defined, in particular $\int_\Omega (\varphi \circ f)^- \,\mathrm{d}\mu < +\infty$ and it holds*

$$\varphi\left(\int_\Omega f \,\mathrm{d}\mu\right) \leq \frac{1}{\mu(\Omega)} \int_\Omega \varphi \circ f \,\mathrm{d}\mu$$

Proof. Let $t_0 = \mu(\Omega)^{-1} \int_\Omega f \,\mathrm{d}\mu \in \mathbb{R}$. First we show that $t_0 \in I$. Let $I = (a, b)$ with $a, b \in \overline{\mathbb{R}}$ and $a \leq b$. If $b \in I$, then $I = (a, b]$ and being $f(x) \leq b$ for every $x \in \Omega$, it holds $\int_\Omega f \,\mathrm{d}\mu \leq b\mu(\Omega)$ and hence $t_0 \leq b$. If $b \notin I$, then $I = (a, b[$, and we can assume $b < +\infty$ (indeed if $b = +\infty$, it is clear that $t_0 < b$) and being $f(x) < b$ it holds again $\int_\Omega f \,\mathrm{d}\mu \leq b\mu(\Omega)$. Now $\int_\Omega f \,\mathrm{d}\mu = b\mu(\Omega)$ implies $\int_\Omega (b - f) \,\mathrm{d}\mu = 0 \implies f = b$ μ-q.o. $\implies \mu(\Omega) = 0$ which leads to a contraddiction. We proved therefore that $t_0 < b$. The same reasoning can be pursued also for the other end point of I and hence we get $t_0 \in I$.

The functions φ is convex and finite, therefore it is continuous and subdifferentiable and for every $t \in \mathbb{R}$ it holds

$$\varphi(t) \geq \varphi(t_0) + (t - t_0)a$$

with $a \in \mathbb{R}$. Then letting $b = \varphi(t_0) - t_0 a$, one has $at + b \leq \varphi(t)$ and $\varphi(t_0) = at_0 + b$. Therefore $af(x) + b \leq \varphi(f(x)) := h(x)$ for every $x \in \Omega$ and hence also $-h(x) \leq |a||f(x)| + |b| := g$, from which it follows $h^- = \max\{0, -\varphi \circ f\} \leq g$ and, being g μ-integrable, it is $\int_\Omega h^- \,\mathrm{d}\mu < +\infty$. Thus, one can define the integral

$$\int_\Omega h \,\mathrm{d}\mu = \int_\Omega h^+ \,\mathrm{d}\mu - \int_\Omega h^- \,\mathrm{d}\mu$$

If h is μ-integrable, (that is $\int_\Omega h^+ \,\mathrm{d}\mu < +\infty$), being $af + b \leq h$ it holds

$$\int_\Omega af + b \,\mathrm{d}\mu \leq \int_\Omega h \,\mathrm{d}\mu \tag{A.5}$$

If on the contrary $\int_\Omega h^+ \,\mathrm{d}\mu = +\infty$, then $\int_\Omega h \,\mathrm{d}\mu = +\infty$ and (A.5) is still valid. Therefore in any case one has

$$\mu(\Omega)\varphi(t_0) = a \int_\Omega f \,\mathrm{d}\mu + b\mu(\Omega) = \int_\Omega af + b \,\mathrm{d}\mu \leq \int_\Omega \varphi \circ f \,\mathrm{d}\mu\,. \qquad \square$$

Corollay A.2.2. *Let $f : \mathbb{R}^d \to \mathbb{R}_+$ be a probability density function and suppose $\int_{\mathbb{R}^d} f(x)^2 \,\mathrm{d}x < +\infty$. Then one can define the* differential entropy *as*

$$\boxed{H(f) := \int_{\mathbb{R}^d} -f(x) \log f(x) \,\mathrm{d}x} \tag{A.6}$$

(using the convention $0 \log 0 = 0$) in the sense that the above integral is well-defined, and moreover

$$H(f) \geq -\log \left(\int_{\mathbb{R}^d} f^2 \, \mathrm{d}x \right) > -\infty$$

Proof. Let $\Omega = \{x \in \mathbb{R}^d \mid f(x) > 0\}$. From the definition it holds

$$H(f) = \int_{\Omega} (-\log) f(x) \, \mathrm{d}\mu(x)$$

where $\mu = f_{|\Omega} \, \mathrm{d}x$ is a probability measure, since $\mu(\Omega) = \int_{\Omega} f(x) \, \mathrm{d}x = 1$. Then clearly $-\log : \mathbb{R}_+^* \to \mathbb{R}$ is a convex function and by hypothesis $\int_{\Omega} f(x) \, \mathrm{d}\mu = \int_{\Omega} f(x)^2 \, \mathrm{d}x < +\infty$. Thus, due to Jensen inequality, the integral which defines the entropy is well-defined and

$$H(f) \geq -\log \left(\int_{\Omega} f(x) \, \mathrm{d}\mu(x) \right) = -\log \left(\int_{\mathbb{R}^d} f(x)^2 \, \mathrm{d}x \right) . \qquad \square$$

Corollay A.2.3. *Let $f, g : \mathbb{R}^d \to \mathbb{R}_+$ be two continuous probability density functions, such that $f(x), g(x) > 0$ for every $x \in \mathbb{R}^d$. Then one can define the* Kullback-Leibler distance *as follows*

$$\boxed{D(f \| g) := \int_{\mathbb{R}^d} f(x) \log \frac{f(x)}{g(x)} \, \mathrm{d}x} \tag{A.7}$$

(that is the integral above is well-defined) and moreover $D(f \| g) \geq 0$.

