

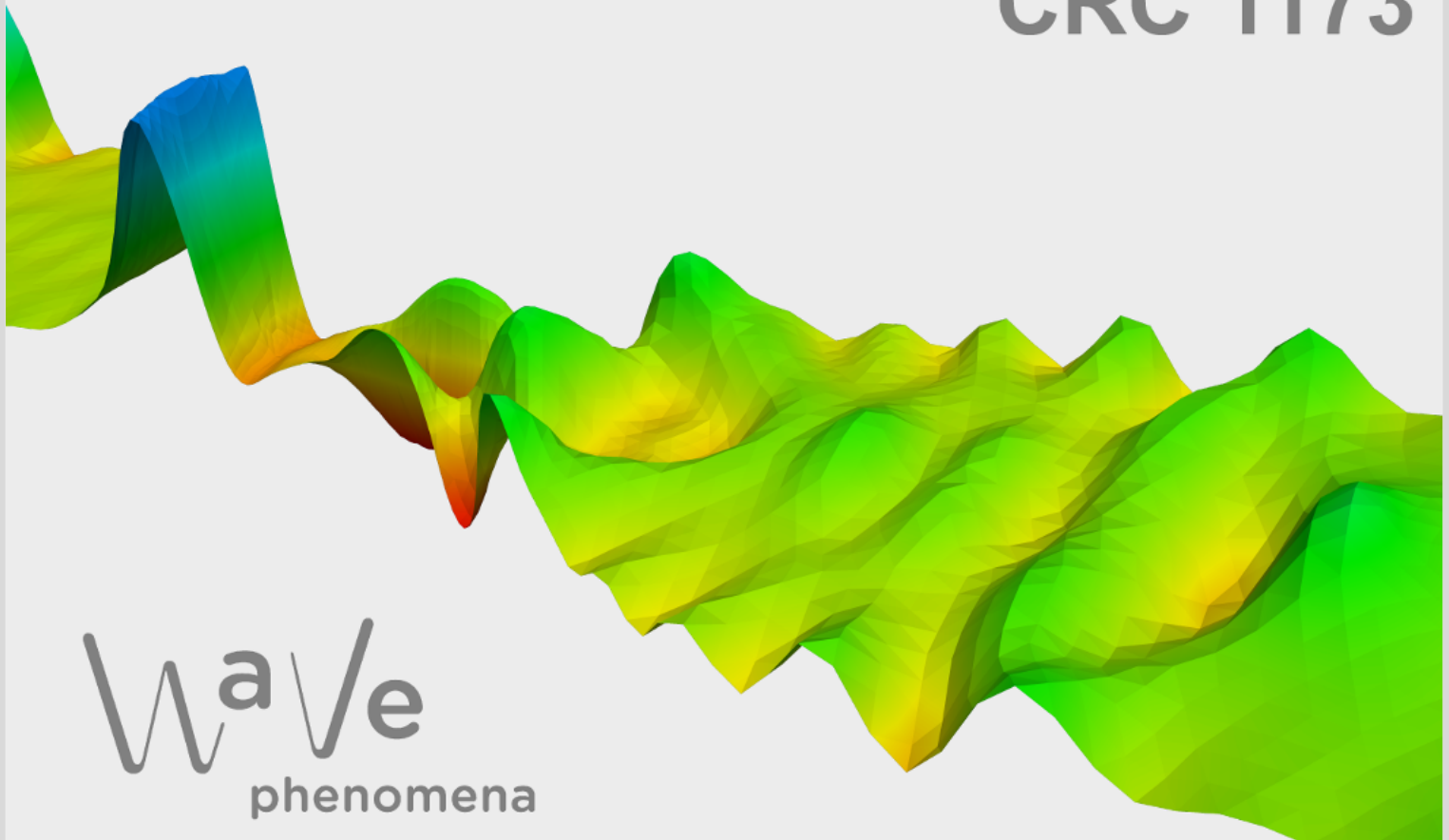
Solving highly underdetermined inverse problems by an inexact penalty method and learned distances with an application to seismic imaging

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SOLVING HIGHLY UNDERDETERMINED INVERSE PROBLEMS BY AN INEXACT PENALTY METHOD AND LEARNED DISTANCES WITH AN APPLICATION TO SEISMIC IMAGING

DAVID HÄMMERLING[†]  AND ANDREAS RIEDER[†] 

ABSTRACT. Inverse problems are often solved by minimizing problem-specific distance functionals. In many applications, such as full waveform inversion (FWI), the leading technology in seismic imaging, standard functionals are non-convex and thus hard to optimize. Consequently, many convex replacements have been proposed, including learned distance functionals. However, even if one can find a minimizer of such a functional, it is likely not unique, particularly when the inverse problem is underdetermined, as is often the case in practical settings. To overcome this challenge, we propose and theoretically backup an inexact penalty method, that is computationally realizable and finds a solution to the inverse problem with physically preferred properties, that are described by a given regularization term. To validate this method, we apply it to FWI in the acoustic regime using the Marmousi model, a proven geophysical benchmark problem. We observe a significant enhancement in the reconstruction quality compared to standard methods.

1. INTRODUCTION

We consider a general inverse problem formulated as a nonlinear equation

$$(1) \quad F(x) = y,$$

which is described by some operator $F: D(F) \subset X \rightarrow Y$ acting between Hilbert spaces X and Y and a data vector $y \in Y$. Our declared goal is to find a parameter vector $x \in D(F)$, which fulfills (1), at least approximately. One way to address this type of problem is to rewrite the strict equality in (1) as an optimization problem

$$(2) \quad \min_{x \in D(F)} d_y(x),$$

with some objective functional $d_y: X \rightarrow [0, \infty)$, that works as an abstract distance functional to quantify the distance between the predicted data $F(x)$ and the measured data y . An essential property of such a distance d_y is that it only attains its minimal value in a solution of (1), i.e.

$$d_y(x) = 0 \iff F(x) = y.$$

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A common but generally poor choice is the standard least-squares functional

$$J_y(x) := \frac{1}{2} \|F(x) - y\|^2.$$

In many areas of application this functional is known for being notoriously difficult to minimize without knowledge of an unreasonably well-chosen initial guess. One of these applications is full waveform inversion (FWI) in seismic imaging. The inverse problem in FWI is to gain information about the earth's subsurface by reconstructing a material multi-parameter x , containing, for instance, wave velocity or mass density. The desired subsurface information is encoded in seismogram data y measured on the earth's exterior and linked to the parameters by the used wave propagation model, such as the acoustic wave equation, resulting in the nonlinear forward modeling operator F .

This combination of the measurement process and the wave equation constructs a nonlinearity F for which the associated least-squares functional J_y is highly non-convex. As a result considerable effort has been devoted to replacing this non-convex objective J_y by a problem-tailored convex distance measure d_y . Alternatives for reconstructing better-suited distance functionals include:

- optimal transport based distances [11, 12, 16, 32, 33, 36, 45],
- cross-correlation based traveltimes misfits [30, 44],
- machine-learning based distances [9, 20, 41, 42, 46].

The most recent and promising of these approaches are neural network based distances. A common technique among the cited sources is training a neural network $\Phi: Y \rightarrow Z$ that acts as a simplifier such that the new least squares functional

$$d_y(x) := \frac{1}{2} \|\Phi(F(x)) - \Phi(y)\|^2$$

becomes convex.

However, even if we are given a convex objective functional d_y and we are able to solve problem (2) with some optimization algorithm, two main issues remain, inherited by the operator F :

- Equation (1) is typically ill-posed, which makes the inversion process unstable when confronted with perturbed data y^δ , since small variations in the measurements can lead to huge errors in the reconstruction.
- In general we cannot expect F to be injective. Or at least in a numerical realization the inversion process can become almost singular, which results in (1) being underdetermined, i.e., not uniquely solvable.

The first issue can be addressed by standard regularization techniques such as an appropriate early-stopping-criterion for an iterative method.

The second issue can be avoided by replacing the unconstrained optimization problem (2) with a constraint problem that includes a uniformly convex regularization term $R: X \rightarrow [0, \infty)$ that encapsulates physical a-priori knowledge about the desired solution. The uniform convexity of R should 'injectify' the problem, i.e., render it uniquely solvable. A common strategy for such a constraint optimization problem is

$$\min_{x,u} R(x), \quad \mathcal{F}x = u, \quad Mu = y,$$

in case the forward operator $F = M\mathcal{F}$ consists of a (PDE) model operator $\mathcal{F}$ and a measurement operator M . Such tasks can, for example, be solved by reinterpreting them as a Tikhonov methods in an all-at-once setting [24, 38, 40], or by an alternating direction

method of multipliers (ADMM), which works reasonably well for FWI [1, 2, 15], although it lacks a theoretical justification. Introducing the second optimization parameter u can alter theoretical restrictions on the forward operator F , but it also requires significantly more computational effort. In the case of FWI, u corresponds to one wave field over the full space-time domain, which often requires excessive computer memory.

To avoid this complication we rely on the following reduced optimization problem, which only requires a one-dimensional constraint:

$$(3) \quad \min_{x \in D(F)} R(x), \quad d_y(x) = 0.$$

Under reasonable assumptions on R and d_y , that will be thoroughly discussed in the next section, we will verify that (3) admits a unique solution (Proposition 2.3). Our method of choice to find this unique solution is the penalty method. Here the idea is to iteratively approximate (3) by the unconstrained optimization problem,

$$(4) \quad \min_{x \in D(F)} f_n(x) := R(x) + v_n d_y(x),$$

for progressively increasing parameters $v_n > 0$. This is essentially equivalent to a non-stationary iterated Tikhonov method, where one solves

$$(5) \quad \min_{x \in D(F)} T_n(x) := d_y(x) + \alpha_n R(x),$$

for parameters $\alpha_n > 0$. This method has been thoroughly studied for linear inverse problem [6, 17, 21, 22] as well as nonlinear problems [23, 34, 35, 47]. Despite the rigorous and well-developed Banach space theory established in these sources, a few major caveats regarding its computational side remain: The theory only considers norm-based distance functionals of the form

$$d_y(x) = \frac{1}{s} \|F(x) - y\|^s,$$

for which strong restrictions on the nonlinearity F are required, such as the tangential cone condition (TCC) (see [43, (3.1) & (3.2)] or [25]). Moreover, it does not cover the newly emerged distance functionals addressed above. To the best of our knowledge, it is always assumed that at the n -th iteration step the optimization problem (5) is solved exactly, i.e., each iterate is defined as

$$x_n := \arg \min_{x \in D(F)} T_n(x),$$

which is generally not realizable, since an explicit expression for this minimizer does not exist. Lastly, the numerical examples of nonlinear inverse problems presented in the above-cited literature are highly academic; they were fabricated with no connection to real-world applications.

For these reasons we introduce an early-stopped inexact penalty method as a replacement for the nonlinear iterated Tikhonov method which allows the following generalizations:

- We avoid the theoretical restriction of the TCC by replacing it with a local convexity assumption on d_y , a property that is more natural for a generalized distance functional. This assumption can be demonstrated using constructed examples of ill-posed problems, as shown in Appendix A or [19, Section 5].

- We consider the penalty functional f_n instead of the Tikhonov functional T_n , which allows us to relax the exact solvability of (4) at the n -th optimization step to finding an approximation $x_n \in D(F)$ close to a stationary point, that means we only have to realize

$$\|\nabla f_n(x_n)\| \leq \varepsilon_n,$$

for some tolerance level $\varepsilon_n > 0$. The idea for this relaxation and the associated theoretical results are inspired by inexact penalty decomposition methods as presented in [26, 29].

In this paper we explore theoretical and computational aspects of the penalty scheme (4). In particular,

- We conduct a full convergence analysis in Section 2 for inverse problems in Hilbert spaces, given exact and noisy data. In case of noisy data the optimization method becomes a regularization method by incorporating the discrepancy principle as stopping rule.
- We discuss the numerical realization of the optimization step in Section 3 and we prove global convergence of the penalty method under arguably weak assumptions on the objective functional d_y .
- Finally, in Section 4, we test our method on a well-established benchmark model for full waveform inversion and numerically validate its clear improvement upon standard methods when combined with the learned distance functionals from [20].

2. AN EARLY STOPPED INEXACT PENALTY METHOD

There is a huge variety of methods well suited to solve constrained optimization problems such as (3). In our case we choose the penalty method. Here we iteratively calculate solutions x_n to the optimization problem

$$\min_{x \in X} f_n(x) := R(x) + v_n d_y(x),$$

for an increasing sequence of penalty parameters $v_n \rightarrow \infty$. Since this optimization problem can in general not be solved exactly and not on the full space, we loosen the problem to finding an $x_n \in \mathcal{U}_n$ for some subset $\mathcal{U}_n \subset X$ such that $\|\nabla f_n(x_n)\| \leq \varepsilon_n$ for some tolerance $\varepsilon_n > 0$.

Since we are mainly interested in finding a solution of an ill-posed problem we additionally employ the discrepancy principle as a stopping criterion, which in the context of a generalized distance functional d_y means that for a given noise level $\delta > 0$ and a proportionality constant $\tau > 0$ we choose the first $N(\delta) \in \mathbb{N}$ as a stopping index for which the corresponding $x_{N(\delta)}$ of the penalty method fulfills $d_y(x_{N(\delta)}) \leq \tau\delta$, i.e.,

$$d_y(x_{N(\delta)}) \leq \tau\delta, \quad \text{and} \quad d_y(x_n) > \tau\delta, \quad \text{for } n \in \{0, \dots, N(\delta) - 1\}.$$

This regularizing solution approach for (3) results in total in Algorithm 1.

We will provide a convergence and regularization analysis of the penalty method under certain hypotheses on R and d_y which we collect in the following assumption and which we discuss in Remark 2.2.

