# Iterative parameter choice by discrepancy principle 

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This work is concerned with the numerical implementation of the discrepancy principle for nonsmooth Tikhonov regularization for linear inverse problems. First, some theoretical properties of the solutions to the discrepancy equation, i.e., uniqueness and upper bounds, are discussed. Then, the idea of Padé approximation is exploited for designing model functions with model parameters iteratively updated. Two algorithms are proposed for its efficient numerical realization, i.e., a two-parameter algorithm based on model functions and a quasi-Newton method, and their convergence properties are briefly discussed. Numerical results for four nonsmooth models are presented to demonstrate the accuracy of the principle and to illustrate the efficiency and robustness of the proposed algorithms.

Keywords: discrepancy principle; regularization parameter; uniqueness; model function approach; Tikhonov regularization.

## 1. Introduction

This work considers determining regularization parameters in nonsmooth Tikhonov regularization. We will focus on linear inverse problems that can be written

$$
\begin{equation*}
K x=y^{\delta}, \tag{1.1}
\end{equation*}
$$

where $x \in X$ and $y^{\delta} \in Y$ refer to the unknown and the noisy data, respectively. The spaces $X$ and $Y$ are Banach spaces with their respective norms denoted by $\|\cdot\|_{X}$ and $\|\cdot\|_{Y}$, with $X$ being reflexive. The reflexivity of $X$ is not essential. In the case of a Hilbert space, its norm will simply be denoted by $\|\cdot\|$. The operator $K: X \rightarrow Y$ is linear and bounded. The accuracy of the data $y^{\delta}$ relative to the exact data $y^{\dagger}=K x^{\dagger}$ is measured by the noise level $\delta^{2}=\phi\left(x^{\dagger}, y^{\delta}\right)$, where the fidelity $\phi\left(x, y^{\delta}\right)$ : $X \times Y \mapsto\{0\} \cup \mathbb{R}_{+}$measures the proximity of the model output $K x$ to the data $y^{\delta}$. Some widely-used choices include $\frac{1}{2}\left\|K x-y^{\delta}\right\|_{L^{2}}^{2},\left\|K x-y^{\delta}\right\|_{L^{1}}$ and $\int\left(K x-y^{\delta} \log K x\right)+C$, which are statistically suitable for Gaussian, (impulsive) Laplacian and Poissonian noise, respectively.

Inverse problems are numerically challenging due to their inherent ill-posedness in the sense that small perturbations of the data can cause large deviations in the solution. One standard procedure is regularization, which minimizes the Tikhonov functional

$$
\begin{equation*}
J_{\eta}(x)=\phi\left(x, y^{\delta}\right)+\eta \psi(x), \tag{1.2}
\end{equation*}
$$

and takes its minimizer $x_{\eta}$ as an approximation, where $\eta$ is the regularization parameter. The penalty $\psi(x)$ encodes the a priori information, and some common choices include $\frac{1}{v}\|x\|_{L^{v}}^{\nu}, \frac{1}{2}\|x\|_{H^{m}}^{2}$ and $|x|_{T V}$. Nonsmooth models have attracted considerable attention; see Burger \& Osher (2004); Resmerita (2005); Hofmann et al. (2007); Hein \& Hofmann (2009); Hofmann \& Yamamoto (2010), for theoretical studies.

The choice of $\eta$ represents one of the most challenging issues; see Engl et al. (1996); Vogel (2002); Jin \& Zou (2009). The discrepancy principle (Morozov, 1966) is very popular due to its rigorous foundation and a posteriori nature. Theoretically, existence and consistency of the rule were studied in Tikhonov et al. (1998). In Bonesky (2009), convergence rates were derived under appropriate source conditions. The principle determines the parameter $\eta(\delta)$ such that it solves

$$
\begin{equation*}
\phi\left(x_{\eta}, y^{\delta}\right)=\delta^{2} . \tag{1.3}
\end{equation*}
$$

Since $x_{\eta}$ is only implicitly defined via the functional $J_{\eta}$, in practice the principle amounts to solving a highly nonlinear and potentially nonsmooth equation in $\eta$.

The numerical realization of the principle has not received due attention despite its practical significance. This is especially important for nonsmooth models since their efficient minimization can be highly nontrivial and their repeated solutions can be computationally very demanding. Among existing approaches the model function approach (MFA) stands out prominently (Ito \& Kunisch, 1992; Kunisch \& Zou, 1998; Xie \& Zou, 2002). Ito \& Kunisch (1992) proposed a four-parameter model function for nonlinear parameter identification problems. Later, Kunisch \& Zou (1998) derived a two-parameter model function for linear inverse problems, which was further improved in Xie \& Zou (2002). Recently, it has also been applied to other choice rules (Heng et al., 2010). Nonetheless, all these studies focus on the $L^{2}-L^{2}$ model, and a direct extension to nonsmooth models is not viable because these derivations hinge essentially on the inner product structure of Hilbert spaces.

In this paper we provide some light on the aforementioned numerical aspects of the principle. First, we provide some properties (uniqueness and upper bound) of the discrepancy equation, i.e., equation (1.3). Then, we discuss differentiability of the value function and generalize MFA in Kunisch \& Zou (1998) and Xie \& Zou (2002) via Padé approximants, which enables us to develop analogous strategies for general nonsmooth models. These represent our essential contributions. A hybrid algorithm combining the steady global convergence of the MFA and the fast local convergence of a quasi-Newton method is also proposed.

The rest of the paper is structured as follows. Section 2 discusses the discrepancy equation and derives some theoretical results. Section 3 studies the differentiability of the value function and the numerical solution of the discrepancy equation. Section 4 presents some numerical results for four nonsmooth models, i.e., $L^{2}-T V, L^{2}-\ell^{1}, L^{1}-T V$ and elastic net, to demonstrate the accuracy and optimality of the principle and to illustrate the efficiency and robustness of the algorithms.

## 2. Properties of discrepancy equation

This section discusses uniqueness and bounds of solutions to equation (1.3). We shall make the following assumptions: (a) and (b) are standard for the existence of minimizers to $J_{\eta}$, and $\tilde{x}$ in (c) can often be set to $\tilde{x}=0$.

ASSUMPTIONS 2.1 The non-negative functionals $\phi$ and $\psi$ in equation (1.2) satisfy
(a) for any $\eta>0$ the functional $J_{\eta}(x)$ in (1.2) is coercive;
(b) the functionals $\phi(x, y)$ and $\psi(x)$ are weakly lower semicontinuous, i.e., $\phi(x, y) \leqslant \liminf _{n \rightarrow \infty}$ $\phi\left(x_{n}, y\right)$ and $\psi(x) \leqslant \liminf _{n \rightarrow \infty} \psi\left(x_{n}\right)$ for any sequence $\left\{x_{n}\right\} \subset X$ converging weakly to $x$;
(c) there exists an $\tilde{x} \in X$ such that it minimizes $\psi(x)$ over $X$ with $\psi(\tilde{x})=0$.

The minimizers $x_{\eta}$, with the set denoted by $S(\eta)$, of $J_{\eta}$ may be nonunique. Hence, the functions $\eta \mapsto$ $\phi\left(x_{\eta}, y^{\delta}\right)$ and $\eta \mapsto \psi\left(x_{\eta}\right)$ may be set-valued. However, they are monotone (Tikhonov \& Arsenin, 1977; Tikhonov et al., 1998).

Lemma 2.2 The functions $\phi\left(x_{\eta}, y^{\delta}\right)$ and $\psi\left(x_{\eta}\right)$ are monotone in $\eta$ in that for any $x_{\eta_{1}} \in S\left(\eta_{1}\right)$ and any $x_{\eta_{2}} \in S\left(\eta_{2}\right)$ there hold

$$
\left(\eta_{1}-\eta_{2}\right)\left(\psi\left(x_{\eta_{1}}\right)-\psi\left(x_{\eta_{2}}\right)\right) \leqslant 0 \quad \text { and } \quad\left(\eta_{1}-\eta_{2}\right)\left(\phi\left(x_{\eta_{1}}, y^{\delta}\right)-\phi\left(x_{\eta_{2}}, y^{\delta}\right)\right) \geqslant 0
$$

There exists at least a positive solution to equation (1.3) if $\lim _{\eta \rightarrow 0} \phi\left(x_{\eta}, y^{\delta}\right)<\delta^{2}, \lim _{\eta \rightarrow \infty} \phi\left(x_{\eta}, y^{\delta}\right)>$ $\delta^{2}$ and $\phi\left(x_{\eta}, y^{\delta}\right)$ is continuous in $\eta$. The continuity of $\phi\left(x_{\eta}, y^{\delta}\right)$ in $\eta$ is ensured by the uniqueness of the minimizer to $J_{\eta}$, and it holds for strictly convex models, e.g., $L^{2}-L^{p}$ with $1<p \leqslant 2$ and $L^{2}-T V$ and $L^{2}-\ell^{1}$ with injective $K$. Uniqueness is necessary for the continuity of $\phi\left(x_{\eta}, y^{\delta}\right)$; see Chan \& Esedoglu (2005) for $L^{1}-T V$.