Proof. The integral can be written in an equivalent way as

$$D(f \| g) = \int_{\mathbb{R}^d} f(x)(-\log) \frac{g(x)}{f(x)} \, \mathrm{d}x = \int_{\mathbb{R}^d} -\log \frac{g(x)}{f(x)} \, \mathrm{d}\mu(x)$$

where $\mu = f \, \mathrm{d}x$ is a probability measure on $\mathbb{R}^d$ and $\mu(\mathbb{R}^d) = \int f(x) \, \mathrm{d}x = 1 < +\infty$. Since

$$\int_{\mathbb{R}^d} \frac{g(x)}{f(x)} \, \mathrm{d}\mu = \int_{\mathbb{R}^d} g(x) \, \mathrm{d}x = 1$$

i.e. g/f is μ-integrabile, due to Jensen's inequality, the integral defining the Kullback-Leibler distance is well-defined and it holds $D(f \| g) \geq -\log(1) = 0$. $\square$

A.3 Proofs of Section 4.3.1

Let us start with the study of the continuity of the mutual information (4.8) w.r.t. I_1 and I_2. Evidently from (4.7), it follows that $p_{I_1,I_2}(\mathbf{i})$ is a function defined by integrals and in any case the integrand is continuous in the variable $\mathbf{i}$ and it is also dominated by $|\Omega|^{-1}G_\sigma(0,0)$, which is an integrable function over Ω. Therefore, due to the classical Lebesgue dominated convergence theorem (or Theorem A.1.2), the function $p_{I_1,I_2}(\mathbf{i})$ is continuous. Reasoning in the same way, one can prove that p_{I_1} and p_{I_2} are continuous. Let us show that the function p_I can be bounded from below and above by integrable functions independently form I if the image I is bounded. More precisely let $A > 0$ and set

$$\underset{\smile}{\varphi} : \mathbb{R} \to \mathbb{R} \qquad \underset{\smile}{\varphi}(i) = \begin{cases} g_\sigma(i-A) & \text{se } i \leq -A \\ g_\sigma(2A) & \text{se } |i| \leq A \\ g_\sigma(i+A) & \text{se } A \leq i \end{cases} \tag{A.8}$$

and

$$\hat{\varphi} : \mathbb{R} \to \mathbb{R} \qquad \hat{\varphi}(i) = \begin{cases} g_\sigma(i+A) & \text{se } i \leq -A \\ g_\sigma(0) & \text{se } |i| \leq A \\ g_\sigma(i-A) & \text{se } A \leq i \end{cases} \tag{A.9}$$

Then the following result holds

Proposition A.3.1. *For every $I \in L^\infty(\Omega)$ with $\|I\|_\infty \leq A$, it is $0 < \underset{\smile}{\varphi} \leq p_I \leq \hat{\varphi}$, where both $\underset{\smile}{\varphi}, \hat{\varphi}$ are integrable functions over Ω.*

Proof. The integrability of the functions $\underset{\smile}{\varphi}, \hat{\varphi}$ is clear. We have $|I(\mathbf{x})| \leq A$ for a.e. $\mathbf{x} \in \Omega$. If $i \leq -A$, then $0 \leq -i - A \leq -i + I(\mathbf{x}) \leq -i + A$, which implies $g_\sigma(A-i) \leq g_\sigma(I(\mathbf{x}) - i) \leq g_\sigma(i+A)$ for a.e. $\mathbf{x} \in \Omega$. Thus computing the integrals, it holds $g_\sigma(A-i) \leq p_I(i) \leq g_\sigma(i+A)$ for each $i \in \mathbb{R}$. If $|i| \leq A$, then $0 \leq |i - I(\mathbf{x})| \leq 2A$, from which it follows $g_\sigma(2A) \leq g_\sigma(I(\mathbf{x}) - i) \leq g_\sigma(0)$ for a.e. $\mathbf{x} \in \Omega$ and hence $g_\sigma(2A) \leq p_I(i) \leq g_\sigma(0)$. Finally if $i \geq A$, then $0 \leq i - A \leq i - I(\mathbf{x}) \leq i + A$, which implies $g_\sigma(i+A) \leq g_\sigma(I(\mathbf{x}) - i) \leq g_\sigma(A-i)$ for a.e. $\mathbf{x} \in \Omega$ and thus $g_\sigma(A+i) \leq p_I(i) \leq g_\sigma(A-i)$. We proved that $0 < \underset{\smile}{\varphi} \leq p_I \leq \hat{\varphi}$. $\square$