Assumption 2.1. *For the regularization term $R: X \rightarrow [0, \infty)$ we require:*

(R1) *R is continuously (Fréchet)-differentiable.*

Algorithm 1 Penalty method

Input: $R, d_y: X \rightarrow [0, \infty)$, $x_0 \in X$, $\tau, \delta \geq 0$, $(\varepsilon_n)_{n \in \mathbb{N}}, (v_n)_{n \in \mathbb{N}} \in (0, \infty)^{\mathbb{N}}$, $(\mathcal{U}_n)_{n \in \mathbb{N}} \in (2^X)^{\mathbb{N}}$.
 $n := 0$
while $d_y(x_n) > \tau\delta$ **do**
 $n++$
 $f_n(x) := R(x) + v_n d_y(x)$
 Choose $x_n \in \mathcal{U}_n$ **such that** $\|\nabla f_n(x_n)\| \leq \varepsilon_n$
end while
 $N(\delta) := n$
Output: $x_{N(\delta)}$

(R2) R is μ -strongly convex, i.e. there is an $\mu > 0$, such that for all $x, z \in X$ we have

$$R(z) \geq R(x) + \langle \nabla R(x), z - x \rangle + \mu \|x - z\|^2.$$

(R3) The gradient $\nabla R: X \rightarrow X$ is Lipschitz-continuous and hence bounded on bounded sets.

For a given $y \in Y$, the objective functional $d_y: X \rightarrow [0, \infty)$ fulfills:

(D1) d_y is continuously (Fréchet)-differentiable.

(D2) There is a non-empty, closed and convex set $\mathcal{U}(y) \subset D(F)$ such that d_y is convex on $\mathcal{U}(y)$, i.e., for all $x, z \in \mathcal{U}(y)$ we have

$$d_y(z) \geq d_y(x) + \langle \nabla d_y(x), z - x \rangle.$$

Further, $d_y^{-1}(0) \subset \text{int}(\mathcal{U}(y))$ if $d_y^{-1}(0) \neq \emptyset$ and, otherwise,

$$\emptyset \neq \arg \min_{x \in \mathcal{U}(y)} d_y(x) \subset \text{int}(\mathcal{U}(y)).$$

(D3) For all $x \in X$,

$$d_y(x) = 0 \iff F(x) = y.$$

(D4) There is a continuously (Fréchet)-differentiable functional $d: Y \times X \rightarrow [0, \infty)$ such that $d(y, x) = d_y(x)$ for all $x \in X$ and $y \in Y$. Further, there is a well-defined functional $\eta: Y \rightarrow [0, \infty)$ such that

$$\|\partial_y d(F(x), x)\|_{Y \rightarrow \mathbb{R}} \leq \eta(F(x)), \quad \text{for all } x \in X.$$

As announced above, we now motivate and discuss the made hypotheses.

Remark 2.2. The assumptions (R1)-(R3) on the regularization term are quite standard. They are, for example, satisfied by any potentiated and translated Hilbert space norm

$$R(x) = \|x - \bar{x}\|^p,$$

with $p \geq 2$ and a reference element $\bar{x}$ [5, Example 10.16]. In our analysis we will heavily rely on the strong convexity (R2) which can be guaranteed for more general R in a finite-dimensional setting after an appropriate discretization. Indeed all L^p -norms are strictly convex and thus also strongly convex on non-empty, bounded and closed convex subsets [5, Corollary 10.18]. Also, combining any convex function such as the total variation (TV) with a strongly convex regularization term always yields a strongly convex functional. So, from a practical point of view, (R2) is less restrictive than it seems at first glance. In our

numerical experiments we combine a smooth approximation of the TV-seminorm with the p -th power of an L^p -norm, see (13), which is convex on the bounded domain $D(F)$ in the given example.

Requirements (D1), (D3), and (D4) on the distance functional are taken from [20, Assumption 2.1 (i), (iii), and (v)], where they are also motivated in Remark 2.2. They are met by the learned, neural-net-based distances proposed in [20, Section 3].

On the other hand, (D2) is non-trivial and requires additional justification. It is a relaxation of Assumption 2.1(ii) from [20] adapted to the highly underdetermined situation we consider in this work, where we take into account that $d_y^{-1}(0)$ is not obliged to be single-valued. Further, it is also a natural property of alternative distance functionals, like those mentioned in the introduction, since the whole idea behind replacing the standard least-squares functional is to expand the area of convexity $\mathcal{U}(y)$ to include the set of exact solutions $d_y^{-1}(0)$ or, in case it is empty, to include the set of minimizers.

Conditions similar to (D2) have for instance been discussed in [19] where the authors also give (academic) examples of nonlinear operators F for which the resulting least-squares functionals J_y are locally convex. Moreover, they discuss the relation of the convexity of J_y to the tangential cone condition (TCC), a structural restriction on F , and gave an example [19, Example 4.1] of an F for which the TCC does not hold, yet J_y is globally convex.

Whether the TCC of F implies local convexity of J_y and thus local convexity is a weaker assumption than the TCC or whether these concepts are fundamentally different remains an open problem to date, see [19, Section 4] and the references therein for further discussion.

Lastly to even further support Assumption 2.1, we give an academic example in Appendix A of a non-injective operator F for which $d_y := J_y$ satisfies (D1)-(D4). This example is heavily inspired by [19, Example 5.1].

The first result we can validate under above assumptions is the unique solvability of (3).

Proposition 2.3 (Unique solvability). *If $d_y^{-1}(0) \subset X$ is non-empty under Assumption 2.1, then the optimization task (3) has a unique solution $x^+ \in d_y^{-1}(0)$.*

Proof. Since R is continuous (R1) and convex (R2), it is also lower semicontinuous [7, Corollary 3.9]. Further, from (R2) we also find that

$$R(x) \geq R(0) + \langle \nabla R(0), x - 0 \rangle + \mu \|x - 0\|^2 \geq -\|\nabla R(0)\| \|x\| + \mu \|x\|^2 \rightarrow \infty, \\ \text{as } \|x\| \rightarrow \infty,$$

which means that R is coercive. Next we know that the pre-image $d_y^{-1}(0)$ is closed since $\{0\} \subset \mathbb{R}$ is closed and d_y is continuous by (D1). From (D2) we further conclude that $d_y^{-1}(0)$ is convex and thus by [7, Corollary 3.23] there exists a minimizer $x^+ \in X$, which is unique due to R being strongly convex. $\square$

To ensure that the iterates $(x_n)_{n \in \mathbb{N}}$ from Algorithm 1 are actually computable and converge to x^+ we impose a structural property on our sequence of subsets $(\mathcal{U}_n)_{n \in \mathbb{N}}$, which we will call *U-compatibility*.

Definition 2.4 (U-compatibility). *Let $R: X \rightarrow [0, \infty)$ and $d_y: X \rightarrow [0, \infty)$ fulfill Assumption 2.1. Let $(v_n)_{n \in \mathbb{N}}$ be a sequence of positive numbers such that*

$$v_n \rightarrow \infty, \quad n \rightarrow \infty.$$

Then, we call a sequence $(\mathcal{U}_n)_{n \in \mathbb{N}}$ of closed and convex subsets of X U -compatible to R , d_y and $(v_n)_{n \in \mathbb{N}}$ provided the following three properties hold true:

- (U1) For every $n \in \mathbb{N}$ the penalty functional $f_n(x) = R(x) + v_n d_y(x)$ is μ_n -strongly convex on $\mathcal{U}_n$, i.e. there is a constant $\mu_n > 0$ such that

$$f_n(z) \geq f_n(x) + \langle \nabla f_n(x), z - x \rangle + \mu_n \|x - z\|^2 \quad \forall x, z \in \mathcal{U}_n.$$

- (U2) We have for every $n \in \mathbb{N}$: $\mathcal{U}(y) \subset \mathcal{U}_n$.

- (U3) There exists a $K \in \mathbb{N}$ such that $\mathcal{U}_n = \mathcal{U}(y)$ for all $n \geq K$.

We highlight this definition with a few comments.

Remark 2.5.

- (a) By Assumption 2.1(D2) there always exists a U -compatible sequence $(\mathcal{U}_n)_{n \in \mathbb{N}}$ for any arbitrary sequence $(v_n)_{n \in \mathbb{N}}$, namely the constant setting $\mathcal{U}_n = \mathcal{U}(y)$. However, this choice is generally too restrictive. Therefore, in Algorithm 1, we allow a relaxation with which the functional f_n can be strongly convex on bigger subsets for finitely many optimization steps.
- (b) Note that for every U -compatible sequence by (U3) we have $\mu_n \geq \mu$ for $n \geq K$ or equivalently

$$\liminf_{n \rightarrow \infty} \mu_n \geq \mu.$$

This uniform boundedness of the moduli will be essential for the subsequent proofs.

In the following we distinguish between a sequence $(x_n)_{n \in \mathbb{N}}$ generated by Algorithm 1 and its output $x_{N(\delta)}$. By a sequence generated by Algorithm 1 we denote any sequence $(x_n)_{n \in \mathbb{N}}$ satisfying

$$\|\nabla f_n(x_n)\| \leq \varepsilon_n,$$

for a given input configuration $(R, d_y, x_0, \tau, \delta, (\varepsilon_n)_{n \in \mathbb{N}}, (v_n)_{n \in \mathbb{N}}, (\mathcal{U}_n)_{n \in \mathbb{N}})$. The output $x_{N(\delta)}$ is defined by the first element of the sequence $(x_n)_{n \in \mathbb{N}}$, for which the stopping criterion

$$d_y(x_{N(\delta)}) \leq \tau \delta$$

is fulfilled.

Having introduced the necessary terminology, we are in a position to verify the well-definedness of Algorithm 1, i.e. the computability of the sequence $(x_n)_{n \in \mathbb{N}}$.

Proposition 2.6 (Well-definedness). *Let Assumption 2.1 hold and let the sequence $(v_n)_{n \in \mathbb{N}}$ be chosen such that*

$$v_n \rightarrow \infty, \quad n \rightarrow \infty.$$

Further let $(\mathcal{U}_n)_{n \in \mathbb{N}}$ be U -compatible to R , d_y and $(v_n)_{n \in \mathbb{N}}$. Then, there is an index $M \in \mathbb{N}$ such that for any $n \geq M$ there exists a $x_n \in \mathcal{U}_n$ with $\|\nabla f_n(x_n)\| \leq \varepsilon_n$ for any given $\varepsilon_n > 0$.

Proof. By construction f_n is coercive, since

$$f_n(x) = R(x) + v_n d_y(x) \geq R(x) \rightarrow \infty \quad \text{as} \quad \|x\| \rightarrow \infty.$$

Further, by (U1), f_n is convex and continuous on $\mathcal{U}_n$ and thus also lower semi-continuous [7, Corollary 3.9]. In view of [7, Corollary 3.23] there exists a minimizer $x_n^* \in \mathcal{U}_n$ of f_n , which is unique due to the uniform convexity. We now show that this minimizer x_n^* lies

in the interior of $(\mathcal{U}_n)$ for n large enough: To this end let $x^+ \in \text{int}(\mathcal{U}(y))$ be the unique solution of

$$\min R(x) \quad \text{for } x \in \arg \min_{x \in \mathcal{U}(y)} d_y(x),$$

which coincides with the unique solution of (3) from Proposition 2.3 if $d_y^{-1}(0) \neq \emptyset$ and otherwise also exists and is unique according to (D2). Next, since $\mathcal{U}_n$ is closed and convex the minimizer x_n^* fulfills the variational inequality

$$\langle \nabla f_n(x_n^*), x - x_n^* \rangle \geq 0 \quad \text{for all } x \in \mathcal{U}_n.$$

Combining this inequality with the uniform convexity of f_n , we can deduce for the unique solution $x^+ \in \mathcal{U}(y) \subset \mathcal{U}_n$ (see (U2) and (U3)) of (3):

$$\begin{aligned} \mu_n \|x_n^* - x^+\|^2 &\leq f_n(x^+) - f_n(x_n^*) - \langle \nabla f_n(x_n^*), x^+ - x_n^* \rangle \\ &\leq R(x^+) - R(x_n^*) + v_n(d_y(x^+) - d_y(x_n^*)). \end{aligned}$$

Rearranging the terms and taking the limit yields

$$\limsup_{n \rightarrow \infty} \mu_n \|x_n^* - x^+\|^2 + R(x_n^*) + v_n(d_y(x_n^*) - d_y(x^+)) \leq R(x^+) < \infty,$$

from which we immediately draw three consequences:

- The sequence $(x_n^*)_{n \in \mathbb{N}}$ is bounded,
- $\limsup_{n \rightarrow \infty} R(x_n^*) \leq R(x^+)$,
- $\lim_{n \rightarrow \infty} d_y(x_n^*) = d_y(x^+)$, since $v_n \rightarrow \infty$.