The solution to equation (1.3) may be nonunique, even if it does exist. Under the continuity condition, the set of solutions can form a closed interval. We shall examine the uniqueness issue, which has rarely been discussed. The next result reveals one simple uniqueness condition.
Lemma 2.3 Let the functional $J_{\eta}$ satisfy $S\left(\eta_{1}\right) \cap S\left(\eta_{2}\right)=\emptyset$ for distinct $\eta_{1}, \eta_{2}>0$. Then, equation (1.3) has a unique solution $\eta(\delta)>0$.

Proof. We proceed by means of contradiction. Assume that there exist two distinct solutions $\eta_{1}$ and $\eta_{2}$ to equation (1.3), i.e., $\phi\left(x_{\eta_{1}}, y^{\delta}\right)=\phi\left(x_{\eta_{2}}, y^{\delta}\right)=\delta^{2}$. By the minimizing property of the minimizers $x_{\eta_{1}} \in S\left(\eta_{1}\right)$ and $x_{\eta_{2}} \in S\left(\eta_{2}\right)$ and the fact that $x_{\eta_{2}} \notin S\left(\eta_{1}\right)$ from the assumption $S\left(\eta_{1}\right) \cap S\left(\eta_{2}\right)=\emptyset$, we have

$$
\phi\left(x_{\eta_{1}}, y^{\delta}\right)+\eta_{1} \psi\left(x_{\eta_{1}}\right)<\phi\left(x_{\eta_{2}}, y^{\delta}\right)+\eta_{1} \psi\left(x_{\eta_{2}}\right),
$$

which consequently implies that $\psi\left(x_{\eta_{1}}\right)<\psi\left(x_{\eta_{2}}\right)$. However, reversing the roles of $\eta_{1}$ and $\eta_{2}$ gives a contradictory inequality $\psi\left(x_{\eta_{2}}\right)<\psi\left(x_{\eta_{1}}\right)$.

To exploit Lemma 2.3, we first derive a result characterizing the solution $x_{\eta}$. It also gives an explicit formula for computing $\eta^{*}$ from the data $y^{\delta}$ for Hilbertian $Y$ and $\psi(x)$ being a norm on $X$ (or its power). We denote by $\|\cdot\|_{X^{*}}$ the norm of the dual space $X^{*}$ of the space $X$, and by $\langle\cdot, \cdot\rangle$ both the duality pairing between $X^{*}$ and $X$ and the inner product on a Hilbert space. Also we recall the subdifferential $\partial \psi(x)$ of $\psi$ at $x$, i.e., $\partial \psi(x)=\left\{\zeta \in X^{*}: \psi\left(x^{\prime}\right) \geqslant \psi(x)+\left\langle\zeta, x^{\prime}-x\right\rangle\right.$ for all $\left.x^{\prime} \in X\right\}$.
THEOREM 2.4 Let $Y$ be a Hilbert space, $\phi\left(x, y^{\delta}\right)=\frac{1}{2}\left\|K x-y^{\delta}\right\|^{2}, \psi(x)=\frac{1}{p}\|x\|_{X}^{p}$ with $p \geqslant 1$, and $\left\|K^{*} y^{\delta}\right\|_{X^{*}} \neq 0$. Furthermore, let $\eta^{*}=\left\|K^{*} y^{\delta}\right\|_{X^{*}}$ if $p=1$ and $\eta^{*}=+\infty$ if $p>1$. Then, for $\eta \geqslant \eta^{*}$, $x_{\eta}=0$ and for $\eta<\eta^{*}$, there hold

$$
\left\langle K^{*}\left(K x_{\eta}-y^{\delta}\right), x_{\eta}\right\rangle=-p \eta \psi\left(x_{\eta}\right) \quad \text { and } \quad\left\|K^{*}\left(y^{\delta}-K x_{\eta}\right)\right\|_{X^{*}}=\eta\left\|x_{\eta}\right\|_{X}^{p-1}
$$

Conversely, if the above relations hold, then $x_{\eta}$ is a minimizer of $J_{\eta}$.

Proof. First, we note that the optimality condition for $x_{\eta}$ reads

$$
K^{*}\left(K x_{\eta}-y^{\delta}\right)+\eta \zeta_{\eta}=0,
$$

where $\zeta_{\eta} \in \partial \psi\left(x_{\eta}\right)$. We discuss the cases $p>1$ and $p=1$ separately.
For $p>1, \partial \psi\left(x_{\eta}\right)=j_{p}\left(x_{\eta}\right)$, the duality mapping of weight $g(t)=t^{p-1}$ (Cioranescu, 1990, Theorem 4.4). It satisfies

$$
\left\|j_{p}\left(x_{\eta}\right)\right\|_{X^{*}}=\left\|x_{\eta}\right\|_{X}^{p-1} \quad \text { and } \quad\left\langle j_{p}\left(x_{\eta}\right), x_{\eta}\right\rangle=\|x\|_{X}^{p} .
$$

Consequently, the desired relations follow directly. Conversely, the two relations imply directly that (Cioranescu, 1990)

$$
\eta^{-1} K^{*}\left(y^{\delta}-K x_{\eta}\right)=j_{p}\left(x_{\eta}\right) \in \partial \psi\left(x_{\eta}\right),
$$

which is a sufficient condition for the optimality of $x_{\eta}$ by noting the convexity of $J_{\eta}$.
Meanwhile, for $p=1$, by Cioranescu (1990, Proposition 3.4), we have $\partial \psi(x)=\left\{x^{*} \in X^{*}\right.$ : $\left.\left\langle x^{*}, x\right\rangle=\|x\|_{X},\left\|x^{*}\right\|_{X^{*}}=1\right\}$ for $x \neq 0$. Therefore, at $x_{\eta} \neq 0$, the two relations obviously hold, and the converse follows as before. If $x_{\eta}=0$, the minimizing property implies that for any $h \in X$ and $\varepsilon>0$,

$$
\frac{1}{2}\left\|K(\varepsilon h)-y^{\delta}\right\|^{2}+\eta \psi(\varepsilon h) \geqslant \frac{1}{2}\left\|y^{\delta}\right\|^{2} .
$$

Letting $\varepsilon \rightarrow 0^{+}$yields $\eta \psi(h)-\left\langle K h, y^{\delta}\right\rangle \geqslant 0$. Since the inequality holds for arbitrary $h \in X$ and $\left\|K^{*} y^{\delta}\right\|_{X^{*}} \neq 0$, we have $\eta \geqslant \eta^{*}=\left\|K^{*} y^{\delta}\right\|_{X^{*}}$. The converse follows by reversing the arguments.

REMARK 2.5 In the case where $\psi(x)$ is a seminorm (or its power), i.e., $\psi(x)=\frac{1}{p}|x|_{X}^{p}$ with $p \geqslant 1$, then at a minimum $x_{\eta}$, the identity $\left\langle K^{*}\left(K x_{\eta}-y^{\delta}\right), x_{\eta}\right\rangle=-p \eta \psi\left(x_{\eta}\right)$ remains valid. However, an explicit characterization of the critical value $\eta^{*}$ is missing.