Remark A.3.2. *One can easily see that $\|\hat{\varphi}\|_1 = \sqrt{\frac{2}{\pi}\frac{A}{\sigma}} + \|g_\sigma\|_1$. Indeed*

$$\begin{aligned} \int_{\mathbb{R}} |\hat{\varphi}(i)| \,\mathrm{d}i &= \int_{-\infty}^{-A} g_\sigma(i+A) \,\mathrm{d}i + \int_{-A}^{A} g_\sigma(0) \,\mathrm{d}i + \int_{A}^{+\infty} g_\sigma(i-A) \,\mathrm{d}i \\ &= \int_{-\infty}^{0} g_\sigma(i) \,\mathrm{d}i + 2A g_\sigma(0) + \int_{0}^{+\infty} g_\sigma(i) \,\mathrm{d}i \end{aligned}$$

Let us prove now that the mutual information (4.8) is finite if at least one of the two images is (essentially) bounded.

Proof. of Proposition 4.3.1. As in the previous proof, we proceed treating separately different cases according to the values of i_1, assuming $\|I_1\|_\infty \leq A$ (one can proceed in the same way with i_2 in case $\|I_2\|_\infty \leq A$). If $i_1 \leq -A$, then, as before one can show that for a.e. $x \in \Omega$ it is

$$g_\sigma(A - i_1) \leq g_\sigma(I_1(\mathbf{x}) - i_1) \leq g_\sigma(A + i_1) \tag{A.10}$$

from which it follows $g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(A - i_1) \leq g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(I_1(\mathbf{x}) - i_1) \leq g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(A + i_1)$ for a.e. $x \in \Omega$ and dividing by $|\Omega|$ and computing the integrals, one obtains $p_{I_2}(i_2)g_\sigma(A - i_1) \leq p_{I_1,I_2}(\mathbf{i}) \leq p_{I_2}(i_2)g_\sigma(A + i_1)$ for each $\mathbf{i} \in \mathbb{R}^2$. Thus, it holds

$$g_\sigma(A - i_1) \leq \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_2}(i_2)} \leq g_\sigma(A + i_1)$$

But from (A.10), one also has $g_\sigma(A - i_1) \leq p_{I_1}(i_1) \leq g_\sigma(A + i_1)$, and hence

$$\frac{g_\sigma(A - i_1)}{g_\sigma(A + i_1)} \leq \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)} \leq \frac{g_\sigma(A + i_1)}{g_\sigma(A - i_1)}$$

From this, it follows

$$\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \leq \log \frac{g_\sigma(A + i_1)}{g_\sigma(A - i_1)} = -\frac{2Ai_1}{\sigma^2}$$

and thus

$$p_{I_1,I_2}(\mathbf{i})\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \leq p_{I_2}(i_2)g_\sigma(i_1 + A)\frac{-2Ai_1}{\sigma^2}$$

If $|i_1| \leq A$, then

$$g_\sigma(2A) \leq g_\sigma(I_1(\mathbf{x}) - i_1) \leq g_\sigma(0) \tag{A.11}$$

which implies $g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(2A) \leq g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(I_1(\mathbf{x}) - i_1) \leq g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(0)$ for a.e. $x \in \Omega$ and computing the integrals $p_{I_2}(i_2)g_\sigma(2A) \leq p_{I_1,I_2}(\mathbf{i}) \leq p_{I_2}(i_2)g_\sigma(0)$ for each $\mathbf{i} \in \mathbb{R}^2$. Thus

$$g_\sigma(2A) \leq \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_2}(i_2)} \leq g_\sigma(0)$$

But from (A.11), one has also $g_\sigma(2A) \leq p_{I_1}(i_1) \leq g_\sigma(0)$, and thus

$$\frac{g_\sigma(2A)}{g_\sigma(0)} \leq \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)} \leq \frac{g_\sigma(0)}{g_\sigma(2A)}$$

From this it follows

$$\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \leq \log \frac{g_\sigma(0)}{g_\sigma(2A)} = \frac{2A^2}{\sigma^2}$$

and thus

$$p_{I_1,I_2}(\mathbf{i})\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \leq p_{I_2}(i_2)g_\sigma(0)\frac{2A^2}{\sigma^2}$$

Finally if $A \le i_1$, it is

$$g_\sigma(i_1 + A) \le g_\sigma(I_1(\mathbf{x}) - i_1) \le g_\sigma(A - i_1) \tag{A.12}$$

from which it follows $g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(i_1 + A) \le g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(I_1(\mathbf{x}) - i_1) \le g_\sigma(I_2(\mathbf{x}) - i_2)g_\sigma(A - i_1)$ for a.e. $x \in \Omega$ and integrating one has $p_{I_2}(i_2)g_\sigma(i_1 + A) \le p_{I_1,I_2}(\mathbf{i}) \le p_{I_2}(i_2)g_\sigma(A - i_1)$. Thus

$$g_\sigma(i_1 + A) \le \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_2}(i_2)} \le g_\sigma(A - i_1)$$

But from (A.12), it is also $g_\sigma(i_1 + A) \le p_{I_1}(i_1) \le g_\sigma(A - i_1)$, and hence

$$\frac{g_\sigma(i_1 + A)}{g_\sigma(A - i_1)} \le \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)} \le \frac{g_\sigma(A - i_1)}{g_\sigma(i_1 + A)}$$