The boundedness yields the existence of a weak limit $x_n^* \rightharpoonup \tilde{x}$. Since for convex sets closedness in the strong and in the weak topology are equivalent [7, Theorem 3.7], we derive from (U2) and (U3):

$$\tilde{x} \in \mathcal{U}(y) = \bigcap_{n \in \mathbb{N}} \mathcal{U}_n.$$

For this limit we conclude, based on the three properties of $(x_n^*)_{n \in \mathbb{N}}$ from above,

$$\begin{aligned} d_y(\tilde{x}) &= d_y(\tilde{x}) - d_y(x_n^*) + d_y(x_n^*) = v_n^{-1}(f_n(\tilde{x}) - f_n(x_n^*) + R(x_n^*) - R(\tilde{x})) + d_y(x_n^*) \\ &\leq v_n^{-1}(\langle \nabla f_n(\tilde{x}), \tilde{x} - x_n^* \rangle + R(x_n^*) - R(\tilde{x})) + d_y(x_n^*) \\ &= \langle \nabla d_y(\tilde{x}), \tilde{x} - x_n^* \rangle + \frac{\langle \nabla R(\tilde{x}), \tilde{x} - x_n^* \rangle + R(x_n^*) - R(\tilde{x})}{v_n} + d_y(x_n^*) \rightarrow d_y(x^+). \end{aligned}$$

Hence, by (D2),

$$\tilde{x} \in \arg \min_{x \in \mathcal{U}(y)} d_y(x) \subset \text{int}(\mathcal{U}(y)) \subset \text{int}(\mathcal{U}_n)$$

and $R(x^+) \leq R(\tilde{x})$ by definition of x^+ . This inequality implies the strong convergence of x_n^* to $\tilde{x}$:

$$\limsup_{n \rightarrow \infty} \mu \|x_n^* - \tilde{x}\|^2 \leq \limsup_{n \rightarrow \infty} [R(x_n^*) - R(\tilde{x}) - \langle \nabla R(\tilde{x}), x_n^* - \tilde{x} \rangle] \leq R(x^+) - R(\tilde{x}) \leq 0.$$

Thus, $x_n^* \in \text{int}(\mathcal{U}_n)$ for n large enough. Next, since x_n^* is an inner point we have $x_n^* + t \nabla f_n(x_n^*) \in \mathcal{U}_n$ for $t > 0$ small enough. With this knowledge the function $\varphi(t) := f_n(x_n^* + t \nabla f_n(x_n^*))$ attains its minimum in zero, which gives us

$$0 = \varphi'(0) = \|\nabla f_n(x_n^*)\|^2.$$

This finally yields the existence of a stationary point in $\mathcal{U}_n$ for n large enough and concludes the proof. $\square$

Without loss of generality we identify $(v_n)_{n \in \mathbb{N}}$ with $(v_{n+M})_{n \in \mathbb{N}}$ as well as $(\mathcal{U}_n)_{n \in \mathbb{N}}$ with $(\mathcal{U}_{n+M})_{n \in \mathbb{N}}$ for M from Proposition 2.6 in the remainder of this work. Thus, we have a well-defined Algorithm 1 that produces a sequence $(x_n)_{n \in \mathbb{N}}$. This sequence converges in the case of noise-free data.

Theorem 2.7 (Noise-free convergence). *Under Assumption 2.1 let $y \in Y$ such that $d_y^{-1}(0) \neq \emptyset$. Further, let $\delta = 0$,*

$$\varepsilon_n \rightarrow 0 \quad \text{and} \quad v_n \rightarrow \infty \quad \text{as} \quad n \rightarrow \infty.$$

Additionally, assume $(\mathcal{U}_n)_{n \in \mathbb{N}}$ to be a U -compatible sequence for R , d_y and $(v_n)_{n \in \mathbb{N}}$. Then, the sequence $(x_n)_{n \in \mathbb{N}}$ generated by Algorithm 1 converges to the unique solution $x^+ \in X$ of (3).

Proof. First, we assume for the limes superior of $(R(x_n))_{n \in \mathbb{N}}$ the lower bound

$$(6) \quad \limsup_{n \rightarrow \infty} R(x_n) > R(x^+).$$

Now let $(x_{n_k})_{k \in \mathbb{N}}$ be a subsequence such that

$$\lim_{k \rightarrow \infty} R(x_{n_k}) = \limsup_{n \rightarrow \infty} R(x_n).$$

We identify $(x_{n_k})_{k \in \mathbb{N}} = (x_n)_{n \in \mathbb{N}}$. Then, $\|x_n - x^+\| > 0$ and $R(x_n) > R(x^+)$ for n large enough. Using $x^+ \in \mathcal{U}(y) \subset \mathcal{U}_n$ we, in combination with the uniform convexity of f_n , obtain

$$\begin{aligned} \mu_n \|x_n - x^+\|^2 &\leq f_n(x^+) - f_n(x_n) - \langle \nabla f_n(x_n), x^+ - x_n \rangle \\ &\leq R(x^+) - R(x_n) - v_n d_y(x_n) + \|\nabla f_n(x_n)\| \|x_n - x^+\| \\ &\leq \varepsilon_n \|x_n - x^+\|. \end{aligned}$$

Dividing by $\|x_n - x^+\|$, recalling Remark 2.5(b), and taking the limit yields

$$\lim_{n \rightarrow \infty} \|x_n - x^+\| = 0$$

and, by continuity, $R(x_n) \rightarrow R(x^+)$, which contradicts (6).

Thus,

$$\limsup_{n \rightarrow \infty} R(x_n) \leq R(x^+),$$

which implies that $(R(x_n))_{n \in \mathbb{N}}$ is bounded. Now, let x^* be the global minimizer of R , which exists due to the uniform convexity (R2) and fulfills $\nabla R(x^*) = 0$, then we also get

$$\mu \|x_n - x^*\|^2 \leq R(x_n) - R(x^*) - \langle \nabla R(x^*), x_n - x^* \rangle \leq \sup_{n \in \mathbb{N}} R(x_n) - R(x^*) < \infty,$$

which immediately yields that also $(x_n)_{n \in \mathbb{N}}$ is bounded.

Next, the limit $v_n \rightarrow \infty$ and the boundedness of $(\|\nabla R(x_n)\|)_{n \in \mathbb{N}}$ (see (R3) in Assumption 2.1) yield

$$\begin{aligned} \|\nabla d_y(x_n)\| &= \frac{\|\nabla R(x_n)\|}{v_n} - \frac{\|\nabla R(x_n)\|}{v_n} + \|\nabla d_y(x_n)\| \leq \frac{\|\nabla R(x_n)\|}{v_n} + \left\| \frac{\nabla R(x_n)}{v_n} + \nabla d_y(x_n) \right\| \\ &= \frac{\|\nabla R(x_n)\|}{v_n} + \frac{\|\nabla f_n(x_n)\|}{v_n} \leq \frac{\|\nabla R(x_n)\|}{v_n} + \frac{\varepsilon_n}{v_n} \rightarrow 0. \end{aligned}$$

So, $\nabla d_y(x_n) \rightarrow 0$. With the convexity of d_y on $\mathcal{U}_n = \mathcal{U}(y)$ for n large enough and the boundedness of $(x_n)_{n \in \mathbb{N}}$ we further get

$$d_y(x_n) \leq d_y(x^+) - \langle \nabla d_y(x_n), x^+ - x_n \rangle \leq \|\nabla d_y(x_n)\| \|x_n - x^+\| \rightarrow 0.$$

Since $(x_n)_{n \in \mathbb{N}}$ is bounded, there exists a weakly convergent subsequence $(x_{n_k})_{k \in \mathbb{N}}$ with weak limit $\tilde{x} \in \mathcal{U}(y)$ (see proof of Proposition 2.6). Again we set $(x_{n_k})_{k \in \mathbb{N}} = (x_n)_{n \in \mathbb{N}}$ and we estimate with the convexity of d_y for n large enough

$$d_y(\tilde{x}) \leq d_y(x_n) - \langle \nabla d_y(\tilde{x}), x_n - \tilde{x} \rangle \rightarrow 0.$$

Thus, $d_y(\tilde{x}) = 0$. Since x^+ is the minimizer of (3) we have $R(\tilde{x}) \geq R(x^+)$ and, combined with the uniform convexity of R , we obtain

$$0 \leq \limsup_{n \rightarrow \infty} \mu \|x_n - \tilde{x}\|^2 \leq \limsup_{n \rightarrow \infty} [R(x_n) - R(\tilde{x}) - \langle \nabla R(\tilde{x}), x_n - \tilde{x} \rangle] \leq R(x^+) - R(\tilde{x}) \leq 0.$$

This inclusion simultaneously yields that $(x_n)_{n \in \mathbb{N}}$ converges strongly to $\tilde{x}$ and that $R(\tilde{x}) \leq R(x^+)$, which gives us $\tilde{x} = x^+$ by uniqueness.

We have basically shown that any limit point of $(x_n)_{n \in \mathbb{N}}$ must be x^+ . Hence, the whole sequence $(x_n)_{n \in \mathbb{N}}$ converges to x^+ . $\square$

Remark 2.8. *The convergence in Theorem 2.7 only applies to the sequence $(x_n)_{n \in \mathbb{N}}$ generated by Algorithm 1. Note that the algorithm could terminate prematurely with an iterate x_K such that $d_y(x_K) = 0$ but $x_K \neq x^+$. We could avoid this nuisance by modifying the stopping criterion to*

while $d_y(x_n) > 0$ **or** $\varepsilon_n > 0$ **do**

Since we are primarily interested in the regularization property of Algorithm 1, we refrained from doing so.

Having established the convergence in the case of noise-free data, we proceed by showing convergence for noisy data. That is, we show that the output $x_{N(\delta)}^\delta$ for noisy data y^δ is well-defined and converges to the solution x^+ of (3) for $\delta \rightarrow 0$:

Theorem 2.9 (Convergence under noise). *Let $y \in Y$ be such that (3) has a unique solution $x^+ \in X$ and, for every $\delta > 0$, we are given noisy data $y^\delta \in Y$ with*

$$\|y - y^\delta\| \leq \delta.$$

Let Assumption 2.1 hold for R , d_y , and d_{y^δ} for every $\delta > 0$. Choose $\tau > \eta(y)$ (see (D4)), and let $(\varepsilon_n)_{n \in \mathbb{N}}, (v_n)_{n \in \mathbb{N}} \in (0, \infty)^\mathbb{N}$ satisfy

$$\varepsilon_n \rightarrow 0 \quad \text{and} \quad v_n \rightarrow \infty \quad \text{as} \quad n \rightarrow \infty,$$

as well as $v_{n+1} - v_n \leq V$ for some $V > 0$. We define

$$\varepsilon_n^\delta := \min \{\varepsilon_n, \delta\}, \quad \text{for all } \delta > 0.$$

Let $(\mathcal{U}_n)_{n \in \mathbb{N}}$ and $(\mathcal{U}_n^\delta)_{n \in \mathbb{N}}$ be U -compatible sequences to R , d_y and $(v_n)_{n \in \mathbb{N}}$ and to R , d_{y^δ} and $(v_n)_{n \in \mathbb{N}}$, respectively. Moreover, let $K = K(\delta) \in \mathbb{N}$ from (U3) for $(\mathcal{U}_n^\delta)_{n \in \mathbb{N}}$ be uniformly bounded by some $\bar{K} \in \mathbb{N}$:

$$K(\delta) \leq \bar{K} \quad \text{for } \delta > 0 \text{ sufficiently small,}$$

and assume the compatibility condition

$$\mathcal{U}_n^\delta = \mathcal{U}_n \text{ for } \delta > 0 \text{ sufficiently small.}$$

Choose $x_0 \in D(F)$ such that $d_y(x_0) > 0$.

Then, a call of Algorithm 1 with input $(R, d_{y^\delta}, x_0, \tau, \delta, (\varepsilon_n)_{n \in \mathbb{N}}, (v_n)_{n \in \mathbb{N}}, (\mathcal{U}_n^\delta)_{n \in \mathbb{N}})$ terminates with $x_{N(\delta)}^\delta$ after finitely many steps $N(\delta) \in \mathbb{N}$ for all $\delta > 0$ sufficiently small. Moreover,

$$x_{N(\delta)}^\delta \rightarrow x^+ \quad \text{as } \delta \rightarrow 0.$$

Proof. In the subsequent analysis we denote by $(x_n^\delta)_{n \in \mathbb{N}}$ a sequence generated with Algorithm 1 for the input configuration $(R, d_{y^\delta}, x_0, \tau, \delta, (\varepsilon_n)_{n \in \mathbb{N}}, (v_n)_{n \in \mathbb{N}}, (\mathcal{U}_n^\delta)_{n \in \mathbb{N}})$.

We start with

$$d_{y^\delta}(x^+) = d(y^\delta, x^+) - d(y, x^+) - \partial_y d(y, x^+)[y^\delta - y] + \partial_y d(y, x^+)[y^\delta - y] \leq o(\delta) + \eta(y)\delta,$$

where we used (D4) of Assumption 2.1.

By the choice of τ we thus get $d_{y^\delta}(x^+) < \tau\delta$ for δ small enough. For such δ 's, we assume Algorithm 1 not to terminate: $d_{y^\delta}(x_n^\delta) > \tau\delta$ for all $n \in \mathbb{N}$. Hence, $\|x_n^\delta - x^+\| > 0$.