Now we can state the uniqueness for some nonsmooth models, e.g., $\frac{1}{p}\|\cdot\|_{L^{p}}^{p}$ and $|\cdot|_{T V}$.
Corollary 2.6 Assume that $\eta^{*}>0$. Let $\phi\left(x, y^{\delta}\right)=\frac{1}{2}\left\|K x-y^{\delta}\right\|^{2}$ and $\psi(x)=\frac{1}{p}\|x\|_{X}^{p}\left(\right.$ or $\left.\frac{1}{p}|x|_{X}^{p}\right)$ with $p \geqslant 1$. If there exists an $\eta<\eta^{*}$ satisfying equation (1.3), then it is unique.
Proof. In the light of Remark 2.5 it suffices to show the norm case. Assume that there exist two distinct $\eta_{1}, \eta_{2}<\eta^{*}$ both satisfying equation (1.3). Then, by Theorem 2.4, the solutions $x_{\eta_{1}} \in S\left(\eta_{1}\right)$ and $x_{\eta_{2}} \in S\left(\eta_{2}\right)$ satisfy

$$
\left\langle K^{*}\left(y^{\delta}-K x_{\eta_{i}}\right), x_{\eta_{i}}\right\rangle=\eta_{i}\left\|x_{\eta_{i}}\right\|_{X}^{p}, \quad i=1,2 .
$$

This implies $S\left(\eta_{1}\right) \cap S\left(\eta_{2}\right)=\emptyset$, and the assertion follows from Lemma 2.3.
The next corollary is a direct consequence of Theorem 2.4.
Corollary 2.7 Assume that $\eta^{*}>0$. Let $\phi\left(x, y^{\delta}\right)=\frac{1}{2}\left\|K x-y^{\delta}\right\|^{2}$ and $\psi(x)=\frac{1}{p}\|x\|_{X}^{p}\left(\right.$ or $\left.\frac{1}{p}|x|_{X}^{p}\right)$ with $p \geqslant 1$. Then, $\phi\left(x_{\eta}, y^{\delta}\right)$ and $\psi\left(x_{\eta}\right)$ are strictly monotone on the interval $\left.] 0, \eta^{*}\right]$.

Finally, we derive an upper bound for the solution to equation (1.3) for the case $\phi\left(x, y^{\delta}\right)=\frac{1}{2} \| K x-$ $y^{\delta} \|^{2}$ and $\psi(x)=\frac{1}{p}\|x\|_{X}^{p}$. It may be used as an initial guess in iterative algorithms for solving equation (1.3).

THEOREM 2.8 Let $\phi\left(x, y^{\delta}\right)=\frac{1}{2}\left\|K x-y^{\delta}\right\|^{2}$ and $\psi(x)=\frac{1}{p}\|x\|_{X}^{p}(p \geqslant 1)$. Then, for the choice $\eta=\frac{\|K\|_{L(X, Y)}^{p}}{\left(\left\|y^{\delta}\right\|-\delta\right)^{p-1}} \delta$, there holds the estimate $\left\|K x_{\eta}-y^{\delta}\right\|^{2} \geqslant \delta^{2}$.

Proof. From Theorem 2.4 we have $\eta p \psi\left(x_{\eta}\right)=-\left\langle K^{*}\left(K x_{\eta}-y^{\delta}\right), x_{\eta}\right\rangle=\left\langle y^{\delta}-K x_{\eta}, K x_{\eta}\right\rangle$. Applying the Cauchy-Schwarz inequality gives

$$
\eta \leqslant \frac{\left\|K x_{\eta}-y^{\delta}\right\|\left\|K x_{\eta}\right\|}{p \psi\left(x_{\eta}\right)} .
$$

Consequently, we have

$$
\eta \leqslant \frac{\left\|K x_{\eta}-y^{\delta}\right\|\left\|K x_{\eta}\right\|}{p \psi\left(x_{\eta}\right)}=\frac{\left\|K x_{\eta}-y^{\delta}\right\|\left\|K x_{\eta}\right\|^{p}}{\left\|x_{\eta}\right\|_{X}^{p}\left\|K x_{\eta}\right\|^{p-1}} .
$$

Now the inequality $\left\|K x_{\eta}\right\| \leqslant\|K\|_{L(X, Y)}\left\|x_{\eta}\right\|_{X}$ implies that

$$
\eta \leqslant \frac{\left\|K x_{\eta}-y^{\delta}\right\|\|K\|_{L(X, Y)}^{p}}{\left\|K x_{\eta}\right\|^{p-1}} \leqslant \frac{\left\|K x_{\eta}-y^{\delta}\right\|\|K\|_{L(X, Y)}^{p}}{\left(\left\|y^{\delta}\right\|-\left\|K x_{\eta}-y^{\delta}\right\|\right)^{p-1}},
$$

by noting that $\left\|K x_{\eta}\right\| \geqslant\left\|y^{\delta}\right\|-\left\|K x_{\eta}-y^{\delta}\right\|$. The desired estimate follows from the inequality.

Hence, the value $\eta$ by the principle is at most of order $\delta$, i.e., $\mathcal{O}(\delta)$. This shows suboptimality of the principle in Hilbert spaces: it cannot achieve optimal convergence rates for the source parameter $v$ within the range $\left.] \frac{1}{2}, 1\right]$ since then optimality can only be realized for $\eta$ larger than $\mathcal{O}(\delta)$ (Engl et al., 1996).

## 3. Numerical algorithms

In this section we develop efficient algorithms for solving equation (1.3). Generally, equation (1.3) is highly nonlinear, nonconvex and potentially nonsmooth, and thus, its numerical treatment is nontrivial. We will exploit the idea of model functions (Ito \& Kunisch, 1992; Kunisch \& Zou, 1998; Xie \& Zou, 2002). Our essential contributions here include a differentiability result and interpreting model functions via Padé approximation. First, we introduce the value function

$$
F(\eta):=J_{\eta}\left(x_{\eta}\right)=\min _{x \in X} J_{\eta}(x) .
$$

### 3.1 Value function

Here we collect some important analytical properties of the function $F(\eta)$.
Lemma 3.1 The function $F(\eta)$ is continuous and monotonically increasing.
Proof. The assertion follows directly from the minimizing property of $x_{\eta}$.
Lemma 3.2 The following limits hold for the function $F(\eta)$ :

$$
\begin{equation*}
\lim _{\eta \rightarrow 0^{+}} F(\eta)=\lim _{\eta \rightarrow 0^{+}} \phi\left(x_{\eta}, y^{\delta}\right) \equiv \phi^{0} \quad \text { and } \quad \lim _{\eta \rightarrow+\infty} F(\eta)=\lim _{\eta \rightarrow+\infty} \phi\left(x_{\eta}, y^{\delta}\right) \equiv \phi^{\infty} \tag{3.1}
\end{equation*}
$$

Proof. Assumption 2.1(c) and the minimizing property of $x_{\eta}$ imply

$$
\begin{equation*}
F(\eta) \equiv \phi\left(x_{\eta}, y^{\delta}\right)+\eta \psi\left(x_{\eta}\right) \leqslant \phi\left(\tilde{x}, y^{\delta}\right)+\eta \psi(\tilde{x})=\phi\left(\tilde{x}, y^{\delta}\right)<+\infty \tag{3.2}
\end{equation*}
$$

and a trivial lower bound for $F(\eta)$ is 0 , i.e., $F(\eta)$ is uniformly bounded. Hence, both limits in (3.1) make sense. There exists an $x^{\varepsilon} \in X$ such that $\phi^{0} \leqslant \phi\left(x^{\varepsilon}, y^{\delta}\right) \leqslant \phi^{0}+\varepsilon$ and by the extremal property of $x_{\eta}$,

$$
\phi^{0} \leqslant \phi\left(x_{\eta}, y^{\delta}\right)+\eta \psi\left(x_{\eta}\right) \leqslant \phi\left(x^{\varepsilon}, y^{\delta}\right)+\eta \psi\left(x^{\varepsilon}\right) \leqslant \phi^{0}+\varepsilon+\eta \psi\left(x^{\varepsilon}\right) .
$$

Letting $\eta \rightarrow 0^{+}$gives $\phi^{0} \leqslant \lim _{\eta \rightarrow 0^{+}} F(\eta) \leqslant \phi^{0}+\varepsilon$. This shows the first assertion.
Let $\left\{\eta_{n}\right\}_{n}$ be a sequence tending to infinity. By Lemma 2.2 and inequality (3.2), $\psi\left(x_{\eta_{n}}\right) \rightarrow 0$ and $\phi\left(x_{\eta_{n}}, y^{\delta}\right) \rightarrow \phi^{\infty}$. Hence, by Assumption 2.1(a), $\left\{x_{\eta_{n}}\right\}_{n}$ is uniformly bounded, and there exists a subsequence, also denoted $\left\{x_{\eta_{n}}\right\}_{n}$, and some $x^{*} \in X$, such that $x_{\eta_{n}} \rightarrow x^{*}$ weakly and $\psi\left(x^{*}\right)=0$. Now Assumption 2.1(b) and the minimizing property of $x_{\eta_{n}}$ yield

$$
\begin{aligned}
\phi\left(x^{*}, y^{\delta}\right) & \leqslant \liminf _{n \rightarrow \infty} \phi\left(x_{\eta_{n}}, y^{\delta}\right) \leqslant \limsup _{n \rightarrow \infty} \phi\left(x_{\eta_{n}}, y^{\delta}\right) \\
& \leqslant \limsup _{n \rightarrow \infty}\left\{\phi\left(x_{\eta_{n}}, y^{\delta}\right)+\eta_{n} \psi\left(x_{\eta_{n}}\right)-\eta_{n} \psi\left(x^{*}\right)\right\} \\
& \leqslant \limsup _{n \rightarrow \infty}\left\{\phi\left(x^{*}, y^{\delta}\right)+\eta_{n} \psi\left(x^{*}\right)-\eta_{n} \psi\left(x^{*}\right)\right\}=\phi\left(x^{*}, y^{\delta}\right),
\end{aligned}
$$

i.e., $\lim _{n \rightarrow \infty} \phi\left(x_{\eta_{n}}, y^{\delta}\right)=\phi\left(x^{*}, y^{\delta}\right)$. Letting $n \longrightarrow \infty$ in the inequality $\phi\left(x_{\eta_{n}}, y^{\delta}\right) \leqslant \phi\left(x_{\eta_{n}}, y^{\delta}\right)+$ $\eta_{n} \psi\left(x_{\eta_{n}}\right) \leqslant \phi\left(x^{*}, y^{\delta}\right)$ establishes the second assertion.