From which it follows

$$\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \le \log \frac{g_\sigma(A - i_1)}{g_\sigma(i_1 + A)} = \frac{2Ai_1}{\sigma^2}$$

and hence

$$p_{I_1,I_2}(\mathbf{i}) \left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \le p_{I_2}(i_2)g_\sigma(A - i_1)\frac{2Ai_1}{\sigma^2}$$

Summarizing if we define the function

$$\psi : \mathbb{R} \to \mathbb{R} \qquad \psi(i) = \begin{cases} \dfrac{-2Ai}{\sigma^2} & \text{se } i \le -A \\ \dfrac{2A^2}{\sigma^2} & \text{se } |i| \le A \\ \dfrac{2Ai}{\sigma^2} & \text{se } A \le i \end{cases}$$

it holds

$$\left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \le \psi(i_1) \qquad p_{I_1,I_2}(\mathbf{i}) \le p_{I_2}(i_2)\hat{\varphi}(i_1)$$

and hence

$$p_{I_1,I_2}(\mathbf{i}) \left|\log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}\right| \le p_{I_2}(i_2)\hat{\varphi}(i_1)\psi(i_1) \tag{A.13}$$

Letting $h(i_1, i_2) = p_{I_2}(i_2)\hat{\varphi}(i_1)\psi(i_1)$, it is

$$\int_{\mathbb{R}^2} h(i_1, i_2)\,\mathrm{d}\mathbf{i} = \int_{\mathbb{R}} p_{I_2}(i_2)\,\mathrm{d}i_2 \int_{\mathbb{R}} \hat{\varphi}(i_1)\psi(i_1)\,\mathrm{d}i_1 = \int_{\mathbb{R}} \hat{\varphi}(i_1)\psi(i_1)\,\mathrm{d}i_1 < +\infty$$

therefore h is integrable over $\mathbb{R}^2$ e $\mathbf{MI}(I_1, I_2) \le \int_{\mathbb{R}^2} h(\mathbf{i})\,\mathrm{d}\mathbf{i} < +\infty$ and $\int_{\mathbb{R}^2} h(\mathbf{i})\,\mathrm{d}\mathbf{i}$ does not depend on I_1 and I_2 but just on the constant A. $\square$

Remark A.3.3. *Note that* $\psi(i) = 2A/\sigma^2 \max\{|i|, A\} \leq 2A/\sigma^2(|i| + A)$.

In the following we give the proof of the continuity property for the mutual information.

Proof. of Proposition 4.3.2. We already noted that $p_{I_1,I_1}, p_{I_1}, p_{I_2}$ are all continuous functions. Letting $\mathbf{I}^k(x) = (I_1^k(\mathbf{x}), I_2^k(\mathbf{x}))$ and $\mathbf{I}(x) = (I_1(\mathbf{x}), I_2(\mathbf{x}))$, it is $\mathbf{I}^k(x) \to \mathbf{I}(x)$ a.e. on Ω. Moreover, being G_σ continuous, for each $\mathbf{i} \in \mathbb{R}^2$ it holds $G_\sigma(\mathbf{I}^k(x) - \mathbf{i}) \to G_\sigma(\mathbf{I}(x) - \mathbf{i})$ for a.e. $x \in \Omega$ and clearly $G_\sigma(\mathbf{I}^k(x) - \mathbf{i}) \leq g_\sigma(0)^2$ for each $x \in \Omega$. Therefore by the Lebesgue's dominated convergence theorem $p_{I_1^k,I_2^k}(\mathbf{i}) \to p_{I_1,I_2}(\mathbf{i})$ and this is true for each $\mathbf{i} \in \mathbb{R}^2$. In the same manner one can prove that $p_{I_1^k}(i_1) \to p_{I_1}(i_1)$ and $p_{I_2^k}(i_2) \to p_{I_2}(i_2)$ and from the continuity of log, it holds

$$p_{I_1^k,I_2^k}(\mathbf{i}) \log \frac{p_{I_1^k,I_2^k}(\mathbf{i})}{p_{I_1^k}(i_1)p_{I_2^k}(i_2)} \to p_{I_1,I_2}(\mathbf{i}) \log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)}$$

pointwise. In the previous proposition we proved that

$$p_{I_1^k,I_2^k}(\mathbf{i}) \left| \log \frac{p_{I_1^k,I_2^k}(\mathbf{i})}{p_{I_1^k}(i_1)p_{I_2^k}(i_2)} \right| \leq h_k(i_1, i_2)$$

with $h_k : \mathbb{R}^2 \to \mathbb{R}$ integrable function, $h_k(\mathbf{i}) = p_{I_2^k}(i_2)\hat{\varphi}(i_1)\psi(i_1)$ and $h_k(\mathbf{i}) \to h(\mathbf{i}) = p_{I_2}(i_2)\hat{\varphi}(i_1)\psi(i_1)$. Since $\int_\Omega h_k \, \mathrm{d}\mathbf{i} = \int_\mathbb{R} \hat{\varphi}(i_1)\psi(i_1) \, \mathrm{d}i_1 = \int_\Omega h \, \mathrm{d}\mathbf{i}$, by (the extended dominated convergence) Theorem A.1.1, one gets the conclusion. □

We finish with the study of the partial differentiability of $\mathbf{MI}(I_1, I_2)$ w.r.t. the variable I_2.