The compatibility condition yields, for δ sufficiently small,

$$x^+ \in \mathcal{U}(y) \subset \mathcal{U}_n = \mathcal{U}_n^\delta,$$

and we may estimate, relying on the μ_n^δ -strong convexity of $f_n^\delta := R + v_n d_{y^\delta}$ on $\mathcal{U}_n^\delta$, as follows

$$\begin{aligned} \mu_n^\delta \|x_n^\delta - x^+\|^2 &\leq f_n^\delta(x^+) - f_n^\delta(x_n^\delta) - \langle \nabla f_n^\delta(x_n^\delta), x^+ - x_n^\delta \rangle \\ &\leq R(x^+) - R(x_n^\delta) + v_n(d_{y^\delta}(x^+) - d_{y^\delta}(x_n^\delta)) + \|\nabla f_n^\delta(x_n^\delta)\| \|x_n^\delta - x^+\| \\ &\leq \langle \nabla R(x^+), x^+ - x_n^\delta \rangle - \mu_n^\delta \|x_n^\delta - x^+\|^2 + \varepsilon_n \|x_n^\delta - x^+\| \\ &\leq (\|\nabla R(x^+)\| + \varepsilon_n) \|x_n^\delta - x^+\| - \mu_n^\delta \|x_n^\delta - x^+\|^2. \end{aligned}$$

Rearranging the terms, dividing by $2\mu_n^\delta \|x_n^\delta - x^+\|$ and taking the limit with the knowledge

$$\liminf_{n \rightarrow \infty} \mu_n^\delta \geq \mu,$$

for sufficiently small δ yields

$$\limsup_{n \rightarrow \infty} \|x_n^\delta - x^+\| \leq \frac{\|\nabla R(x^+)\|}{2\mu},$$

i.e., $(x_n^\delta)_{n \in \mathbb{N}}$ is bounded. From this boundedness and the convergence $\|\nabla f_n^\delta(x_n^\delta)\| \rightarrow 0$ we conclude, as in the proof of Theorem 2.7, that $\nabla d_{y^\delta}(x_n^\delta) \rightarrow 0$ as $n \rightarrow \infty$. Since, for sufficiently large $n \in \mathbb{N}$ and small $\delta > 0$, the objective d_{y^δ} is convex on $\mathcal{U}(y^\delta) = \mathcal{U}_n^\delta = \mathcal{U}_n = \mathcal{U}(y)$ we obtain

$$d_{y^\delta}(x_n^\delta) \leq d_{y^\delta}(x^+) - \langle \nabla d_{y^\delta}(x_n^\delta), x^+ - x_n^\delta \rangle \rightarrow d_{y^\delta}(x^+) < \tau\delta,$$

contradicting the above assumed non-termination of Algorithm 1. Hence, $d_{y^\delta}(x_n^\delta) \leq \tau\delta$ for n sufficiently large. This implies that $x_{N(\delta)}^\delta$ is well-defined for δ small enough, since the while-loop terminates after finitely many steps, if it actually starts.

To guarantee the latter we prove that $d_{y^\delta}(x_0) > \tau\delta$ for all $\delta > 0$ sufficiently small. Since $d_y(x_0) > 0$ there exist $\gamma, \delta_1 > 0$ such that

$$\gamma + \tau\delta < d_y(x_0) \quad \text{for all } \delta \in [0, \delta_1].$$

Next, with the continuity from (D4) in Assumption 2.1 we find a $\delta_2 > 0$ such that

$$|d_y(x_0) - d_{y^\delta}(x_0)| \leq \gamma \quad \text{for all } \delta \in [0, \delta_2].$$

In total, for $\delta < \min\{\delta_1, \delta_2\}$,

$$d_{y^\delta}(x_0) = d_{y^\delta}(x_0) - d_y(x_0) + d_y(x_0) > -|d_y(x_0) - d_{y^\delta}(x_0)| + \gamma + \tau\delta \geq \tau\delta.$$

Thus, the while-loop starts for δ sufficiently small and terminates with a well-defined $x_{N(\delta)}^\delta \in D(F)$ and $N(\delta) > 0$.

Now to validate the convergence of $x_{N(\delta)}^\delta$ we distinguish two cases:

Case 1: $N(\delta) \rightarrow \infty$ as $\delta \rightarrow 0$. This allows us to choose a function $m: (0, \infty) \rightarrow \mathbb{N}$ with $m(\delta) \rightarrow \infty$ as $\delta \rightarrow 0$ and $m(\delta) < N(\delta)$. By definition of $N(\delta)$ we have $d_{y^\delta}(x_{m(\delta)}^\delta) > \tau\delta$ and additionally, for δ sufficiently small, we can make $m(\delta)$ large enough to ensure $\mu_{m(\delta)}^\delta \geq \mu$ as well as $x^+ \in \mathcal{U}_{m(\delta)}^\delta$. Then,

$$\begin{aligned} \mu \|x_{m(\delta)}^\delta - x^+\|^2 &\leq f_{m(\delta)}^\delta(x^+) - f_{m(\delta)}^\delta(x_{m(\delta)}^\delta) - \langle \nabla f_{m(\delta)}^\delta(x_{m(\delta)}^\delta), x^+ - x_{m(\delta)}^\delta \rangle \\ &\leq R(x^+) - R(x_{m(\delta)}^\delta) + v_{m(\delta)} (d_{y^\delta}(x^+) - d_{y^\delta}(x_{m(\delta)}^\delta)) + \varepsilon_{m(\delta)} \|x_{m(\delta)}^\delta - x^+\| \\ &\leq (\|\nabla R(x^+)\| + \varepsilon_{m(\delta)}) \|x_{m(\delta)}^\delta - x^+\| - \mu \|x_{m(\delta)}^\delta - x^+\|^2 \\ &\quad + v_{m(\delta)} (o(\delta) + \eta(y)\delta - \tau\delta) \\ &\leq (\|\nabla R(x^+)\| + \varepsilon_{m(\delta)}) \|x_{m(\delta)}^\delta - x^+\| - \mu \|x_{m(\delta)}^\delta - x^+\|^2. \end{aligned}$$

This estimate implies as before boundedness of the set $M := \{x_{m(\delta)}^\delta : \delta > 0 \text{ sufficiently small}\}$.

With the same argument as in the beginning of Theorem 2.7 we first get

$$\limsup_{\delta \rightarrow 0} R(x_{m(\delta)}^\delta) \leq R(x^+),$$

then

$$\|\nabla d_{y^\delta}(x_{m(\delta)}^\delta)\| \leq \frac{\|\nabla R(x_{m(\delta)}^\delta)\| + \varepsilon_{m(\delta)}}{v_{m(\delta)}} \rightarrow 0 \quad \text{as } \delta \rightarrow 0,$$

and finally for $\delta \rightarrow 0$:

$$d_{y^\delta}(x_{m(\delta)}^\delta) \leq d_{y^\delta}(x^+) - \langle \nabla d_{y^\delta}(x_{m(\delta)}^\delta), x^+ - x_{m(\delta)}^\delta \rangle \rightarrow 0.$$

The boundedness of M guarantees the existence of a weak accumulation point $\tilde{x} \in \mathcal{U}(y)$ with corresponding sequence $\delta_n \rightarrow 0$. With $x_{m(\delta_n)}^{\delta_n}$, $\tilde{x} \in \mathcal{U}(y^{\delta_n})$ for n large enough we conclude

$$\begin{aligned} (7) \quad d_{y^{\delta_n}}(\tilde{x}) &\leq d_{y^{\delta_n}}(x_{m(\delta_n)}^{\delta_n}) - \langle \nabla d_{y^{\delta_n}}(\tilde{x}), x_{m(\delta_n)}^{\delta_n} - \tilde{x} \rangle \\ &= d_{y^{\delta_n}}(x_{m(\delta_n)}^{\delta_n}) - \langle \nabla d_{y^{\delta_n}}(\tilde{x}) - \nabla d_y(\tilde{x}), x_{m(\delta_n)}^{\delta_n} - \tilde{x} \rangle - \langle \nabla d_y(\tilde{x}), x_{m(\delta_n)}^{\delta_n} - \tilde{x} \rangle. \end{aligned}$$

and, by the continuity due to (D4),

$$\begin{aligned} \langle \nabla d_{y^{\delta_n}}(\tilde{x}) - \nabla d_y(\tilde{x}), x_{m(\delta_n)}^{\delta_n} - \tilde{x} \rangle &= \partial_x d(y^{\delta_n}, \tilde{x})[x_{m(\delta_n)}^{\delta_n} - \tilde{x}] - \partial_x d(y, \tilde{x})[x_{m(\delta_n)}^{\delta_n} - \tilde{x}] \\ &\leq \|\partial_x d(y^{\delta_n}, \tilde{x}) - \partial_x d(y, \tilde{x})\|_{X \rightarrow \mathbb{R}} \|x_{m(\delta_n)}^{\delta_n} - \tilde{x}\| \rightarrow 0. \end{aligned}$$

Taking the limit in (7) we find $d_y(\tilde{x}) = 0$. As in the Theorem 2.7 we also have

$$\begin{aligned} 0 \leq \limsup_{n \rightarrow \infty} \mu \left\| x_{m(\delta_n)}^{\delta_n} - \tilde{x} \right\|^2 &\leq \limsup_{n \rightarrow \infty} \left[R(x_{m(\delta_n)}^{\delta_n}) - R(\tilde{x}) - \langle \nabla R(\tilde{x}), x_{m(\delta_n)}^{\delta_n} - \tilde{x} \rangle \right] \\ &\leq R(x^+) - R(\tilde{x}) \leq 0, \end{aligned}$$

which yields $R(\tilde{x}) \leq R(x^+)$ as well as the strong convergence $x_{m(\delta_n)}^{\delta_n} \rightarrow \tilde{x} = x^+$. This also implies $\hat{x} = x^+$ for any accumulation point $\hat{x}$ of M , since the previous arguments apply to any accumulation point as well. Therefore,

$$x_{m(\delta)}^\delta \rightarrow x^+ \quad \text{as } \delta \rightarrow 0.$$

For the next step we specifically choose $m(\delta) := N(\delta) - 1$ and δ small enough to guarantee $x_{m(\delta)}^\delta, x_{N(\delta)}^\delta \in \mathcal{U}(y^\delta)$. We have

$$\begin{aligned} \mu \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\|^2 &\leq f_{m(\delta)}^\delta(x_{N(\delta)}^\delta) - f_{m(\delta)}^\delta(x_{m(\delta)}^\delta) - \langle \nabla f_{m(\delta)}^\delta(x_{m(\delta)}^\delta), x_{N(\delta)}^\delta - x_{m(\delta)}^\delta \rangle \\ &\leq R(x_{N(\delta)}^\delta) - R(x_{m(\delta)}^\delta) \\ &\quad + v_{m(\delta)} (d_{y^\delta}(x_{N(\delta)}^\delta) - d_{y^\delta}(x_{m(\delta)}^\delta)) + \varepsilon_{m(\delta)} \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\| \end{aligned}$$

as well as

$$\begin{aligned} \mu \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\|^2 &\leq f_{N(\delta)}^\delta(x_{m(\delta)}^\delta) - f_{N(\delta)}^\delta(x_{N(\delta)}^\delta) - \langle \nabla f_{N(\delta)}^\delta(x_{N(\delta)}^\delta), x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \rangle \\ &\leq R(x_{m(\delta)}^\delta) - R(x_{N(\delta)}^\delta) \\ &\quad + v_{N(\delta)} (d_{y^\delta}(x_{m(\delta)}^\delta) - d_{y^\delta}(x_{N(\delta)}^\delta)) + \varepsilon_{N(\delta)} \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\| \end{aligned}$$

Summing up both inequalities and using $v_{n+1} - v_n \leq V$ we obtain

$$\begin{aligned} 2\mu \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\|^2 &\leq (v_{N(\delta)} - v_{m(\delta)}) (d_{y^\delta}(x_{m(\delta)}^\delta) - d_{y^\delta}(x_{N(\delta)}^\delta)) + (\varepsilon_{N(\delta)} + \varepsilon_{m(\delta)}) \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\| \\ &\leq V \langle \nabla d_{y^\delta}(x_{m(\delta)}^\delta), x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \rangle + (\varepsilon_{N(\delta)} + \varepsilon_{m(\delta)}) \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\| \\ &\leq (V \left\| \nabla d_{y^\delta}(x_{m(\delta)}^\delta) \right\| + \varepsilon_{N(\delta)} + \varepsilon_{m(\delta)}) \left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\|. \end{aligned}$$

Dividing by $\left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\|$ and taking the limit yield

$$\left\| x_{m(\delta)}^\delta - x_{N(\delta)}^\delta \right\| \rightarrow 0 \quad \text{as } \delta \rightarrow 0.$$

In total we have shown

$$\left\| x_{N(\delta)}^\delta - x^+ \right\| \leq \left\| x_{N(\delta)}^\delta - x_{m(\delta)}^\delta \right\| + \left\| x_{m(\delta)}^\delta - x^+ \right\| \rightarrow 0 \quad \text{as } \delta \rightarrow 0,$$

which is the claimed regularization property of Algorithm 1.