In practice, $\phi^{0}$ and $\phi^{\infty}$ are often straightforward to obtain: $\phi^{0}$ is the minimal value of $\phi\left(x, y^{\delta}\right)$ over the space $X$, while $\phi^{\infty}$ is the minimal value of $\phi\left(x, y^{\delta}\right)$ over the subset of $X$ which annihilates $\psi$.

Finally, we show a differentiability result for $F(\eta)$.
THEOREM 3.3 If the function $\psi\left(x_{\eta}\right)$ is continuous at $\tilde{\eta}>0$, then $F(\eta)$ is differentiable at $\tilde{\eta}$ and

$$
F^{\prime}(\tilde{\eta})=\psi\left(x_{\tilde{\eta}}\right) .
$$

Proof. For $\eta>\tilde{\eta}$, from the minimizing property of $x_{\tilde{\eta}}$, the relation

$$
\begin{equation*}
F(\eta)-F(\tilde{\eta})=\left[\phi\left(x_{\eta}, y^{\delta}\right)-\phi\left(x_{\tilde{\eta}}, y^{\delta}\right)+\tilde{\eta}\left(\psi\left(x_{\eta}\right)-\psi\left(x_{\tilde{\eta}}\right)\right)\right]+(\eta-\tilde{\eta}) \psi\left(x_{\eta}\right) \geqslant(\eta-\tilde{\eta}) \psi\left(x_{\eta}\right) \tag{3.3}
\end{equation*}
$$

follows. Similarly, by the minimizing property of $x_{\eta}$, we deduce

$$
\begin{equation*}
F(\eta)-F(\tilde{\eta})=\phi\left(x_{\eta}, y^{\delta}\right)-\phi\left(x_{\tilde{\eta}}, y^{\delta}\right)+\eta\left(\psi\left(x_{\eta}\right)-\psi\left(x_{\tilde{\eta}}\right)\right)+(\eta-\tilde{\eta}) \psi\left(x_{\tilde{\eta}}\right) \leqslant(\eta-\tilde{\eta}) \psi\left(x_{\tilde{\eta}}\right) . \tag{3.4}
\end{equation*}
$$

Hence, inequalities (3.3)-(3.4) yield

$$
\psi\left(x_{\eta}\right) \leqslant \frac{F(\eta)-F(\tilde{\eta})}{\eta-\tilde{\eta}} \leqslant \psi\left(x_{\tilde{\eta}}\right) .
$$

The claim now follows from the continuity of $\psi\left(x_{\eta}\right)$ at $\tilde{\eta}$.
Throughout, we shall assume that $\psi\left(x_{\eta}\right)$ is continuous in $\eta$.

### 3.2 Two numerical algorithms

We shall develop two algorithms, i.e., MFA and a quasi-Newton method.

The idea of the MFA is as follows (Kunisch \& Zou, 1998; Xie \& Zou, 2002). First, by Theorem 3.3, one rewrites equation (1.3) equivalently as

$$
\begin{equation*}
F(\eta)-\eta F^{\prime}(\eta)=\delta^{2} \tag{3.5}
\end{equation*}
$$

and approximates $F(\eta)$ with a model function $m_{k}(\eta)$ at the $k$ th iteration given by

$$
m_{k}(\eta)=b+\frac{c_{k}}{t_{k}+\eta}
$$

where $b, c_{k}$ and $t_{k}$ are constants to be determined. In existing MFA implementations the constant $b$ is fixed by imposing further assumptions on the asymptotes of $m_{k}(\eta)$ : in Kunisch \& Zou (1998) the condition $m_{k}(0)=0$ was enforced, whereas in Xie \& Zou (2002), $b$ was set to $\frac{1}{2}\left\|y^{\delta}\right\|^{2}$, i.e., $b=\phi^{\infty}$.

We interpret the model $m_{k}(\eta)$ as a Padé approximation of $F(\eta)$ with suitable constraint on the asymptotes. Then, existing algorithms (Kunisch \& Zou, 1998; Xie \& Zou, 2002) are reproduced by enforcing the asymptotes $m_{k}(0)=0$ and $m_{k}(+\infty)=\frac{1}{2}\left\|y^{\delta}\right\|^{2}$, respectively. This interpretation is new and crucial for subsequent developments since the derivations in Kunisch \& Zou (1998) and Xie \& Zou (2002) hinge essentially on the inner product structure. Due to its better theoretical underpinnings and numerical performance, we focus on the variant in Xie \& Zou (2002), i.e., fixing $b$ at $\phi^{\infty}$. So, we arrive at the model

$$
m_{k}(\eta)=\phi^{\infty}+\frac{c_{k}}{t_{k}+\eta} .
$$

Then, by enforcing interpolation conditions at $\eta_{k}$, i.e.,

$$
m_{k}\left(\eta_{k}\right)=\phi^{\infty}+\frac{c_{k}}{t_{k}+\eta_{k}}=F\left(\eta_{k}\right) \quad \text { and } \quad m_{k}^{\prime}\left(\eta_{k}\right)=-\frac{c_{k}}{\left(t_{k}+\eta_{k}\right)^{2}}=F^{\prime}\left(\eta_{k}\right)
$$

we derive

$$
c_{k}=-\frac{\left(F\left(\eta_{k}\right)-\phi^{\infty}\right)^{2}}{F^{\prime}\left(\eta_{k}\right)} \quad \text { and } \quad t_{k}=\frac{\phi^{\infty}-\phi\left(x_{\eta_{k}}, y^{\delta}\right)}{\psi\left(x_{\eta_{k}}\right)}-2 \eta_{k}
$$

Hence, $c_{k}$ is negative for $\eta_{k}<\eta^{*}$, and $t_{k}$ is generally nondeterminate, and positive if and only if

$$
\begin{equation*}
\phi^{\infty}-\phi\left(x_{\eta_{k}}, y^{\delta}\right)-2 \eta_{k} \psi\left(x_{\eta_{k}}\right)>0 \tag{3.6}
\end{equation*}
$$

which, by Lemma 3.2, holds if $\eta_{k}$ is sufficiently small.
If the condition $t_{k}>0$ holds, the definition of $m_{k}$ gives

$$
\begin{aligned}
& \lim _{\eta \rightarrow+\infty} m_{k}(\eta)=\phi^{\infty}=\lim _{\eta \rightarrow+\infty} F(\eta), \\
& \lim _{\eta \rightarrow+\infty} m_{k}^{\prime}(\eta)=0=\lim _{\eta \rightarrow+\infty} F^{\prime}(\eta) .
\end{aligned}
$$

Moreover, by its definition,

$$
m_{k}^{\prime}(\eta)=-\frac{c_{k}}{\left(t_{k}+\eta\right)^{2}}>0 \quad \text { and } \quad m_{k}^{\prime \prime}(\eta)=\frac{2 c_{k}}{\left(t_{k}+\eta\right)^{3}}<0
$$

In view of Lemmas 2.2 and 3.1 and Theorem 3.3 the model $m_{k}(\eta)$ preserves the asymptotic behaviour, monotonicity and concavity of $F(\eta)$. Hence, we arrive at an approximation to equation (3.5),

$$
\begin{equation*}
G_{k}(\eta) \equiv m_{k}(\eta)-\eta m_{k}^{\prime}(\eta)=\delta^{2} \tag{3.7}
\end{equation*}
$$

which is computationally more tractable than equation (1.3) because of the simplicity of $m_{k}(\eta)$. Note that $G_{k}^{\prime}(\eta)=\frac{-2 c_{k} \eta}{\left(t_{k}+\eta\right)^{3}}>0$, i.e., $G_{k}(\eta)$ preserves the monotonicity of $\phi\left(x_{\eta}, y^{\delta}\right)$.