Proof. of Theorem 4.3.4. Let us fix $I_1 \in L^\infty(\Omega), I_2, I \in L^q(\Omega)$ and $t \in]-1, 1[=: U$ and study the differentiability of the function $\phi : U \to \mathbb{R}$

$$\phi(t) = \mathbf{MI}(I_1, I_2 + tI) = \int_{\mathbb{R}^2} F(t, \mathbf{i}) \log \frac{F(t, \mathbf{i})}{F_1(i_1)F_2(t, i_2)} \, \mathrm{d}i_1 \, \mathrm{d}i_2 \tag{A.14}$$

with

$$F(t, \mathbf{i}) = p_{I_1,I_2+tI}(i_1, i_2) = \int_\Omega f(t, x; \mathbf{i}) \, \mathrm{d}x, \quad f(t, x; \mathbf{i}) = \frac{1}{|\Omega|} g_\sigma(I_1(\mathbf{x}) - i_1) g_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)$$

$$F_2(t, i_2) = p_{I_2+tI}(i_2) = \int_\Omega f_2(t, x; i_2) \, \mathrm{d}x, \qquad f_2(t, x; i_2) = \frac{1}{|\Omega|} g_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)$$

$$F_1(i_1) = p_{I_1}(i_1).$$

For each $\mathbf{i} \in \mathbb{R}^2$, the function $F(\cdot, \mathbf{i}) : U \to \mathbb{R}$ is defined by integrals with integrand $f(\cdot, \cdot; \mathbf{i}) : U \times \Omega \to \mathbb{R}$. Thus, if we fix $\mathbf{i} \in \mathbb{R}^2$, clearly for each $x \in \Omega$, the function $f(\cdot, x; \mathbf{i})$

is differentiable with derivative $f'(t, \mathbf{x}; \mathbf{i}) = |\Omega|^{-1} g_\sigma(I_1(\mathbf{x}) - i_1) g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2) I(\mathbf{x})$. Moreover, it holds $|f'(t, \mathbf{x}; \mathbf{i})| \leq |\Omega|^{-1} g_\sigma(0)(\max|g'_\sigma|)|I(\mathbf{x})|$ and hence for each $t \in U$

$$|f'(t, \cdot; \mathbf{i})| \leq |\Omega|^{-1} g_\sigma(0)(\max|g'_\sigma|)|I| \in L^1(\Omega)$$

Therefore one can apply Theorem A.1.3, of differentiation under the integral sign, and conclude that $F(\cdot, \mathbf{i})$ is differentiable on U and for each $t \in U$ it holds

$$\partial_t F(t, \mathbf{i}) = \int_\Omega f'(t, \mathbf{x}; \mathbf{i}) \, \mathrm{d}\mathbf{x}$$

Moreover $\partial_t F(\cdot, \mathbf{i})$ is continuous since $f'(\cdot, \mathbf{x}, \mathbf{i})$ is continuous. In the same way, fixing $i_2 \in \mathbb{R}$, the function $F_2(\cdot, i_2) : U \to \mathbb{R}$ is defined by integrals with integrand $f_2(\cdot, \cdot; i_2) : U \times \Omega \to \mathbb{R}$. For each $x \in \Omega$ the function $f_2(\cdot, x; i_2)$ is differentiable with derivative $f'_2(t, \mathbf{x}; i_2) = |\Omega|^{-1} g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2) I(\mathbf{x})$, and for each $t \in U$ it holds

$$|f_2(t, \cdot; i_2)| \leq |\Omega|^{-1}(\max|g'_\sigma|)|I| \in L^1(\Omega)$$

Again from Theorem A.1.3 it follows that $F_2(\cdot, i_2)$ is differentiable on U and for each $t \in U$ it is

$$\partial_t F_2(t, i_2) = \int_\Omega f'_2(t, \mathbf{x}; i_2) \, \mathrm{d}\mathbf{x}$$

and $\partial_t F_2(\cdot, i_2)$ is continuous since so is $f'_2(\cdot, \mathbf{x}; i_2)$. Thus, if we denote for brief the integrand in (A.14) with $\Phi(t, \mathbf{i})$, the function $\Phi(t, \mathbf{i})$ is differentiable w.r.t. the variable t and

$$\begin{aligned}
\Phi'(t, \mathbf{i}) &= \partial_t F(t, \mathbf{i}) \left[\log \frac{F(t, \mathbf{i})}{F_1(i_1) F_2(t, i_2)} + 1 \right] - \frac{F(t, \mathbf{i})}{F_2(t, i_2)} \partial_t F_2(t, i_2) \\
&= \partial_t F(t, \mathbf{i}) \left[\log \frac{p_{I_1, I_2 + tI}(\mathbf{i})}{p_{I_1}(i_1) p_{I_2 + tI}(i_2)} + 1 \right] - \frac{p_{I_1, I_2 + tI}(\mathbf{i})}{p_{I_2 + tI}(i_2)} \partial_t F_2(t, i_2)
\end{aligned}$$