Case 2: Now we assume $N(\delta) \rightarrow M \in \mathbb{N}$. This is synonymous to $N(\delta) = M$ for $\delta < \bar{\delta}$ for some $\bar{\delta} > 0$, since we are dealing with a sequence of natural numbers. For such a $\delta < \bar{\delta}$ sufficiently small we once more estimate with $x^+ \in \mathcal{U}_M = \mathcal{U}_M^\delta$ for $\delta > 0$ sufficiently small:

$$\begin{aligned} (8) \quad \mu_M \left\| x_M^\delta - x^+ \right\|^2 &\leq R(x^+) - R(x_M^\delta) + v_M (d_{y^\delta}(x^+) - d_{y^\delta}(x_M^\delta)) + \varepsilon_M^\delta \left\| x_M^\delta - x^+ \right\| \\ &\leq (\left\| \nabla R(x^+) \right\| + v_M d_{y^\delta}(x^+) + \varepsilon_M^\delta) \left\| x_M^\delta - x^+ \right\|, \end{aligned}$$

which yields the boundedness of $\{x_M^\delta : \delta > 0\}$. Rearranging the terms in (8), then taking the limit, where we consider the continuity of d in (D4) and the definition of ε_M^δ , yields

$$(9) \quad \limsup_{\delta \rightarrow 0} R(x_M^\delta) \leq \liminf_{\delta \rightarrow 0} [R(x^+) + (v_M d_{y^\delta}(x^+) + \varepsilon_M^\delta) \left\| x_M^\delta - x^+ \right\|] = R(x^+).$$

Furthermore, $d_{y^\delta}(x_M^\delta) \leq \tau\delta \rightarrow 0$. The proof now proceeds by taking again a weak accumulation point $\tilde{x}$ of $\{x_M^\delta : \delta > 0\}$ assuming $x_M^\delta \rightharpoonup \tilde{x}$ as $\delta \rightarrow 0$. We conclude from the boundedness of x_M^δ and (D4) that

$$\begin{aligned} f_M^\delta(\tilde{x}) - f_M^\delta(x_M^\delta) &\leq \langle \nabla f_M^\delta(\tilde{x}), \tilde{x} - x_M^\delta \rangle \\ &= \langle \nabla f_M^\delta(\tilde{x}) - \nabla f_M(\tilde{x}), \tilde{x} - x_M^\delta \rangle + \langle \nabla f_M(\tilde{x}), \tilde{x} - x_M^\delta \rangle \\ &\leq \|\nabla f_M^\delta(\tilde{x}) - \nabla f_M(\tilde{x})\| \|\tilde{x} - x_M^\delta\| + \langle \nabla f_M(\tilde{x}), \tilde{x} - x_M^\delta \rangle \rightarrow 0 \end{aligned}$$

implying

$$\limsup_{\delta \rightarrow 0} f_M^\delta(\tilde{x}) - f_M^\delta(x_M^\delta) \leq 0.$$

Combining this bound with the uniform convexity of f_M^δ , we obtain

$$\begin{aligned} 0 \leq \mu_M \|x_M^\delta - \tilde{x}\|^2 &\leq f_M^\delta(\tilde{x}) - f_M^\delta(x_M^\delta) - \langle \nabla f_M^\delta(x_M^\delta), \tilde{x} - x_M^\delta \rangle \\ &\leq f_M^\delta(\tilde{x}) - f_M^\delta(x_M^\delta) + \varepsilon_M^\delta \|\tilde{x} - x_M^\delta\| \rightarrow 0 \quad \text{as } \delta \rightarrow 0, \end{aligned}$$

which is the strong convergence $x_M^\delta \rightarrow \tilde{x}$. Next we observe

$$d_y(\tilde{x}) = \lim_{\delta \rightarrow 0} d_{y^\delta}(x_M^\delta) \leq \lim_{\delta \rightarrow 0} \tau\delta = 0.$$

In view of (9) and with the continuity of R we get

$$R(\tilde{x}) = \lim_{\delta \rightarrow 0} R(x_M^\delta) \leq R(x^+).$$

Connecting the last two results to the uniqueness of x^+ , gives $\tilde{x} = x^+$ and thus

$$x_{N(\delta)}^\delta = x_M^\delta \rightarrow \tilde{x} = x^+,$$

for every accumulation point $\tilde{x}$. □

We conclude the section with a remark on the assumptions of Theorem 2.9.

Remark 2.10. Assuming the existence of U -compatible subsets $(\mathcal{U}_n^\delta)_{n \in \mathbb{N}}$ for every sufficiently small noise level $\delta > 0$ is not a restriction on the degree of ill-posedness of the problem, as it seems at first glance, but rather a restriction on the structure of the forward operator F . A justifying example would be the least-squares functional $x \mapsto \frac{1}{2} \|Ax - y\|^2$ for any linear operator A , which is globally convex and thus the existence of such subsets is trivial. In Section 3 we will present a general procedure for constructing such subsets and in Appendix A we will provide explicit examples. For more examples of nonlinear problems for which such subsets exist, see [19, Section 5].

Note that the requirement $d_y(x_0) > 0$ can be omitted if we change the while-loop in Algorithm 1 to a repeat-until-loop.

3. NUMERICAL REALIZATION

We now turn our attention to the numerical realization of Algorithm 1. To this end we assume that the forward operator F , the regularization term R , and the distance functional d_y are appropriately discretized. In particular, we consider X and Y to be finite-dimensional Hilbert spaces..

The success of the proposed penalty method is solely determined by the realization of the optimization step

$$\text{Choose } x_n \in \mathcal{U}_n \text{ such that } \|\nabla f_n(x_n)\| \leq \varepsilon_n$$

from Algorithm 1. Here we have to approximate a stationary point of the current penalty objective f_n . The most natural way to compute a stationary point in finite dimensions is to use an iterative optimization method like gradient descent, nonlinear cg, Newton's method, or BFGS. In the subsequent analysis we will mainly focus on Quasi-Newton methods such as BFGS or L-BFGS. Fortunately, there is an abundance of convergence results for these methods in finite-dimensional spaces (see standard literature on optimization methods like [14, 27]). Therefore we will not go into detail on the convergence analysis here. However, we must discuss how to guarantee the assumptions necessary for the convergence of a standard optimization method to a minimizer of the strongly convex functional f_n .

Most of these iterative methods operate with descent directions. A common assumption that ensures convergence to a minimizer of f_n is that the level set of the initial guess $x_n^0 \in X$, defined as

$$\mathcal{L}_n(x_n^0) := \{x \in X : f_n(x) \leq f_n(x_n^0)\},$$

is closed and convex (see [27, Theorem 4.1.9] for BFGS or [14, Satz 12.10] for L-BFGS). In the context of our penalty method, we define $\mathcal{U}_n$ as the smallest closed and convex superset of $\tilde{\mathcal{U}}_n := \mathcal{L}_n(x_n^0) \cup \mathcal{U}(y)$, which is the closure of the convex hull:

$$\mathcal{U}_n := \overline{\text{conv } \tilde{\mathcal{U}}_n} = \overline{\{\lambda x + (1 - \lambda)z \mid x, z \in \tilde{\mathcal{U}}_n, \lambda \in [0, 1]\}}.$$

Now, we can guarantee both convergence for the outer penalty iteration as well as for the inner optimization method, as long as f_n is strongly convex on the whole of $\mathcal{U}_n$.

Translating this observation into the setting of Section 2 means that, for a fixed sequence of penalty parameters $(v_n)_{n \in \mathbb{N}}$, we have to generate a sequence of initial guesses $(x_n^0)_{n \in \mathbb{N}}$, for which the corresponding sequence $(\mathcal{U}_n)_{n \in \mathbb{N}}$ of optimization neighborhoods is U-compatible. The simplest way to construct such a sequence of initial guesses using an optimization algorithm is through the iterative procedure, which we describe in the following.

For the time being we assume that we are at an iteration step $n \in \mathbb{N}$ at which f_n is strongly convex on $\mathcal{U}_n$ with some $x_n^0 \in X$. We denote by $(x_n^k)_{k \in \mathbb{N}}$ the sequence generated by a suitable optimization method, which fulfills

$$x_n^k \rightarrow x_n^*, \quad \text{as } k \rightarrow \infty,$$

with x_n^* being the unique minimizer of f_n over $\mathcal{U}_n$. Since the optimizing sequence $(x_n^k)_{k \in \mathbb{N}}$ only has to be generated until the gradient norm falls below the given tolerance threshold ε_n , we define the output of the inner iteration $x_n^{K_n}$ with the first index K_n for which we have

$$\|\nabla f_n(x_n^{K_n})\| \leq \varepsilon_n.$$

We use this inner output $x_n^{K_n}$ as initial guess for the optimization method applied to the next penalty functional, i.e.,

$$x_{n+1}^0 = x_n^{K_n},$$

and $x_1^0 = x_0$, for some well chosen $x_0 \in X$.

The implicitly generated sequence of convex hulls $\mathcal{U}_n = \overline{\text{conv}(\mathcal{L}_n(x_n^0) \cup \mathcal{U}(y))}$ automatically satisfies assumption (U2). The other two requirements, (U1) and (U3), do not follow immediately and require further analysis.

In order to achieve (U3) we need $\mathcal{U}_n = \mathcal{U}(y)$ for n large enough and thus $\mathcal{L}_n(x_n^0) \subset \mathcal{U}(y)$ for v_n large enough. This non-trivial yet natural property arises from certain additional structural conditions on d_y , combined with a technical estimate on R and $(v_n)_{n \in \mathbb{N}}$.

Lemma 3.1. *Let $d_y^{-1}(0) \neq \emptyset$, Assumption 2.1 hold and x^+ be the unique solution of (3). Further, assume the following properties of the objective functional:*

- d_y is globally weakly convex, that is,

$$d_y(z) \geq d_y(x) + \langle \nabla d_y(x), z - x \rangle - \beta_y \|x - z\|^2, \quad \text{for all } x, z \in X,$$

for some constant $\beta_y > 0$.

- d_y is bounded from below on $X \setminus \mathcal{U}(y)$, i.e.

$$\gamma_y := \inf_{x \in X \setminus \mathcal{U}(y)} d_y(x) > 0.$$

If R and v_n are chosen such that $v_n \beta_y < \mu$ (see (R2) for μ) and

$$(10) \quad \frac{R(x^+)}{v_n} < \gamma_y,$$

then f_n is globally uniformly convex on X . Moreover, for every penalty parameter $v_{n+1} = v_n + V$ with $V > 0$ and initial guess x_n^0 we can find an $\varepsilon_n > 0$ small enough such that:

$$\mathcal{L}_{n+1}(x_{n+1}^0) = \mathcal{L}_{n+1}(x_n^{K_n}) \subset \mathcal{U}(y).$$

Proof. By the assumptions on d_y and μ the penalized objective f_n is globally μ_n -strongly convex with $\mu_n := (\mu - v_n \beta_y)$. We define x_n^* to be the global minimizer of f_n and with $\rho_n^* := \|x_n^{K_n} - x_n^*\|$ we deduce

$$\begin{aligned} d_y(x_n^{K_n}) &= v_n^{-1} (f_n(x_n^{K_n}) - f_n(x^+) + R(x^+) - R(x_n^{K_n})) \\ &\leq v_n^{-1} (f_n(x_n^{K_n}) - f_n(x_n^*) + R(x^+) - R(x_n^{K_n})) \\ &\leq v_n^{-1} \left(\langle \nabla f_n(x_n^{K_n}), x_n^{K_n} - x_n^* \rangle - \mu_n \|x_n^{K_n} - x_n^*\|^2 + R(x^+) \right) \\ &\leq \frac{R(x^+) + \varepsilon_n \rho_n^* - \mu_n (\rho_n^*)^2}{v_n}. \end{aligned}$$

Next, we find, for any $x \in \mathcal{L}_{n+1}(x_n^{K_n})$,

$$\begin{aligned} d_y(x) &= v_{n+1}^{-1} (f_{n+1}(x) - f_{n+1}(x_n^{K_n}) + f_{n+1}(x_n^{K_n}) - R(x)) \\ &\leq v_{n+1}^{-1} (f_{n+1}(x_n^{K_n}) - R(x)) \\ &= v_{n+1}^{-1} (f_n(x_n^{K_n}) + V d_y(x_n^{K_n}) - f_n(x) + v_n d_y(x)) \\ &\leq v_{n+1}^{-1} (f_n(x_n^{K_n}) + V d_y(x_n^{K_n}) - f_n(x_n^*) + v_n d_y(x)). \end{aligned}$$

This inequality regroups to

$$\begin{aligned} \left(1 - \frac{v_n}{v_{n+1}}\right) d_y(x) &\leq v_{n+1}^{-1} (f_n(x_n^{K_n}) + V d_y(x_n^{K_n}) - f_n(x_n^*)) \\ &\leq \frac{V}{v_{n+1}} d_y(x_n^{K_n}) + v_{n+1}^{-1} \left(\langle \nabla f_n(x_n^{K_n}), x_n^{K_n} - x_n^* \rangle - \mu_n \|x_n^{K_n} - x_n^*\|^2 \right) \\ &\leq \frac{V}{v_{n+1}} d_y(x_n^{K_n}) + \frac{\varepsilon_n \rho_n^* - \mu_n (\rho_n^*)^2}{v_{n+1}}. \end{aligned}$$

Using the identity $\left(1 - \frac{v_n}{v_{n+1}}\right) = \frac{V}{v_{n+1}}$ we obtain

$$\begin{aligned} d_y(x) &\leq d_y(x_n^{K_n}) + \frac{\varepsilon_n \rho_n^* - \mu_n(\rho_n^*)^2}{V} \\ &\leq \frac{R(x^+) + \varepsilon_n \rho_n^* - \mu_n(\rho_n^*)^2}{v_n} + \frac{\varepsilon_n \rho_n^* - \mu_n(\rho_n^*)^2}{V} \\ &= \frac{R(x^+)}{v_n} + \left(\frac{1}{v_n} + \frac{1}{V}\right) (\varepsilon_n \rho_n^* - \mu_n(\rho_n^*)^2). \end{aligned}$$

Since ε_n can be chosen arbitrarily small and $\rho_n^* \rightarrow 0$ for $\varepsilon_n \rightarrow 0$, the second term can be made small enough to ensure with (10) $d_y(x) < \gamma_y$ and thus $x \in \mathcal{U}(y)$. $\square$

In the situation of Lemma 3.1, the sequence $(\mathcal{U}_n)_{n \in \mathbb{N}}$ defined by

$$\mathcal{U}_1 = X, \quad \mathcal{U}_n = \mathcal{U}(y), \quad \text{for all } n \geq 2,$$

is U-compatible to R , d_y and any sequence $(v_n)_{n \in \mathbb{N}}$ with $v_1 < \mu/\beta_y$. Furthermore, it can be generated with any standard optimization scheme as inner iteration for an arbitrary initial guess $x_0 \in X$ provided $\varepsilon_1 > 0$ is small enough. In this context, Algorithm 1 is even globally convergent.