The next result shows the local solvability of equation (3.7).

LEMMA 3.4 If $t_{k}>0$ and $\phi\left(x_{\eta_{k}}, y^{\delta}\right)$ is close to $\delta^{2}$, then there exists a unique positive solution to equation (3.7).
Proof. The approximate equation (3.7) at the $k$ th step reads $\phi^{\infty}+\frac{c_{k}}{t_{k}+\eta}+\eta \frac{c_{k}}{\left(t_{k}+\eta\right)^{2}}=\delta^{2}$. We discuss two cases separately, i.e., $F\left(\eta_{k}\right)-\eta_{k} F^{\prime}\left(\eta_{k}\right)>\delta^{2}$ and $F\left(\eta_{k}\right)-\eta_{k} F^{\prime}\left(\eta_{k}\right)<\delta^{2}$. In the former case, by the monotonicity, it suffices to show

$$
\lim _{\eta \rightarrow 0^{+}}\left(m_{k}(\eta)-\eta m_{k}^{\prime}(\eta)\right)=\phi^{\infty}+\frac{c_{k}}{t_{k}}<\delta^{2} .
$$

Substituting the formulas for $c_{k}$ and $t_{k}$ and observing Theorem 3.3 gives

$$
\left(\phi\left(x_{\eta_{k}}, y^{\delta}\right)-\delta^{2}\right)\left(\phi^{\infty}-\phi\left(x_{\eta_{k}}, y^{\delta}\right)-2 \eta_{k} \psi\left(x_{\eta_{k}}\right)\right)<\eta_{k}^{2} \psi\left(x_{\eta_{k}}\right)^{2}
$$

which together with the assumption yields the assertion. In the latter case the assertion follows directly from $\lim _{\eta \rightarrow+\infty}\left(\phi^{\infty}+\frac{c_{k}}{t_{k}+\eta}+\eta \frac{c_{k}}{\left(t_{k}+\eta\right)^{2}}\right)=\phi^{\infty}>\delta^{2}$.

A direct implementation of the procedure is at best locally convergent because equation (3.7) is only locally solvable. To construct a globally convergent algorithm we replace $G_{k}(\eta)$ by its relaxation (Xie \& Zou, 2002)

$$
\hat{G}_{k}(\eta)=G_{k}(\eta)+\alpha_{k}\left(G_{k}(\eta)-\phi\left(x_{\eta_{k}}, y^{\delta}\right)\right)
$$

where the relaxation constant $\alpha_{k}$ is chosen such that

$$
\begin{equation*}
\hat{G}_{k}(\eta)=\delta^{2} \tag{3.8}
\end{equation*}
$$

always has a unique solution. If $\phi\left(x_{\eta_{k}}, y^{\delta}\right)>\delta^{2}$, this can be achieved by prescribing $\hat{G}_{k}(0)=\hat{\alpha} \delta^{2}$ for all $\hat{\alpha} \in[0,1)$, which consequently suggests $\alpha_{k}=\frac{G_{k}(0)-\hat{\alpha} \delta^{2}}{\phi\left(x_{\eta_{k}}, y^{\delta}\right)-G_{k}(0)}$. It follows from the monotonicity of $G_{k}(\eta)$ that $1+\alpha_{k}>0$ if $\phi\left(x_{\eta_{k}}, y^{\delta}\right)>\delta^{2}$, and thus, $\hat{G}_{k}(\eta)$ preserves monotonicity. Now, we can describe a two-parameter algorithm (TPA for short); see Algorithm 1. The algorithm terminates if the relative change $\left|\eta_{k+1}-\eta_{k}\right| /\left|\eta_{k}\right|$ falls below a given tolerance.

```
Algorithm 1 Two-parameter algorithm (TPA)
    Choose \(\eta_{0}, \hat{\alpha}\) and \(K\), and set \(k=1\).
    for \(k=1, \ldots, K\) do
        Solve (1.2) for \(x_{\eta_{k}}\), compute \(F\left(\eta_{k}\right)\) and \(F^{\prime}\left(\eta_{k}\right)\), and update \(t_{k}\) and \(c_{k}\);
        set the \(k\) th model function \(m_{k}(\eta)=\phi^{\infty}+\frac{c_{k}}{t_{k}+\eta}\), and set \(G_{k}=m_{k}(\eta)-\eta m_{k}^{\prime}(\eta)\);
        solve for \(\eta_{k+1}\) from the relaxed discrepancy equation
\[
\left(1+\frac{G_{k}(0)-\hat{\alpha} \delta^{2}}{\phi\left(x_{\eta_{k}}, y^{\delta}\right)-G_{k}(0)}\right) G_{k}(\eta)=\delta^{2}+\frac{G_{k}(0)-\hat{\alpha} \delta^{2}}{\phi\left(x_{\eta_{k}}, y^{\delta}\right)-G_{k}(0)} \phi\left(x_{\eta_{k}}, y^{\delta}\right) ;
\]
check the stopping criterion.
end for
output approximations \(\eta_{K}\) and \(x_{\eta_{K}}\).
```

The next theorem shows the monotone convergence of the algorithm for 'large' initial guesses. Its proof parallels that in Xie \& Zou (2002), and hence, it is omitted.

THEOREM 3.5 Let the solution $\eta^{\dagger}$ to equation (1.3) be unique, and let $\eta_{0}$ satisfy $\phi\left(x_{\eta_{0}}, y^{\delta}\right)>\delta^{2}$. Then, the sequence $\left\{\eta_{k}\right\}_{k}$ generated by the TPA is well defined. Moreover, the sequence is either finite, i.e., it terminates at some $\eta_{k}$ satisfying $\phi\left(x_{\eta_{k}}, y^{\delta}\right) \leqslant \delta^{2}$, or it is infinite and converges to $\eta^{\dagger}$ strictly monotonically decreasingly.

Numerically, the TPA converges robustly, but the local convergence is slow. To improve the overall performance we hybridize it with the secant method. The variant of secant method adopted is shown in Algorithm 2, where the stopping criterion is identical to Algorithm 1. It computes $\eta_{k+1}$ in the $\eta^{-1}$ coordinate when $\eta_{k}$ over-regularizes and in the $\eta$ coordinate when $\eta_{k}$ under-regularizes. Despite the nonlinearity of equation (1.3), Algorithm 2 has a large convergence basin. The next result sheds some light on the $L^{2}-L^{2}$ model.

```
Algorithm 2 Secant method
    Choose \(\eta_{0}, \eta_{1}\) and \(K\), and set \(k=1\).
    for \(k=1, \ldots, K\) do
        Compute the residual \(\phi\left(x_{\eta_{k}}, y^{\delta}\right)\);
        if \(\phi\left(x_{\eta_{k}}, y^{\delta}\right)>\delta^{2}\), compute \(\eta_{k+1}\) by
                                    \(\tilde{\eta}_{k+1}=\frac{1}{\eta_{k}}-\frac{\left(\phi\left(x_{\eta_{k}}, y^{\delta}\right)-\delta^{2}\right)\left(\eta_{k-1}-\eta_{k}\right)}{\eta_{k-1} \eta_{k}\left(\phi\left(x_{\eta_{k}}, y^{\delta}\right)-\phi\left(x_{\eta_{k-1}}, y^{\delta}\right)\right)}, \quad \eta_{k+1}=\frac{1}{\tilde{\eta}_{k+1}} ;\)
```

        otherwise, compute \(\eta_{k+1}\) by
    $$
\eta_{k+1}=\eta_{k}-\frac{\left(\phi\left(x_{\eta_{k}}, y^{\delta}\right)-\delta^{2}\right)\left(\eta_{k}-\eta_{k-1}\right)}{\phi\left(\eta_{k}, y^{\delta}\right)-\phi\left(\eta_{k-1}, y^{\delta}\right)} ;
$$ solve (1.2) for the Tikhonov solution $x_{\eta_{k+1}}$; check the stopping criterion.

## end for

output approximations $\eta_{K}$ and $x_{\eta_{K}}$.

Lemma 3.6 In the case of $\phi\left(x, y^{\delta}\right)=\frac{1}{2}\left\|K x-y^{\delta}\right\|^{2}$ and $\psi(x)=\frac{1}{2}\|L x\|^{2}$, then $\phi\left(x_{\eta^{-1}}, y^{\delta}\right)$ is convex in $\eta$.