Now, letting $A > 0$ with $\|I_1\|_\infty \leq A$, we proved in Proposition 4.3.1 that

$$\left| \log \frac{p_{I_1, I_2 + tI}(\mathbf{i})}{p_{I_1}(i_1) p_{I_2 + tI}(i_2)} \right| \leq \psi(i_1) \qquad \frac{p_{I_1, I_2 + tI}(\mathbf{i})}{p_{I_2 + tI}(i_2)} \leq \hat{\varphi}(i_1)$$

Then

$$\begin{aligned}
|\Phi'(t, \mathbf{i})| &\leq \frac{1}{|\Omega|} \int_\Omega (\psi(i_1) + 1) g_\sigma(I_1(\mathbf{x}) - i_1) |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)| |I(\mathbf{x})| \, \mathrm{d}\mathbf{x} \\
&\qquad + \frac{1}{|\Omega|} \int_\Omega \hat{\varphi}(i_1) |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)| |I(\mathbf{x})| \, \mathrm{d}\mathbf{x} \\
&\leq \frac{1}{|\Omega|} \int_\Omega \hat{\varphi}(i_1)(\psi(i_1) + 2) |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)| |I(\mathbf{x})| \, \mathrm{d}\mathbf{x} := g(t, \mathbf{i})
\end{aligned}$$

where we took into account that $g_\sigma(I_1(\mathbf{x}) - i_1) \le \hat{\varphi}(i_1)$ for a.e. $\mathbf{x} \in \Omega$ (in fact it holds for all $x \in \Omega$ such that $|I_1(\mathbf{x})| \le A$). Moreover

$$\begin{aligned}
\int_{\mathbb{R}^2} g(t, \mathbf{i})\,\mathrm{d}\mathbf{i} &= \frac{1}{|\Omega|}\int_\Omega |I(\mathbf{x})| \int_{\mathbb{R}^2} \hat{\varphi}(i_1)(\psi(i_1)+2)|g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)|\,\mathrm{d}\mathbf{i}\,\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\int_\Omega |I(\mathbf{x})| \int_{\mathbb{R}} \hat{\varphi}(i_1)(\psi(i_1)+2)\,\mathrm{d}i_1 \int_{\mathbb{R}} |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)|\,\mathrm{d}i_2\,\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\|\hat{\varphi}(\psi+2)\|_1 \|g'_\sigma\|_1 \|I\|_1
\end{aligned}$$

and for each $\mathbf{i} \in \mathbb{R}^2$ the function $g(\cdot, \mathbf{i})$ is continuous — since it is defined by integrals with integrand

$$u_{\mathbf{i}}(t, \mathbf{x}) = \frac{1}{|\Omega|}\hat{\varphi}(i_1)(\psi(i_1)+2)|g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)||I(\mathbf{x})|$$

which is continuous w.r.t. the variable t and $0 \le u_{\mathbf{i}}(t, \mathbf{x}) \le \frac{1}{|\Omega|}\hat{\varphi}(i_1)(\psi(i_1)+2)\max|g'_\sigma||I(\mathbf{x})| \in L^1(\Omega)$. Therefore one can apply Theorem A.1.3 of differentiation under the integral sign and

$$\phi'(t) = \int_{\mathbb{R}^2} \partial_t F(t, \mathbf{i})\left[\log \frac{p_{I_1, I_2+tI}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2+tI}(i_2)} + 1\right]\mathrm{d}i_1\,\mathrm{d}i_2 - \int_{\mathbb{R}^2} \frac{p_{I_1, I_2+tI}(\mathbf{i})}{p_{I_2+tI}(i_2)}\partial_t F_2(t, i_2)\,\mathrm{d}i_1\,\mathrm{d}i_2$$

The second integral is

$$\int_{\mathbb{R}} \frac{\partial_t F_2(t, i_2)}{p_{I_2+tI}(i_2)}\left(\int_{\mathbb{R}} p_{I_1, I_2+tI}(i_1, i_2)\,\mathrm{d}i_1\right)\mathrm{d}i_2 = \int_{\mathbb{R}} \partial_t F_2(t, i_2)\,\mathrm{d}i_2 = \partial_t\left(\int_{\mathbb{R}} F_2(t, i_2)\,\mathrm{d}i_2\right) = 0$$

since $F_2(t, i_2) = p_{I_2+tI}(i_2)$ which has integral constantly equal to 1 — we differentiated under the integral sign again based upon Theorem A.1.3 taking into account that

$$|\partial_t F_2(t, i_2)| \le \frac{1}{|\Omega|}\int_\Omega |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)||I(\mathbf{x})|\,\mathrm{d}\mathbf{x} := g_2(t, i_2)$$

and

$$\int_{\mathbb{R}} g_2(t, i_2)\,\mathrm{d}i_2 = \frac{1}{|\Omega|}\int_\Omega |I(\mathbf{x})| \int_{\mathbb{R}} |g'_\sigma(I_2(\mathbf{x}) + tI(\mathbf{x}) - i_2)|\,\mathrm{d}i_2\,\mathrm{d}\mathbf{x} = \frac{1}{|\Omega|}\|g'_\sigma\|_1\|I\|_1$$