Remark 3.2. Lemma 3.1 is of limited practical use as condition (10) is hard to verify in a concrete setting. Rather, it demonstrates that R and d_y can, in principle, satisfy a compatibility condition, enabling global convergence: If we choose $v_n = \frac{\mu}{C\beta_y}$ for some $C > 1$, then we can rewrite the inequality (10) to

$$\frac{C\beta_y R(x^+)}{\mu} < \gamma_y,$$

which we can interpret as follows. If

- $R(x^+)$ is small enough, i.e., the global optimizer of R and x^+ are close enough,
- μ is large enough, i.e., R is 'uniformly convex enough',
- β_y is small enough, i.e., d_y is 'convex enough',
- γ_y is large enough, i.e., d_y is 'coercive enough',

then we have global convergence for the penalty method, given a well chosen tolerance sequence $(\varepsilon_n)_{n \in \mathbb{N}}$. For an example of an inverse problem that makes estimate (10) realizable, we refer to Appendix A.

Now for our implementation we chose the L-BFGS method as our optimizer to generate the inner iteration and as described above we start the n -th call of this method with the last penalty iterate x_{n-1} as initial guess.

Further to realize the limit behavior $\varepsilon_n \rightarrow 0$ and $v_n \rightarrow \infty$ of the parameter sequences, we distinguish two cases: In the noise-free case $\delta = 0$, we want the convergence to be as fast as possible, i.e., exponential. Therefore we choose $\varepsilon_0, v_0 > 0$ and $\alpha \in (0, 1), \beta \in (1, \infty)$ to define

$$\varepsilon_n := \alpha^n \varepsilon_0, \quad v_n := \beta^n v_0.$$

In the case of noisy data with $\delta > 0$ we are obliged to the requirements of Theorem 2.9. Therefore we choose linear convergence for v_n^δ in n as well as for ε_n^δ in δ :

$$\varepsilon_n^\delta := \min\{\varepsilon_n, \delta\}, \quad v_n^\delta := nv_0.$$

This guarantees $v_{n+1} - v_n = v_0 =: V$.

Algorithm 2 L-BFGS-Penalty method

Input: $R, d_y: X \rightarrow [0, \infty)$, $x_0 \in X$, N_{Penalty} , $N_{\text{L-BFGS}}$, $\varepsilon_0, v_0, \alpha, \beta, \tau, \delta \geq 0$.
 $n := 0$ **while** $d_y(x_n) > \tau\delta$ **and** $n < N_{\text{Penalty}}$ **do** $\varepsilon_{n+1} := \alpha\varepsilon_n$ **if** $\delta = 0$ **then** $v_{n+1} := \beta v_n$ **else** $v_{n+1} := v_n + v_0$ $\varepsilon_{n+1} := \min\{\varepsilon_{n+1}, \delta\}$ **end if** $n++$ $f_n(x) := R(x) + v_n d_y(x)$ $x_n := \text{L-BFGS}(f_n, x_{n-1}, \varepsilon_n, N_{\text{L-BFGS}})$ **end while** $N(\delta) := n$ **Output:** $x_{N(\delta)}$

For practical reasons we limit the maximum numbers of iterations by N_{Penalty} and $N_{\text{L-BFGS}}$ for the penalty method and for each call of the L-BFGS method, respectively. The resulting numerical implementation is summarized in Algorithm 2.

4. FULL WAVEFORM INVERSION

We apply our penalty method to full waveform inversion (FWI) in the acoustic regime. FWI entails the reconstruction of the pressure wave speed in the earth's underground from reflected wave fields. The operator involved in this nonlinear inverse problem is

$$\tilde{F}: \mathcal{X} \rightarrow Y,$$

defined as the concatenation $\tilde{F} = M\mathcal{F}$ of the following two components:

- The state-to-solution map

$$\mathcal{F}: D(\mathcal{F}) \subset \mathcal{X} \rightarrow \mathcal{Y}, \quad \nu \mapsto u,$$

defined between the spaces $\mathcal{X} = L^\infty(\Omega, \mathbb{R})$ and $\mathcal{Y} = L^2([0, T], L^2(\Omega))$, which maps a pressure wave velocity

$$\nu \in D(\mathcal{F}) := \{w \in L^\infty(\Omega, \mathbb{R}) : \nu_{\min} \leq w \leq \nu_{\max} \text{ a.e.}\}$$

to the weak solution $u: [0, T] \rightarrow L^2(\Omega)$ of the acoustic wave equation,

$$(11) \quad \frac{1}{\nu^2} \partial_t^2 u - \Delta u = f, \quad u(0) = 0, \quad \partial_t u(0) = 0.$$

Here, $0 < \nu_{\min} < \nu_{\max}$ are physically meaningful constants and $f: [0, T] \rightarrow L^2(\Omega)$ is the source term. Under sufficient regularity assumptions on f and homogeneous Dirichlet boundary conditions the operator $\mathcal{F}$ is well-defined and Fréchet-differentiable [28].

- The measurement operator

$$M: \mathcal{Y} \rightarrow Y, \quad u \mapsto s,$$

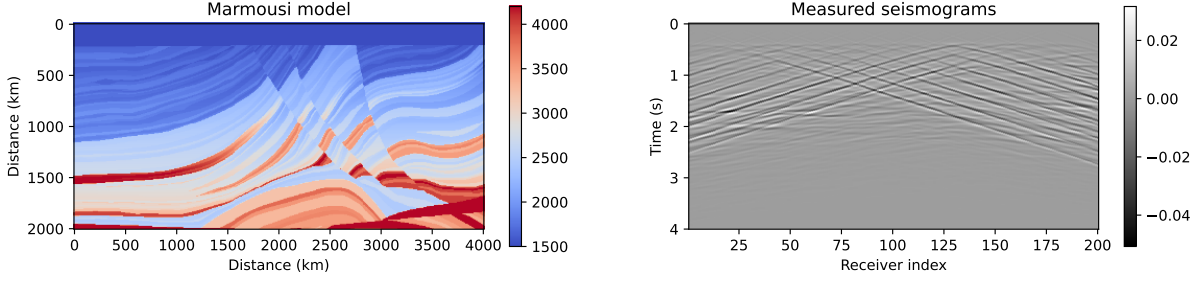


FIGURE 1. Test model (left) with generated reflection seismograms (right).

maps a wave field $u \in \mathcal{Y}$ to the observed collection of seismograms $s \in Y = \mathbb{R}^{N_T \times N_S}$ which is u sampled at N_S receiver locations and N_T points in time. In this finite-dimensional measurement setting we define the norm on Y as the Frobenius-norm for matrices.

In our example we choose the spatial domain as the rectangle $\Omega = [0, 4000] \times [0, 2000]$ and the terminal time is $T = 4.0$.

For our discrete parameter space X we use piecewise constant functions in a certain region of interest Ω_{ROI} located inside of the full domain:

$$\Omega_{\text{ROI}} := [0, 4000] \times [200, 2000] \subset \Omega.$$

The piecewise constant discretization is taken with respect to a uniform grid defined by the spatial discretization levels $N_1, N_2 \in \mathbb{N}$ and thus $X = \mathbb{R}^{N_1 \times N_2}$ and $D(F) = D(\mathcal{F}) \cap X$. In the sequel we identify a piecewise constant velocity $\nu: \Omega_{\text{ROI}} \rightarrow [\nu_{\min}, \nu_{\max}]$ with its piecewise constant values $x \in X$ and thus interpret it as a pixel image. To turn X into a Hilbert space, we equip it with the Frobenius-norm and its corresponding inner product. In the following, $\|\cdot\|$ always refers to the Frobenius-norm for matrices or the Euclidean norm for column vectors on the respective finite-dimensional spaces.

This specific choice of Ω_{ROI} is motivated as follows: We assume that the excited wave signal travels through a known homogeneous medium at first (e.g. water) in the region $\Omega \setminus \Omega_{\text{ROI}}$ and then hits a heterogeneous medium located inside Ω_{ROI} which is represented by the wave speed $\nu|_{\Omega_{\text{ROI}}}$ that we have to reconstruct.

Since this modeling means that all of the information about the unknown medium is carried by the reflections of the emitted wave, we cut off the initial wave traveling through the homogeneous medium $\bar{x} \in X$, which is the constant velocity $\bar{x} \equiv 1500$, and thus define our forward operator $F: X \rightarrow Y$ by

$$F(x) := \tilde{F}(x) - \tilde{F}(\bar{x}), \quad \text{for all } x \in X.$$

The chosen example $x^+ \in X$ for our numerical experiments is a cut off and rescaled version of the Marmousi model [31], which is a widely used benchmark in geophysics. It is shown in Figure 1 together with its corresponding reflection seismograms $y = F(x^+)$.

The displayed seismograms as well as all other examples were calculated with the utilities provided by the software package Deepwave [39]. For the source term f we used 10 identical Ricker wavelets with a central frequency of 10 Hz, as implemented in [39], that are excited at 10 equidistant locations at the top of the spatial domain Ω . The reflected signal is measured at $N_S = 200$ receiver locations also on the top of the domain at a total of $N_T = 800$ temporal sampling points. For the order of the spatial finite

difference method (the used wave solver in [39]) we chose 8 and for the discretization levels $N_1 = 401$ and $N_2 = 181$.

For further implementation details we refer to our GIT repository¹. The code to produce the following examples heavily relies on utilities provided by the PyTorch library [37]. Furthermore we used the L-BFGS method provided by the software package [13]. All of the following experiments were conducted on an NVIDIA RTX A4000.

4.1. Objective functional and regularization term. In our following tests we will compare two choices for the objective functional. The first one is the standard L^2 -objective

$$J_y(x) := \frac{1}{2} \|F(x) - y\|^2,$$

which is known for its notoriously poor convexity properties and an abundance of local minima.

For our second objective we will choose one that reduces the amount of local minima and enlarges the locally convex neighborhood $\mathcal{U}(y)$ of the solution, see Assumption 2.1. We favor a learned distance functional as proposed in [20], where every component of F is concatenated with a neural network $\Phi: \mathbb{R}^{N_T} \rightarrow \mathbb{R}^{N_T}$. This network simplifies the nonlinearity and non-convexity caused by the oscillating nature of waves such that the resulting least-squares functional

$$d_y(x) := \frac{1}{2} \sum_{i=1}^{N_S} \|\Phi(F_i(x)) - \Phi(y_i)\|^2$$

becomes convex. The success of this approach is solely determined by the training of the network Φ , which has been conducted in a supervised manner in [20]. The intended goal is to achieve

$$\|\Phi(y_i(\cdot - t)) - \Phi(y_i)\|^2 \approx t^2$$

for a given time-shifted version $y_i(\cdot - t)$ of a measured seismogram y_i . This approach arguably worked well in the original work for the simple inclusion model with transmission data, but it fails for the subsequent experiments without further adjustments. Since our data stem from multiple scattered reflections in a highly heterogeneous medium, we train the network to fulfill

$$\|\Phi(e^{-t} y_i(\cdot - t)) - \Phi(y_i)\|^2 \approx t^2.$$

The rationale behind introducing the scaling parameter e^{-t} is to dampen reflections that occur later in time, since these are generally smaller in magnitude, see Figure 1. This is an appropriate extension of the method from [20] to reflection data.

We train the network as in [20] with the use of synthetically generated training triplets

$$(y_i, e^{-t_k} y_i(\cdot - t_k), t_k^2)_{i,k}$$

for a given set of time shifts $\{t_k: k = 1, \dots, K\}$ by minimizing the L^1 -loss

$$l(\Phi) = \frac{1}{KN_S} \sum_{i=1}^{N_S} \sum_{k=1}^K \left| \|\Phi(e^{-t_k} y_i(\cdot - t_k)) - \Phi(y_i)\|^2 - t_k^2 \right|.$$

¹<https://gitlab.kit.edu/david.haemmerling/inexact-penalty-method>

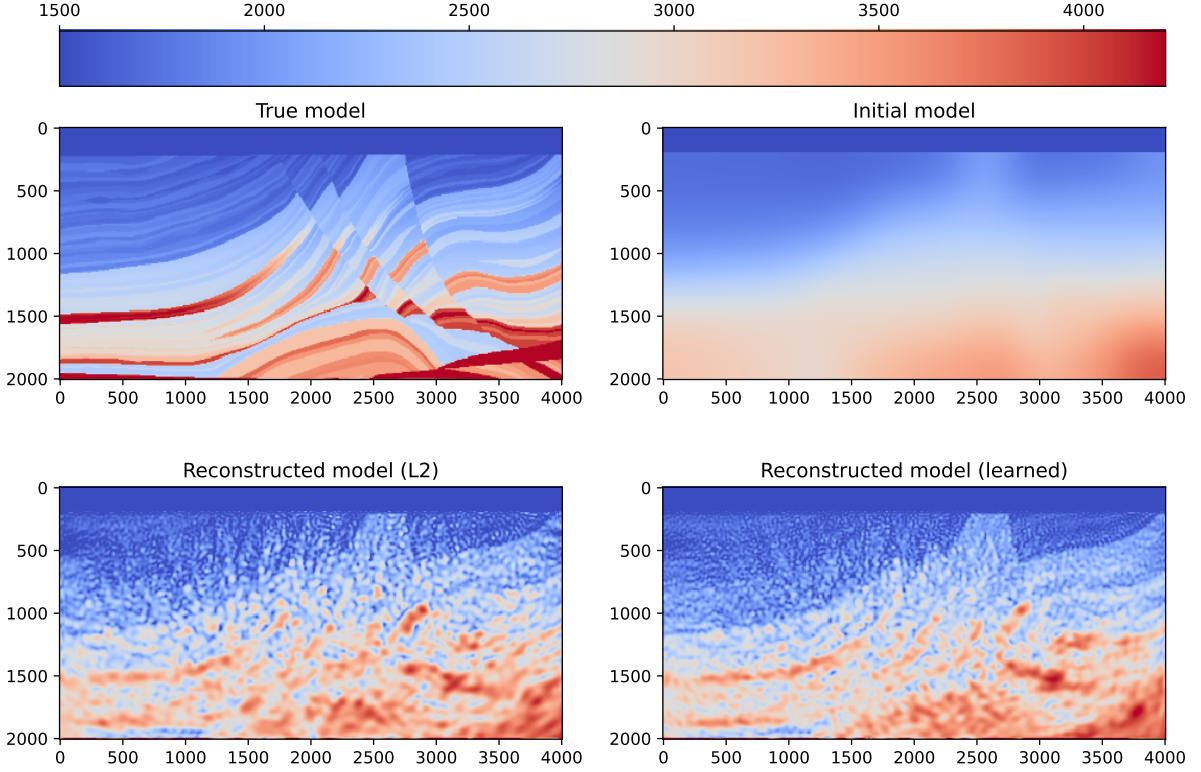


FIGURE 2. Results for the standard L-BFGS method applied to the L^2 - and learned L^2 -misfit with respect to a shared colorbar on top.