Proof. Let $\alpha=\eta^{-1}$, then $x_{\alpha}$ solves $\left(\alpha K^{*} K+L^{*} L\right) x_{\alpha}=\alpha K^{*} y^{\delta}$. Letting $r_{\alpha}=K x_{\alpha}-y^{\delta}$ we can check that $\frac{\mathrm{d} x_{\alpha}}{\mathrm{d} \alpha}$ and $\frac{\mathrm{d}^{2} x_{\alpha}}{\mathrm{d} \alpha^{2}}$ satisfy

$$
\left(\alpha K^{*} K+L^{*} L\right) \frac{\mathrm{d} x_{\alpha}}{\mathrm{d} \alpha}=-K^{*} r_{\alpha} \quad \text { and } \quad\left(\alpha K^{*} K+L^{*} L\right) \frac{\mathrm{d}^{2} x_{\alpha}}{\mathrm{d} \alpha^{2}}=-2 K^{*} K \frac{\mathrm{~d} x_{\alpha}}{\mathrm{d} \alpha} .
$$

Denoting by $Q_{\alpha}$ the bounded inverse operator $\left(\alpha K^{*} K+L^{*} L\right)^{-1}$ gives

$$
\frac{\mathrm{d} x_{\alpha}}{\mathrm{d} \alpha}=-Q_{\alpha} K^{*} r_{\alpha} \quad \text { and } \quad \frac{\mathrm{d}^{2} x_{\alpha}}{\mathrm{d} \alpha^{2}}=2 Q_{\alpha} K^{*} K Q_{\alpha} K^{*} r_{\alpha}
$$

Consequently,

$$
\frac{\mathrm{d}^{2}}{\mathrm{~d} \alpha^{2}} \frac{1}{2}\left\|K x_{\alpha}-y^{\delta}\right\|^{2}=\left\langle K x_{\alpha}-y^{\delta}, K \frac{\mathrm{~d}^{2} x_{\alpha}}{\mathrm{d} \alpha^{2}}\right\rangle+\left\langle K \frac{\mathrm{~d} x_{\alpha}}{\mathrm{d} \alpha}, K \frac{\mathrm{~d} x_{\alpha}}{\mathrm{d} \alpha}\right\rangle=3\left\|K Q_{\alpha} K^{*} r_{\alpha}\right\|^{2} \geqslant 0 .
$$

This concludes the proof of the lemma.
Hence, the function $\phi\left(x_{\eta^{-1}}, y^{\delta}\right)$ is convex in $\eta$ for the $L^{2}-L^{2}$ model, and Newton type methods converge monotonically in exact arithmetic. For nonsmooth models the convexity may not hold, but nonetheless numerical experiments are very encouraging.

## 4. Numerical experiments and discussions

This section presents numerical results for four benchmark inverse problems adapted from the package Regularization Tool (Hansen, 1998) to illustrate the accuracy and optimality of the principle and the robustness and efficiency of the algorithms. These are Fredholm integral equations of the first kind with kernel $k(s, t)$ and solution $x^{\dagger}(t)$. The discretized linear system is of the form $\mathbf{K x}=\mathbf{y}^{\delta}$ with size $300 \times 300$. The model is referred to as $\phi-\psi$ type, e.g., $L^{1}-T V$ denotes $L^{1}$ fidelity and $T V$ penalty. Table 1 summarizes their main features: the degree of ill-posedness (Cond is the condition number) and continuity of $\phi\left(x_{\eta}, y^{\delta}\right)$. The initial guess for $\eta$ is $\eta_{0}=1.0$, and the hybrid algorithm is initialized with four iterations of the TPA. The constant $\hat{\alpha}$ is fixed at $\frac{1}{4}$ as in Xie \& Zou (2002). The minimization problems arising from the $L^{2}-T V, L^{2}-\ell^{1}$ and $L^{1}-T V$ models are solved by an iteratively reweighted least squares method (Clason et al., 2010) and that from the $L^{2}$-elastic net model by a Newton-type method (Jin et al., 2009).

Unless otherwise specified the data $\mathbf{y}^{\delta}$ is generated as follows: $y_{i}^{\delta}=y_{i}+\max _{i}\left\{\left|y_{i}\right|\right\} \varepsilon \xi_{i}$, where the $\xi_{i}$ follow the standard normal distribution and $\varepsilon$ is the relative noise level. The accuracy of the solution $x_{\eta}$ is measured by the relative error $e=\left\|x_{\eta}-x^{\dagger}\right\|_{L^{2}} /\left\|x^{\dagger}\right\|_{L^{2}}$. For each example we also present the optimal choice $\eta_{\text {opt }}$, i.e., the one achieving the minimal error $e$, by solving equation (1.2) for 100 logarithmically-uniformly-distributed points over the interval $\left[1 \times 10^{-15}, 1 \times 10^{-1}\right]$. The subscripts opt and dp denote the optimal solution and that by the discrepancy principle, respectively, whereas tpa and sm denote the results by the TPA and the hybrid algorithm, respectively. The number in the parentheses denotes the number of iterations and that for the hybrid algorithm includes initialization with four iterations of the TPA.

### 4.1 Example 1: $L^{2}-T V$ (Numerical differentiation, adapted from deriv2)

The functions $k$ and $x^{\dagger}$ are given by

$$
k(s, t)=\left\{\begin{array}{l}
s(t-1), s<t, \\
t(s-1), s \geqslant t,
\end{array} \quad \text { and } \quad x^{\dagger}(t)=\left\{\begin{array}{l}
1, \frac{1}{3}<t \leqslant \frac{2}{3}, \\
0, \text { otherwise },
\end{array}\right.\right.
$$

and the integration interval is $[0,1]$. The exact solution $x^{\dagger}$ is piecewise constant, and thus, $T V$ penalty is suitable. The initial guess $\eta_{0}$ is taken to be $1 \times 10^{-2}$.

Table 1 Numerical examples

| Example | Description | $\phi\left(x_{\eta}, y^{\delta}\right)$ | $\operatorname{Cond}(\mathbf{K})$ | Noise | Program | $\phi-\psi$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | Differentiation | Continuous | $1.09 \times 10^{5}$ | Gaussian | deriv2 | $L^{2}-T V$ |
| 2 | Phillips | Continuous | $2.14 \times 10^{8}$ | Gaussian | phillips | $L^{2}-\ell^{1}$ |
| 3 | Deblurring | Discontinuous | $7.35 \times 10^{8}$ | Impulsive | blur | $L^{1}-T V$ |
| 4 | 2D deblurring | Continuous | $3.26 \times 10^{5}$ | Gaussian | blur | $L^{2}$-elastic net |

We observe from Table 2 that the parameter $\eta_{\text {dp }}$ (by the discrepancy principle) agrees very well with the optimal one $\eta_{\text {opt }}$, albeit its value is slightly larger. Furthermore, the accuracy errors $e_{\mathrm{dp}}$ and $e_{\mathrm{opt}}$ do not differ much. The TPA converges steadily and fast, see Fig. 1(a,b), and it yields an acceptable and even very accurate approximation, in terms of the error, within eight iterations. The algorithm tends to accelerate as the noise level decreases. However, its local convergence is slow, and it requires many iterations to reach a very accurate approximation of the solution to equation (1.3) (see Fig. 1(c)) where the symbol G refers to $\left|\phi\left(x_{\eta}, y^{\delta}\right)-\delta^{2}\right|$. The hybrid algorithm converges locally very fast. The initial guesses given by the TPA are smaller than but very close to $\eta^{*}$ beyond which $x_{\eta}$ does not change, and $\phi\left(x_{k-1}, y^{\delta}\right)$ and $\phi\left(x_{k}, y^{\delta}\right)$ are close to $\phi\left(x_{\infty}, y^{\delta}\right)$. Nonetheless, the iterates are rather steady, and the convergence is swift. The secant method is very efficient in decreasing G , which is useful when an accurate estimate of the true noise level is available. The solution is accurate and stable for $\varepsilon$ up to $5 \%$; see Fig. 2 and Table 2. The $T V$ solution exhibits a typical staircasing effect: it is piecewise constant and its magnitude is slightly distorted.