Then, there exists the *directional derivative* of $\mathbf{MI}(I_1, \cdot)$ at I_2 in the direction I and it is

$$\begin{aligned}
\phi'(0) &= \int_{\mathbb{R}^2} \partial_t F(0, \mathbf{i}) L_{I_1, I_2}(i_1, i_2)(i_1, i_2)\,\mathrm{d}i_1\,\mathrm{d}i_2 \\
&= \int_{\mathbb{R}^2} \frac{1}{|\Omega|}\left(\int_\Omega g_\sigma(I_1(\mathbf{x}) - i_1)g'_\sigma(I_2(\mathbf{x}) - i_2)I(\mathbf{x})\,\mathrm{d}\mathbf{x}\right) L_{I_1, I_2}(i_1, i_2)(i_1, i_2)\,\mathrm{d}i_1\,\mathrm{d}i_2
\end{aligned}$$

where we set

$$L_{I_1,I_2}(i_1,i_2) = \log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1)p_{I_2}(i_2)} + 1$$

Exchanging the order of integration and taking into account that $\partial_2 G_\sigma = g_\sigma g'_\sigma$

$$\begin{aligned}
\phi'(0) &= \frac{1}{|\Omega|}\int_\Omega \left(\int_{\mathbb{R}^2} \partial_2 G_\sigma(I_1(\mathbf{x})-i_1, I_2(\mathbf{x})-i_2) L_{I_1,I_2}(i_1,i_2)\,\mathrm{d}i_1\,\mathrm{d}i_2\right) I(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\int_\Omega (\partial_2 G_\sigma * L_{I_1,I_2})(I_1(\mathbf{x}), I_2(\mathbf{x})) I(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\int_\Omega (G_\sigma * \partial_2 L_{I_1,I_2})(I_1(\mathbf{x}), I_2(\mathbf{x})) I(\mathbf{x})\,\mathrm{d}\mathbf{x}
\end{aligned}$$

and

$$\partial_2 L_{I_1,I_2}(i_1,i_2) = \frac{\partial_2 p_{I_1,I_2}(i_1,i_2)}{p_{I_1,I_2}(i_1,i_2)} - \frac{p'_{I_2}(i_2)}{p_{I_2}(i_2)}$$

Let us show that

$$(\partial_2 G_\sigma * L_{I_1,I_2}) \circ (I_1, I_2) \in L^\infty(\Omega) \subseteq L^{q'}(\Omega)$$

Indeed for a.e. $x \in \Omega$ (the ones for which $|I_1(\mathbf{x})| \le A$), it holds

$$\begin{aligned}
|\partial_2 G_\sigma * L_{I_1,I_2}(I_1(\mathbf{x}), I_2(\mathbf{x}))| &\le \int_{\mathbb{R}^2} g_\sigma(I_1(\mathbf{x})-i_1)|g'_\sigma(I_2(\mathbf{x})-i_2)||L_{I_1,I_2}(i_1,i_2)|\,\mathrm{d}i_1\,\mathrm{d}i_2 \\
&\le \int_{\mathbb{R}^2} g_\sigma(I_1(\mathbf{x})-i_1)(\psi(i_1)+1)|g'_\sigma(I_2(\mathbf{x})-i_2)|\,\mathrm{d}i_1\,\mathrm{d}i_2 \\
&\le \int_{\mathbb{R}^2} \hat{\varphi}(i_1)(\psi(i_1)+1)|g'_\sigma(I_2(\mathbf{x})-i_2)|\,\mathrm{d}i_1\,\mathrm{d}i_2 \\
&= \|\hat{\varphi}(\psi+1)\|_1 \|g'_\sigma\|_1 < +\infty
\end{aligned}$$

and hence one can write

$$\phi'(0) = \langle \frac{1}{|\Omega|}(\partial_2 G_\sigma * L_{I_1,I_2}) \circ (I_1, I_2), I\rangle_{q',q}$$

being $\langle\cdot,\cdot\rangle_{q',q}$ the canonical duality between $L^{q'}(\Omega)$ and $L^q(\Omega)$. This shows that $\mathbf{MI}(I_1,\cdot) : L^q(\Omega) \to \mathbb{R}$ is Gâteaux differentiable and it is

$$\nabla\mathbf{MI}(I_1,\cdot)(I_2) = \frac{1}{|\Omega|}(\partial_2 G_\sigma * L_{I_1,I_2}) \circ \mathbf{I} = \frac{1}{|\Omega|}(G_\sigma * \partial_2 L_{I_1,I_2}) \circ \mathbf{I} \in L^{q'}(\Omega)$$

and moreover

$$\|\nabla\mathbf{MI}(I_1,\cdot)(I_2)\|_{q'} \le |\Omega|^{1/q'} \|\nabla\mathbf{MI}(I_1,\cdot)(I_2)\|_\infty \le |\Omega|^{1/q'} \|\hat{\varphi}(\psi+1)\|_1 \|g'_\sigma\|_1$$