For further details on the network architecture, its theoretical properties (injectivity and Lipschitz continuity) as well as the training process we refer to [20, Section 3.1.1].

Before we introduce a useful regularization term, we must clarify the following: Regardless of the chosen objective, this example of an inverse problem is underdetermined². We experimentally justify this claim by optimizing both the L^2 -objective J_y and the learned objective d_y for the exact data from Figure 1 with the L-BFGS method. We denote the initial guess by x_0 which is a blurred version of true model x^+ using a Gaussian filter. Moreover, we call the output of the L-BFGS method $x_{L^2}^{\text{L-BFGS}}$ for J_y and $x_{\Phi}^{\text{L-BFGS}}$ for d_y . The initial guess as well as the reconstructions are displayed³ in Figure 2.

For quantitative comparisons of the reconstructions obtained in our experiments, we compute the relative error with respect to the initial guess as our quality metric, which

²In [10, Section 4] it was shown that the discrete forward operator $\tilde{F}$ is locally injective, given a feasible spatial discretization and an appropriate source term f . However, it is unclear whether the same result holds for the given finite difference discretization or source term. We also do not know if our initial guess is actually in the local injectivity neighborhood. Therefore, we cannot say whether the observed “underdetermination” is due to the theoretical properties of $\tilde{F}$ or to numerical aspects.

³Note that for all plots in this section we clipped the values of the reconstructed models to the range of values of the true model to ensure better visibility. For more details and unclipped plots we refer to our GIT repository.

is

$$\text{err}(x) := \frac{\|x - x^+\|}{\|x_0 - x^+\|}.$$

The reconstructions in Figure 2 have the relatively large errors

$$\text{err}(x_{L^2}^{\text{L-BFGS}}) \approx 1.10 \quad \text{and} \quad \text{err}(x_{\Phi}^{\text{L-BFGS}}) \approx 0.95.$$

Here is an explanation: The L^2 -reconstruction is one of the many local minima of J_y , at which L-BFGS got stuck due to the non-convexity of J_y . The learned reconstruction fulfills $d_y(x_{\Phi}^{\text{L-BFGS}}) \approx 0$ but is still far from x^+ indicating that this inverse problem is underdetermined. In fact, $F(x_{\Phi}^{\text{L-BFGS}})$ matches the seismograms y well with respect to d_y but is not the intended true solution.

Therefore, a decent reconstruction requires a regularization term, that favors desired physical properties of the ground truth. We build a regularization term based on a smooth approximation of the total variation semi-norm

$$(12) \quad \text{TV}_{\theta}(x) = \frac{\sum_{i=1}^{N_1-1} \sum_{j=1}^{N_2} \sqrt{(x_{i+1,j} - x_{i,j})^2 + \theta}}{(N_1 - 1)N_2} + \frac{\sum_{i=1}^{N_1} \sum_{j=1}^{N_2-1} \sqrt{(x_{i,j+1} - x_{i,j})^2 + \theta}}{N_1(N_2 - 1)},$$

with $\theta = 10^{-8}$, which is a convex functional⁴. The uniformly convex regularization term R_c^p is now defined by

$$(13) \quad R_c^p(x) := \text{TV}_{\theta}(x) + c \|x - x_0\|_{L^p}^p,$$

where x_0 is the initial guess from above and

$$\|\xi\|_{L^p}^p := \frac{1}{N_1 N_2} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} |\xi_{i,j}|^p \quad \text{for all } \xi \in \mathbb{R}^{N_1 \times N_2}.$$

The latter norm is strongly convex for $p > 1$ on $D(F)$ as $D(F)$ is non-empty closed, convex, bounded and finite-dimensional [5, Corollary 10.18]. In the following examples we work below with $R = R_{0.01}^{1.1}$, that is, with $p = 1.1$ and $c = 0.01$. This regularization term promotes reconstructions being sparse with jump discontinuities along curves. Both properties are shared by the Marmousi model.

4.2. Exact data. First, we test Algorithm 2 with the introduced objective functionals and the regularization for exact data, that is, $\delta = 0$. The reconstructions $x_{\Phi}^{\text{Penalty}}$ and $x_{L^2}^{\text{Penalty}}$ for d_y and J_y , respectively, can be inspected in Figure 3. The parameters used are listed in Table 1.

It is visually apparent that the reconstruction for the learned distance is superior to that for the standard distance. This observation is confirmed by the relative errors

$$\text{err}(x_{L^2}^{\text{Penalty}}) \approx 1.07 \quad \text{vs.} \quad \text{err}(x_{\Phi}^{\text{Penalty}}) \approx 0.57.$$

The penalty iteration with respect to the learned functional d_y terminated because the maximal number of 20 outer iterations has been reached. Increasing this number does not reduce the error value much. In fact, the minimal value of 0.5699 is reached after 28 iterations, see the plot of the error history of the first 50 iterations at the above mentioned GIT repository.

⁴This can be shown by proving that the Hessian of the two dimensional functional $f_{\theta}: \mathbb{R}^2 \rightarrow \mathbb{R}, (x, y)^{\top} \mapsto \sqrt{(x - y)^2 + \theta}$ is positive semidefinite at any $(x, y)^{\top} \in \mathbb{R}^2$.

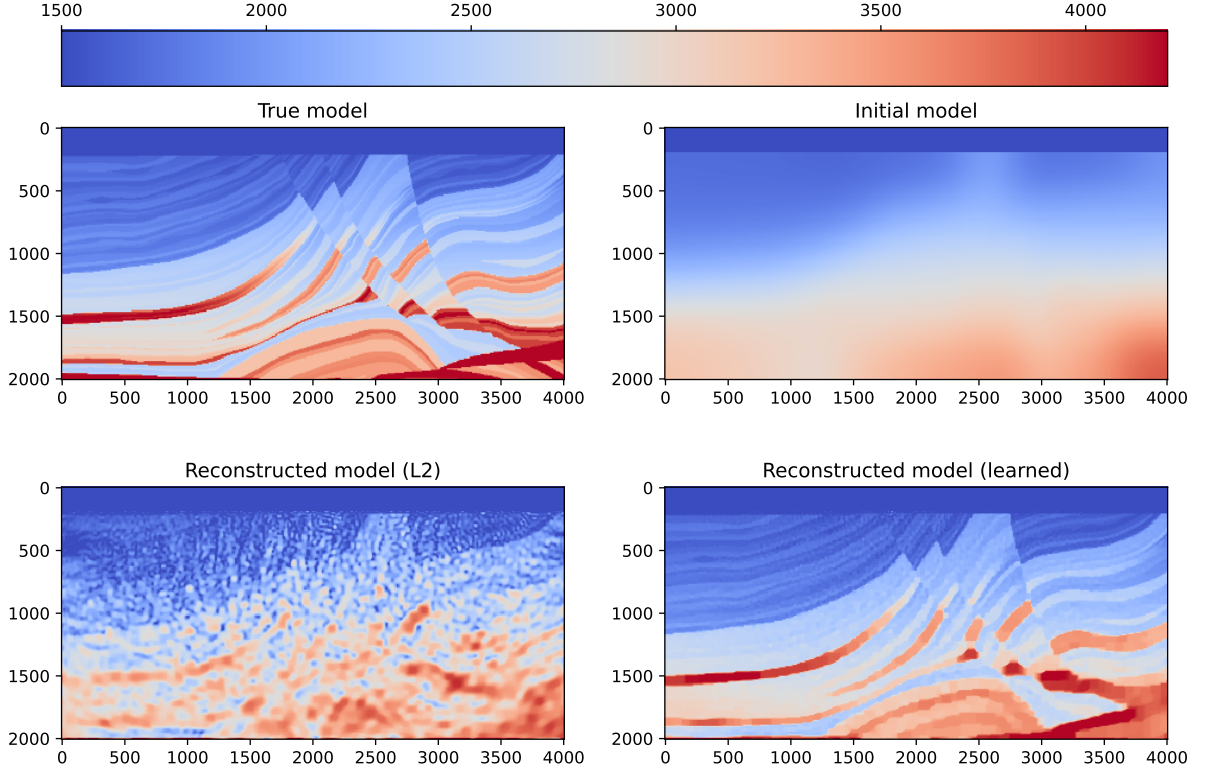


FIGURE 3. Reconstructions obtained with Algorithm 2 for exact data.

Description	Symbol	Value
Max. number of outer iterations	N_{Penalty}	20
Max. number of inner iterations	$N_{\text{L-BFGS}}$	1000
Initial tolerance	ε_0	10^{-4}
Initial penalty parameter	v_0	10^5
Tolerance decay rate	α	0.95
Penalty growth rate	β	1.2
Proportionality constant	τ	None
Noise level	δ	0

TABLE 1. Input configuration for Algorithm 2 with exact data.

The penalty method with the L^2 -objective stagnates after 2 outer iterations, which can be explained by it getting stuck in a local minimum of the now non-convex objective functional $f_n = R + v_n J_y$.

4.3. Noisy data. To numerically justify the applicability of Algorithm 2 to ill-posed problems, we test it for perturbed data $y^\delta \in Y$. This perturbed data vector was again generated with [39] but in order to mitigate the committed inverse crime, we changed the spatial and temporal discretizations by reducing the spatial finite difference order

Description	Symbol	Value
Max. number of outer iterations	N_{Penalty}	9
Max. number of inner iterations	$N_{\text{L-BFGS}}$	5000
Initial tolerance	ε_0	10^{-5}
Initial penalty parameter	v_0	10^4
Tolerance decay rate	α	0.95
Penalty growth rate	β	None
Proportionality constant	τ	10^{-6}
Rel. noise level	δ	≈ 0.094

TABLE 2. Input configuration for Algorithm 2 with perturbed data.

to 4 and using 2000 temporal points for the seismograms, which afterwards have been interpolated to $N_T = 800$ values. Further, we added 1% relative noise to the generated seismograms, which resulted in a total relative error of roughly 9.4%, i.e.,

$$\frac{\|y - y^\delta\|}{\|y\|} \approx 0.094.$$

The reconstruction $x_{N(\delta)}^\delta$ obtained for y^δ can be seen in Figure 4 (bottom right) with parameters from Table 2.

We emphasize that, with the parameter configuration from Table 2, the discrepancy principle is never triggered; that is, all iterates satisfy $d_y(x_n) > \tau\delta$. Nevertheless, $N(\delta)$ is well-defined as the stopping index formulated in Algorithm 2. Due to the lack of practical selection rules for the parameter τ , we determined $N(\delta)$ by the maximum number of iterations N_{Penalty} since lowering τ and raising N_{Penalty} are effectively equivalent.

Comparison with standard Tikhonov regularization. One might argue that increasing the penalty parameter iteratively does not add much value to the reconstruction process as one might just optimize the penalized functional with the last penalty parameter $v_{N(\delta)}$ instead. However, solving the optimization task

$$(14) \quad \min_{x \in \mathcal{U}_{N(\delta)}} R(x) + v_{N(\delta)} d_{y^\delta}(x)$$

requires a well chosen initial guess. For instance, the Gaussian blur x_0 is not a sufficiently good initial guess to solve (14) with $v_{N(\delta)} = v_9$. Figure 4 (bottom left) displays the reconstruction $\tilde{x}_{N(\delta)}^\delta$, obtained by minimizing (14) using the L-BFGS scheme. Comparing qualitatively both reconstructions of Figure 4 yields

$$\text{err}(x_{N(\delta)}^\delta) \approx 0.67 \quad \text{and} \quad \text{err}(\tilde{x}_{N(\delta)}^\delta) \approx 0.90.$$

Thus, we firmly summarize the following facts about our proposed penalty method:

- The regularization term increases the likelihood of finding physically meaningful reconstructions (Figures 2 and 3).
- Successively updating the penalty parameters v_n and the initial guesses x_n^0 enlarges the convergence area compared to standalone minimization (14) at the highest penalty level $v_{N(\delta)}$ (Figure 4).