Now we compare the algorithms with a direct method based on sampling at $\eta_{k}=\eta_{0} q^{k-1}, q \in(0,1)$. Clearly, the efficiency of this method depends crucially on the shrinkage factor $q$ : the smaller is the factor $q$, the more accurate is the selected parameter, but at the expense of increased computing efforts. Also, the attainable accuracy is inherently limited by discrete sampling. We evaluate the method also on the data set with $\varepsilon=5 \%$, and set $q=0.9$ and $\eta_{0}=1 \times 10^{-2}$. The error $e$ after eight iterations of the method is $8.68 \times 10^{-1}$, which is far inferior to those in Table 2. The best possible result is achieved after 35 iterations: the selected parameter $\eta$ and the error $e$ are $2.78 \times 10^{-4}$ and $2.53 \times 10^{-1}$, respectively, which represents a good approximation to $\eta_{\mathrm{dp}}$ and $e_{\mathrm{dp}}$. However, it achieves G at $4.83 \times 10^{-7}$, and this can be realized by the hybrid algorithm within 10 iterations; cf. Fig. 2. Hence, the hybrid algorithm is preferred to the direct method. Although not presented, we would like to note that similar observations can be made for other examples.

### 4.2 Example 2: $L^{2}-\ell^{1}$ (Sparse reconstruction, adapted from Phillips' problem)

Let $\phi(t)=\left[1+\cos \frac{\pi t}{3}\right] \chi_{|t-s|<3}$ with $\chi$ being the indicator function, and $S=[-3,-2.96] \cup[0.6,0.64] \cup$ [3,3.04]. The functions $k$ and $x^{\dagger}$ are given by $k(s, t)=\phi(s-t)$ and $x^{\dagger}(t)=\chi_{S}$, and the integration interval is $[-6,6]$. The exact solution $x^{\dagger}$ has a sparse representation in the pixel basis, and thus, the $\ell^{1}$ penalty is suitable.

The matrix $\mathbf{K}$ is of full rank, and by Corollary 2.6, the solution to equation (1.3) is unique. The parameter $\eta_{\mathrm{dp}}$ is practically identical to the optimal one $\eta_{\mathrm{opt}}$ for all five noise levels; see Table 3. Interestingly, the value of $\eta$ in both cases decreases at the rate $\eta \sim \delta$, and the error $e$ apparently decreases also as $e \sim \delta$. Hence, the $\ell^{1}$ penalty circumvents the well-known saturation phenomenon for Tikhonov regularization in Hilbert spaces. The algorithms achieve a fast and steady convergence; cf. Fig. 3(a). The approximations after eight iterations are already very close to the exact one, and the hybrid algorithm yields more accurate results. Figure 4 shows the prominent feature of the sparsity-promoting $\ell^{1}$ penalty: the locations of all three small spikes are perfectly detected, and their retrieved magnitudes are reasonably accurate.

### 4.3 Example 3: $L^{1}-T V$ (Deblurring one-dimensional image)

The functions $k$ and $x^{\dagger}$ are given by $k(s, t)=\frac{1}{4 \sqrt{2 \pi}} e^{-\frac{(s-t)^{2}}{32}} \chi_{|s-t|<15}$ and $x^{\dagger}(t)=\chi_{[101,200]}$, and the integration interval is $[0,300]$. The data are corrupted by additive random-valued impulsive
TABLE 2 Numerical results for Example 1

| $\varepsilon$ | $\delta^{2}$ | $\eta_{\text {opt }}$ | $\eta_{\text {dp }}$ | $\eta_{\text {tpa }}$ | $\eta_{\text {sm }}$ | $e_{\text {opt }}$ | $e_{\text {dp }}$ | $e_{\text {tpa }}$ | $e_{\text {sm }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $5 \times 10^{-6}$ | $1.52 \times 10^{-11}$ | $7.74 \times 10^{-11}$ | $2.50 \times 10^{-9}$ | $6.26 \times 10^{-9}(8)$ | $5.10 \times 10^{-9}(8)$ | $9.46 \times 10^{-4}$ | $9.69 \times 10^{-3}$ | $1.78 \times 10^{-2}$ | $1.14 \times 10^{-2}$ |
| $5 \times 10^{-5}$ | $1.52 \times 10^{-9}$ | $1.29 \times 10^{-9}$ | $5.98 \times 10^{-8}$ | $3.88 \times 10^{-7}(8)$ | $1.80 \times 10^{-7}(8)$ | $9.80 \times 10^{-3}$ | $4.87 \times 10^{-2}$ | $6.68 \times 10^{-2}$ | $5.20 \times 10^{-2}$ |
| $5 \times 10^{-4}$ | $1.52 \times 10^{-7}$ | $2.78 \times 10^{-8}$ | $2.44 \times 10^{-6}$ | $6.10 \times 10^{-6}(8)$ | $3.81 \times 10^{-6}(8)$ | $5.96 \times 10^{-2}$ | $8.31 \times 10^{-2}$ | $8.82 \times 10^{-2}$ | $8.38 \times 10^{-2}$ |
| $5 \times 10^{-3}$ | $1.52 \times 10^{-5}$ | $1.67 \times 10^{-5}$ | $2.59 \times 10^{-5}$ | $6.48 \times 10^{-5}(8)$ | $3.98 \times 10^{-5}(8)$ | $1.06 \times 10^{-1}$ | $1.08 \times 10^{-1}$ | $1.29 \times 10^{-1}$ | $1.09 \times 10^{-1}$ |
| $5 \times 10^{-2}$ | $1.52 \times 10^{-3}$ | $1.67 \times 10^{-4}$ | $2.81 \times 10^{-4}$ | $7.59 \times 10^{-4}(8)$ | $5.41 \times 10^{-4}(8)$ | $2.42 \times 10^{-1}$ | $2.53 \times 10^{-1}$ | $3.23 \times 10^{-1}$ | $2.65 \times 10^{-1}$ |



FIG. 1. The convergence of (a) $\eta$, (b) $e$ and (c) G for Example 1 with 5\% noise.


FIg. 2. The numerical solutions for Example 1 with 5\% noise: (a) discrepancy principle versus optimal choice and (b) TPA versus hybrid algorithm.
noise as follows:

$$
y_{i}^{\delta}= \begin{cases}y_{i}+\sigma_{m} \xi_{i} \text { with probability } r, \\ y_{i} & \text { with probability } 1-r,\end{cases}
$$

where $\xi_{i}$ follows the standard Gaussian distribution, the constant $\sigma_{m}:=\varepsilon \max _{1 \leqslant i \leqslant 300}\left|y_{i}\right|$. The exact noise level $\delta^{2}$ is dictated by the corruption percentage $r$ and the standard deviation $\sigma_{m}$. The $L^{1}$ fidelity and $T V$ penalty are adopted to cope with impulsive noises and to reconstruct piecewise constant solutions (Chan \& Esedoglu, 2005), respectively. The initial guess $\eta_{0}$ is 10 . We note that the $L^{1}-T V$ model is not covered by the theory herein because of the nonuniqueness of minimizers to the functional $J_{\eta}$ (Chan \& Esedoḡlu, 2005).

The value $\eta_{\mathrm{dp}}$ is close to the optimal one $\eta_{\mathrm{opt}}$ for all noise levels (cf. Table 4), with $\eta_{\mathrm{opt}}$ determined by sampling $\eta$ over the interval $\left[1 \times 10^{-5}, 1 \times 10^{1}\right]$ at 100 points. Interestingly, $\eta_{\text {opt }}$ remains unchanged as the noise level varies by 3 orders of magnitude and also the variation of $\eta_{\mathrm{dp}}$ is negligible. Here, the parameter $\eta$ is characteristic: at some values the solution profile undergoes sudden transition and the profile might change little when $\eta$ varies without crossing these values (Chan \& Esedoğlu, 2005). The
TABLE 3 Numerical results for Example 2