From this, it follows that the gradient $\nabla\mathbf{MI}(I_1,\cdot) : L^q(\Omega) \to L^{q'}(\Omega)$ is a mapping bounded by a constant which depends on A alone.[3]

Finally, let us prove that $\nabla\mathbf{MI}(I_1,\cdot) : L^q(\Omega) \to L^{q'}(\Omega)$ is continuous. Let $(I_2^k)_{k\in\mathbb{N}} \in L^q(\Omega)^{\mathbb{N}}$, $I_2 \in L^q(\Omega)$ with $I_2^k \to I_2$ a.e. and set for brief $f_k = \nabla\mathbf{MI}(I_1,\cdot)(I_2^k)$ and $f = \nabla\mathbf{MI}(I_1,\cdot)(I_2)$. Clearly for every $\mathbf{x} \in \Omega$

$$f_k(\mathbf{x}) = \int_{\mathbb{R}^2} g_\sigma(I_1(\mathbf{x}) - i_1) g'_\sigma(I_2^k(\mathbf{x}) - i_2) L_k(i_1, i_2)\, \mathrm{d}\mathbf{i}$$

$$f(\mathbf{x}) = \int_{\mathbb{R}^2} g_\sigma(I_1(\mathbf{x}) - i_1) g'_\sigma(I_2(\mathbf{x}) - i_2) L(i_1, i_2)\, \mathrm{d}\mathbf{i}$$

where

$$L_k(i_1, i_2) = \log \frac{p_{I_1,I_2^k}(\mathbf{i})}{p_{I_1}(i_1) p_{I_2^k}(i_2)} + 1 \qquad L(i_1, i_2) = \log \frac{p_{I_1,I_2}(\mathbf{i})}{p_{I_1}(i_1) p_{I_2}(i_2)} + 1$$

We already saw that from the hypothesis $I_2^k \to I_2$ a.e. it follows $L_k(\mathbf{i}) \to L(\mathbf{i})$ for every $\mathbf{i} \in \mathbb{R}^2$. Let $\mathbf{x} \in \Omega$ be such that $I_2^k(\mathbf{x}) \to I_2(\mathbf{x})$. Then

$$g_\sigma(I_1(\mathbf{x}) - i_1) g'_\sigma(I_2^k(\mathbf{x}) - i_2) L_k(i_1, i_2) \to g_\sigma(I_1(\mathbf{x}) - i_1) g'_\sigma(I_2(\mathbf{x}) - i_2) L(i_1, i_2)$$

for every $\mathbf{i} \in \mathbb{R}^2$. Next if we take $B > 0$ such that $|I_2^k(\mathbf{x})| \leq B$ for every $k \in \mathbb{N}$,[4] then

$$\begin{aligned} &g_\sigma(I_1(\mathbf{x}) - i_1) |g'_\sigma(I_2^k(\mathbf{x}) - i_2)| |L_k(i_1, i_2)| \\ &\qquad\qquad = g_\sigma(I_1(\mathbf{x}) - i_1) g_\sigma(I_2^k(\mathbf{x}) - i_2) |I_2^k(\mathbf{x}) - i_2| |L_k(i_1, i_2)| \\ &\qquad\qquad \leq \hat{\varphi}_A(i_1)(\psi_A(i_1) + 1)\hat{\varphi}_B(i_2)(|i_2| + B) \end{aligned}$$

and the function on the right side is summable over $\mathbb{R}^2$. Therefore, due to the dominated convergence theorem, it is $f_k(\mathbf{x}) \to f(\mathbf{x})$. We thus, proved that $f_k \to f$ pointwise a.e. Finally we already saw

$$|f_k(\mathbf{x})| \leq \int_{\mathbb{R}^2} g_\sigma(I_1(\mathbf{x}) - i_1) |g'_\sigma(I_2^k(\mathbf{x}) - i_2)| |L_k(i_1, i_2)|\, \mathrm{d}\mathbf{i} = \|\hat{\varphi}(\psi + 1)\|_1 \|g'_\sigma\|_1$$

and on the right side there is a constant function belonging to $L^{q'}(\Omega)$. Another application of the Lebesgue's convergence theorem allows us to conclude $f_k \to f$ in $L^{q'}(\Omega)$. $\square$

[3]Note that $\|g'_\sigma\|_1 = 2g_\sigma(0) = \sqrt{2/(\pi\sigma^2)}$. Indeed $g'_\sigma(i) = -g_\sigma(i) i/\sigma^2$ hence $|g'_\sigma|$ is symmetric and

$$\int_{\mathbb{R}} |g'_\sigma(i)|\, \mathrm{d}i = -2 \int_{\mathbb{R}_+} g'_\sigma(i)\, \mathrm{d}i = -2 \lim_{b\to+\infty} [g_\sigma(b) - g_\sigma(0)] = 2g_\sigma(0)$$

[4]The sequence $(I_2^k(\mathbf{x}))_{k\in\mathbb{N}}$ is bounded, being convergent.

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