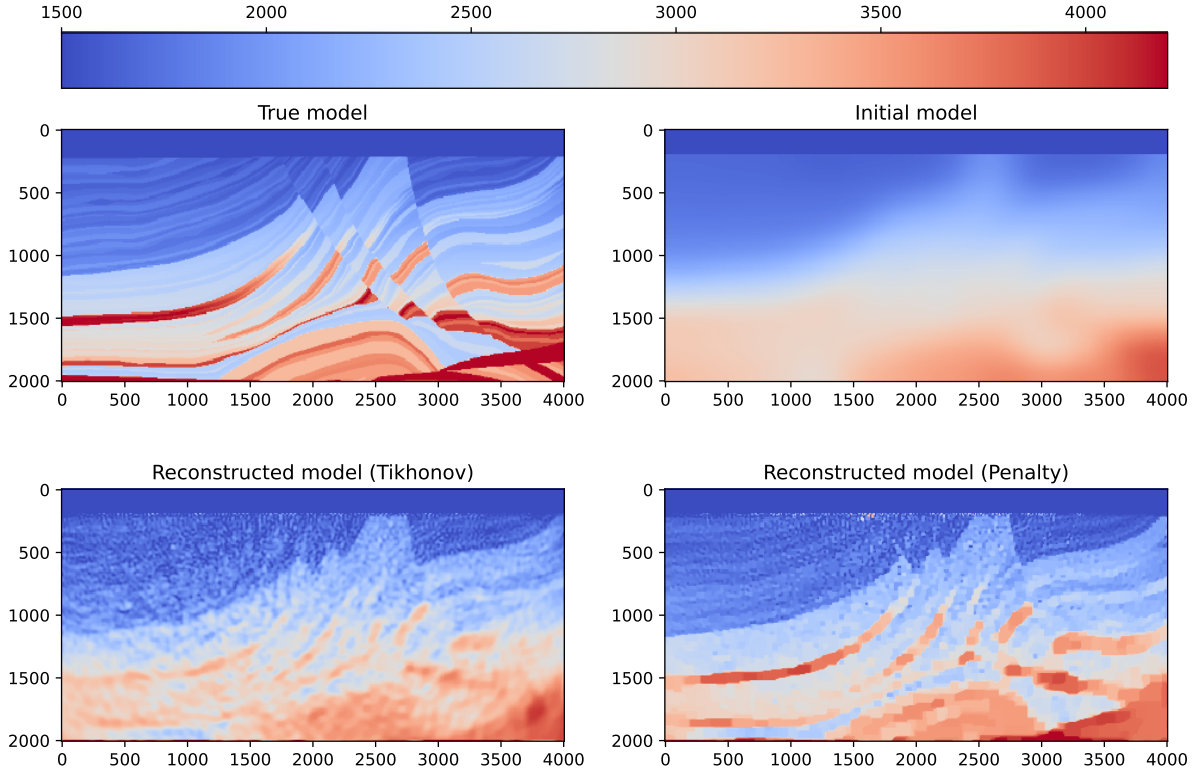


FIGURE 4. Reconstructions obtained for the Tikhonov method (bottom left) and penalty method (bottom right) in the case of noisy data.

- The use of a non-standard objective functional such as machine-learning based ones with improved convexity properties is highly preferable over standard L^2 -objectives (Figure 3).

5. CONCLUSION AND OUTLOOK

Under reasonably well-founded assumptions we established the inexact penalty method as an efficient regularization scheme for highly underdetermined ill-posed problems. The key was the successive, adequate minimization of a weighted sum of locally convex distance functions and well-chosen regularizing terms. Furthermore, we discussed its numerical realizability and even proved global convergence under achievable conditions on the distance functional (Lemma 3.1). Finally, we validated the method with a learned distance functional from [20] on a variation of the Marmousi benchmark model from seismic imaging. We observed significant improvements in the quality of the reconstructions compared to standard regularization schemes.

Potential next research topics include:

- Extending the convergence analysis of Section 2 to a Banach space setting following ideas from [23] for the nonstationary iterated Tikhonov method.
- Generalizing aspects of the numerical realizability from Section 3 to different methods for the inner optimization such as FISTA, for which convergence in general Hilbert spaces has been proven [8].

- Using different distance functionals in the context of FWI or combining learned functionals with knowledge-based functionals to accelerate the convergence speed or improve the reconstruction quality. Also employing retraining strategies during the reconstruction process as in [41, 42] could be beneficial and requires experimental investigation.
- Applying the method to other (possibly underdetermined) inverse problems. One feasible example would be electrical impedance tomography, for which convexity has recently been observed for the standard least-squares distance in special geometries [3].

APPENDIX A. AN ACADEMIC EXAMPLE

To justify Assumption 2.1 as well as the assumptions from Lemma 3.1, we explicitly give an example of an objective functional d_y and a regularization term R that satisfy these assumptions for an inverse problem described by a non-injective operator F . This example is similar to Example 5.1 in [19] and the following results are inspired by this reference but adapted to the context of underdetermined problems.

We consider a nonlinear diagonal operator $F: \ell^2 \rightarrow \ell^2$ which is defined component-wise by

$$F(x)_n = \frac{1}{n} \cdot \begin{cases} \arctan(x_n), & n \leq M, \\ 0, & n > M \text{ and } n \text{ even}, \\ x_n, & n > M \text{ and } n \text{ odd}, \end{cases} \quad \text{for } x \in \ell^2,$$

for some fixed $M \in \mathbb{N}$. This operator not only makes the associated inverse problem ill-posed due to its underdetermined nature, but it also makes the problem ill-posed in the classical sense of local ill-posedness [18]: For any $\rho > 0$ and $x \in \ell^2$ the sequence $(x^n)_{n \in \mathbb{N}}$ in ℓ^2 defined by

$$x_k^n = x_k + \frac{\rho}{2} \delta_{2n+1,k}, \quad \text{for all } n, k \in \mathbb{N},$$

fulfills $x^n \in B_\rho(x) \subset \ell^2$ for all $n \in \mathbb{N}$ and we have

$$F(x) \neq F(x^n) \rightarrow F(x), \quad \text{but } x^n \not\rightarrow x.$$

This makes $F(x) = y$ for $y \in \ell^2$ a fitting example of an inherently ill-posed problem with a severely non-injective forward operator.

We will need first and second order Fréchet-derivatives of F :

$$F'(x)[h]_n = \frac{h_n}{n} \cdot \begin{cases} \frac{1}{x_n^2+1}, & n \leq M, \\ 0, & n > M \text{ and } n \text{ even}, \\ 1, & n > M \text{ and } n \text{ odd}, \end{cases} \quad \text{for } x, h \in \ell^2,$$

$$F''(x)[h, \tilde{h}]_n = \frac{h_n \tilde{h}_n}{n} \cdot \begin{cases} \frac{-2x_n}{(x_n^2+1)^2}, & n \leq M, \\ 0, & n > M, \end{cases} \quad \text{for } x, h, \tilde{h} \in \ell^2.$$

With these derivatives we derive local convexity result for the standard least-squares misfit functional

$$J_y(x) := \frac{1}{2} \|F(x) - y\|^2$$

on the infinite dimensional cylinder

$$\mathcal{U} := \left\{ x \in \ell^2 : |x_n| \leq \frac{\pi}{8}, \text{ for } n \leq M \right\}.$$

The following proposition is similar to Proposition 5.1 in [19].

Proposition A.1. *Let $x^+ \in \mathcal{U}$ with $y := F(x^+)$. Then J_{y^δ} is convex on $\mathcal{U}$ for every $y^\delta \in \ell^2$ with*

$$\|y - y^\delta\| \leq \frac{3}{8} =: \bar{\delta}.$$

Proof. Since J_{y^δ} is twice continuously differentiable, it is sufficient to show that the Hessian operator is positive semidefinite for any $x \in \mathcal{U}$, i.e.,

$$\|F'(x)[h]\|^2 + \langle F(x) - y^\delta, F''(x)[h, h] \rangle \geq 0, \quad \text{for all } x \in \mathcal{U}, h \in \ell^2.$$

To show this, we split the left hand side of the inequality into two terms:

$$\begin{aligned} \|F'(x)[h]\|^2 + \langle F(x) - y^\delta, F''(x)[h, h] \rangle &= \left(\|F'(x)[h]\|^2 + \langle F(x) - y, F''(x)[h, h] \rangle \right) \\ &\quad + \langle y - y^\delta, F''(x)[h, h] \rangle. \end{aligned}$$

For the first term we estimate

$$\begin{aligned} &\|F'(x)[h]\|^2 + \langle F(x) - y, F''(x)[h, h] \rangle \\ &\geq \sum_{n=1}^M \frac{h_n^2}{n^2} \left[\frac{1}{(x_n^2 + 1)^2} + (\arctan(x_n) - \arctan(x_n^+)) \left(\frac{-2x_n}{(x_n^2 + 1)^2} \right) \right] \\ &= \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} [1 - 2x_n \arctan(x_n) - 2x_n \arctan(x_n^+)] \\ &\geq \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} \left[1 - 0.3 - \frac{2\pi}{8} \cdot \frac{1}{2} \right] \\ &\geq \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} [0.3], \end{aligned}$$

where we used the fact that $2t \arctan(t) \leq 0.3$ and $\arctan(t) \leq 0.5$ for $|t| \leq \frac{\pi}{8}$. For the second term we find

$$\begin{aligned} \langle y - y^\delta, F''(x)[h, h] \rangle &= \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} [-2x_n(y_n - y_n^\delta)] \\ &\geq \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} \left[-\frac{\pi}{4} \delta \right] \\ &\geq \sum_{n=1}^M \frac{h_n^2}{n^2(x_n^2 + 1)^2} [-0.8\delta]. \end{aligned}$$

Combining the two estimates yields the claimed convexity since $\delta \leq \frac{3}{8}$. $\square$

From Proposition A.1 we can conclude not only that J_y fulfills Assumption 2.1, but also that we can choose $\mathcal{U}(y) = \mathcal{U}(y^\delta) = \mathcal{U}$ for $x^+ \in \text{int}(\mathcal{U})$ and δ sufficiently small, which was one of the requirements in Theorem 2.9.

Next, we show the weak convexity and boundedness assumed in Lemma 3.1 to yield the practical construction of a U-compatible sequence $(\mathcal{U}_n)_{n \in \mathbb{N}}$ for suitably chosen R and $(v_n)_{n \in \mathbb{N}}$.

Proposition A.2. *Let $x^+ \in \mathcal{U}$ with $|x_n^+| \leq \frac{\pi}{64}$ for $n \leq M$ and $y = F(x^+)$. Then, J_y is weakly convex with $\beta_y \leq \frac{\sqrt{1+\|y\|}}{2}$ and we have*

$$(15) \quad J_y(x) > \frac{1}{20} \sum_{n=1}^M \frac{1}{n^2} \quad \text{for all } x \in \ell^2 \setminus \mathcal{U}.$$

Proof. Since J_y is continuously differentiable with a Lipschitz-continuous gradient, it is also weakly convex and to determine β_y we have to determine the Lipschitz constant of ∇J_y [4, Proposition 2.4]. To this end, let $x, z \in X$. Then,

$$\begin{aligned} \|\nabla J_y(x) - \nabla J_y(z)\| &= \|F'(x)^*[F(x) - y] - F'(z)^*[F(z) - y]\| \\ &\leq \|F'(x)^*F(x) - F'(z)^*F(z)\| + \|(F'(x)^* - F'(z)^*)y\|. \end{aligned}$$

We now estimate both terms separately. Note that $F'(x)$ is self-adjoint for every $x \in \ell^2$ and thus we find for the first term the bound

$$\|F'(x)^*F(x) - F'(z)^*F(z)\|^2 \leq \sum_{n=1}^M \frac{1}{n} \left(\frac{\arctan(x_n)}{x_n^2 + 1} - \frac{\arctan(z_n)}{z_n^2 + 1} \right)^2 + \sum_{n=M+1}^{\infty} \frac{1}{n} (x_n - z_n)^2.$$

Since the function $\mathbb{R} \ni t \mapsto \arctan(t)/(t^2 + 1)$ is Lipschitz-continuous with constant 1, we find

$$\|F'(x)^*F(x) - F'(z)^*F(z)\| \leq \|x - z\|.$$

For the second term we estimate

$$\|(F'(x)^* - F'(z)^*)y\|^2 \leq \sum_{n=1}^M \left(\frac{1}{x_n^2 + 1} - \frac{1}{z_n^2 + 1} \right)^2 y_n^2 + \sum_{n=M+1}^{\infty} \frac{1}{n} (x_n - z_n)^2 y_n^2.$$

As the function $\mathbb{R} \ni t \mapsto 1/(t^2 + 1)$ is Lipschitz continuous with constant $3\sqrt{3}/8$ we conclude

$$\|\nabla J_y(x) - \nabla J_y(z)\| \leq \sqrt{1 + \frac{3\sqrt{3}}{8} \|y\|} \|x - z\|,$$

and, according to [4, Proposition 2.4],

$$\beta_y \leq \frac{\sqrt{1 + \frac{3\sqrt{3}}{8} \|y\|}}{2} \leq \frac{\sqrt{1 + \|y\|}}{2}.$$

To verify (15), let $x \in \ell^2 \setminus \mathcal{U}$: $|x_n| > \frac{\pi}{8}$ for $n \leq M$. Then, by the strict monotonicity of the arctangent,

$$\begin{aligned} J_y(x) &\geq \frac{1}{2} \sum_{n=1}^M \frac{1}{n^2} (\arctan(x_n) - \arctan(x_n^+))^2 \\ &> \sum_{n=1}^M \frac{1}{2n^2} (\arctan(\pi/8) - \arctan(\pi/64))^2 \\ &\geq \sum_{n=1}^M \frac{1}{20n^2}. \end{aligned}$$

□

Fix $M = 100$. Then, from (15),

$$\gamma_y = \sum_{n=1}^M \frac{1}{20n^2} > 0.08.$$

Furthermore, let $x^+ \in \mathcal{U}$ with $\|x^+\| \leq 0.26$ and $|x_n^+| \leq \pi/64$ for $n \leq M$. Choosing $R(x) = \|x\|^2/2$, for which $\mu = 1/2$, we get, with $v \geq \frac{\mu}{2\beta_y} = \frac{1}{2\sqrt{1+\|y\|}}$, that

$$\frac{R(x^+)}{v} \leq \sqrt{1+\|y\|} \|x^+\|^2 \leq \sqrt{1.26} \cdot 0.26^2 < 0.08 < \gamma_y,$$

where we used $\|y\| = \|F(x^+)\| \leq \|x^+\|$. Thus, (10) holds for this specific choice of parameters.

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