| $\varepsilon$ | $\delta^{2}$ | $\eta_{\text {opt }}$ | $\eta_{\text {dp }}$ | $\eta_{\text {tpa }}$ | $\eta_{\text {sm }}$ | $e_{\text {opt }}$ | $e_{\text {dp }}$ | $e_{\text {tpa }}$ | $e_{\text {sm }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $5 \times 10^{-6}$ | $8.19 \times 10^{-11}$ | $1.87 \times 10^{-7}$ | $3.38 \times 10^{-7}$ | $8.12 \times 10^{-7}(8)$ | $5.13 \times 10^{-7}(8)$ | $4.99 \times 10^{-3}$ | $5.84 \times 10^{-3}$ | $7.25 \times 10^{-3}$ | $6.01 \times 10^{-3}$ |
| $5 \times 10^{-5}$ | $8.19 \times 10^{-9}$ | $2.31 \times 10^{-6}$ | $4.26 \times 10^{-6}$ | $1.04 \times 10^{-5}(8)$ | $6.54 \times 10^{-6}(8)$ | $1.17 \times 10^{-2}$ | $1.23 \times 10^{-2}$ | $1.61 \times 10^{-2}$ | $1.26 \times 10^{-2}$ |
| $5 \times 10^{-4}$ | $8.19 \times 10^{-7}$ | $3.51 \times 10^{-5}$ | $4.43 \times 10^{-5}$ | $1.06 \times 10^{-4}(8)$ | $6.69 \times 10^{-5}(8)$ | $3.19 \times 10^{-2}$ | $3.27 \times 10^{-2}$ | $4.12 \times 10^{-2}$ | $3.33 \times 10^{-2}$ |
| $5 \times 10^{-3}$ | $8.19 \times 10^{-5}$ | $5.34 \times 10^{-4}$ | $4.39 \times 10^{-4}$ | $1.06 \times 10^{-3}(8)$ | $6.69 \times 10^{-4}(8)$ | $1.24 \times 10^{-1}$ | $1.25 \times 10^{-1}$ | $1.40 \times 10^{-1}$ | $1.24 \times 10^{-1}$ |
| $5 \times 10^{-2}$ | $8.19 \times 10^{-3}$ | $4.33 \times 10^{-3}$ | $4.32 \times 10^{-3}$ | $1.07 \times 10^{-2}(8)$ | $6.65 \times 10^{-3}(8)$ | $2.83 \times 10^{-1}$ | $2.83 \times 10^{-1}$ | $5.32 \times 10^{-1}$ | $2.80 \times 10^{-1}$ |



FIG. 3. The convergence of (a) $\eta$, (b) $e$ and (c) G for Example 2 with 5\% noise.
(a)

(b)


FIg. 4. The numerical solutions for Example 2 with $5 \%$ noise: (a) discrepancy principle versus optimal choice and (b) TPA versus hybrid algorithm.
numerical results for $r=0.5$ are far more accurate than those for $r=0.3$, which shows the profound effect of the percentage $r$.

The TPA converges steadily (cf. Fig. 5), but very slowly: the 20th iterate represents only a rough approximation. The blame is attributed to clustering points around a solution to equation (1.3), which might render a rational approximation of $F(\eta)$ nearly invalid. A steady and fast convergence of Algorithm 2 is again observed, and the convergence is achieved within 12 iterations. Observing the large amount of noise, the reconstruction agrees well with the exact one; see Fig. 6. Hence, the TPA can provide a rough but visually acceptable estimate, despite the fact that the value $\eta$ and error grossly overestimate the optimal ones.

### 4.4 Example 4: $L^{2}$-elastic net (Two-dimensional image deblurring)

This is the blur example from Hansen (1998). We set the parameters $N=50$, band=5 and sigma=1.2. The true solution is shown in Fig. 8. We used elastic net, i.e., $\psi(x)=\|x\|_{\ell^{1}}+\frac{\gamma}{2}\|x\|_{\ell^{2}}^{2}$, with a fixed $\gamma=1 \times 10^{-3}$, which statistically favours a grouping effect (Zou \& Hastie, 2005).
TABLE 4 Numerical results for Example 3

| $(r, \varepsilon)$ | $\delta^{2}$ | $\eta_{\text {opt }}$ | $\eta_{\text {dp }}$ | $\eta_{\text {tpa }}$ | $\eta_{\text {sm }}$ | $e_{\text {opt }}$ | $e_{\text {dp }}$ | $e_{\text {tpa }}$ | $e_{\text {sm }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| (0.3, $5 \times 10^{-3}$ ) | $1.30 \times 10^{-1}$ | $5.34 \times 10^{-1}$ | $1.01 \times 10^{0}$ | $4.72 \times 10^{0}(20)$ | $1.48 \times 10^{0}(15)$ | $3.74 \times 10^{-7}$ | $5.72 \times 10^{-7}$ | $5.88 \times 10^{-3}$ | $3.81 \times 10^{-6}$ |
| (0.3, $\left.5 \times 10^{-2}\right)$ | $1.30 \times 10^{0}$ | $5.34 \times 10^{-1}$ | $1.19 \times 10^{0}$ | $8.22 \times 10^{0}(20)$ | $1.61 \times 10^{0}(15)$ | $3.72 \times 10^{-7}$ | $4.96 \times 10^{-7}$ | $2.35 \times 10^{-2}$ | $8.76 \times 10^{-6}$ |
| (0.3, $5 \times 10^{-1}$ ) | $1.30 \times 10^{1}$ | $5.34 \times 10^{-1}$ | $1.15 \times 10^{0}$ | $9.75 \times 10^{0}(20)$ | $1.69 \times 10^{0}(15)$ | $3.78 \times 10^{-7}$ | $3.89 \times 10^{-7}$ | $2.95 \times 10^{-2}$ | $1.40 \times 10^{-5}$ |
| (0.5, $\left.5 \times 10^{-3}\right)$ | $2.45 \times 10^{-1}$ | $6.13 \times 10^{-1}$ | $7.14 \times 10^{-1}$ | $6.85 \times 10^{0}(20)$ | $7.14 \times 10^{-1}(15)$ | $2.85 \times 10^{-3}$ | $2.94 \times 10^{-3}$ | $2.45 \times 10^{-2}$ | $2.92 \times 10^{-3}$ |
| (0.5,5 $\times 10^{-2}$ ) | $2.45 \times 10^{0}$ | $7.05 \times 10^{-1}$ | $7.81 \times 10^{-1}$ | $9.41 \times 10^{0}(20)$ | $7.89 \times 10^{-1}(15)$ | $1.89 \times 10^{-2}$ | $1.91 \times 10^{-2}$ | $5.44 \times 10^{-2}$ | $1.91 \times 10^{-2}$ |
| (0.5, $\left.5 \times 10^{-1}\right)$ | $2.45 \times 10^{1}$ | $8.11 \times 10^{-1}$ | $8.24 \times 10^{-1}$ | $9.88 \times 10^{0}(20)$ | $8.07 \times 10^{-1}(15)$ | $2.89 \times 10^{-2}$ | $2.86 \times 10^{-5}$ | $7.50 \times 10^{-2}$ | $2.91 \times 10^{-2}$ |



Fig. 5. The convergence of (a) $\eta$, (b) $e$ and (c) G for Example 3 with $r=0.5$ and $\varepsilon=0.5$ noise.
(a)

(b)


FIG. 6. The numerical solutions for Example 3 with $r=0.5$ and $\varepsilon=0.5$ noise: (a) discrepancy principle versus optimal choice and (b) TPA versus hybrid algorithm.


FIG. 7. The convergence of (a) $\eta$, (b) $e$, and (c) G for Example 4 with $\delta^{2}=1.25 \times 10^{-1}$.


FIg. 8. The numerical solutions for Example 4 with $\delta^{2}=1.25 \times 10^{-1}$.

The TPA and the secant method both converge very steadily and rapidly, but the local convergence of the TPA is far slower; cf. Fig. 7. Nonetheless, three to four iterations of the TPA already agree well with the exact solution. The parameter $\eta_{\mathrm{dp}}$ is $1.41 \times 10^{-2}$, and it is well approximated by eight iterations of either algorithm ( $\eta_{\mathrm{tpa}}=1.44 \times 10^{-2}, \eta_{\mathrm{sm}}=1.41 \times 10^{-2}$ ). It is smaller than the optimal choice, i.e., $3.03 \times 10^{-2}$. Visually, all four solutions are reasonable and fairly close to each other; cf. Fig. 8. This is also indicated by the errors, i.e., $e_{\text {opt }}=4.46 \times 10^{-1}, e_{\text {dp }}=5.05 \times 10^{-1}, e_{\text {tpa }}=5.03 \times 10^{-1}$ and $e_{\mathrm{sm}}=5.05 \times 10^{-1}$. This again shows the feasibility of the principle and the efficiency of the algorithms.

## 5. Concluding remarks

We have studied several numerical aspects of the discrepancy principle. The uniqueness of the solution to the discrepancy equation was shown. This was achieved by deriving an explicit characterization of the solution sets. Two numerical algorithms for its efficient realization were proposed, and their convergence properties were also briefly discussed. The TPA was based on the idea of Padé approximation, generalizing the idea of model functions. The hybrid algorithm drastically enhances its local convergence by the secant method. Numerical results show that the algorithms achieve a fast and steady convergence, and the principle achieves almost optimal convergence rates. Theoretically, it is of much interest to further investigate the convergence of the algorithms in the case of inexact minimization the functional $J_{\eta}$, as often occurs in practical scenarios.

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