

Heuristic parameter-choice rules for convex variational regularization based on error estimates

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Abstract

In this paper, we are interested in heuristic parameter choice rules for general convex variational regularization which are based on error estimates. Two such rules are derived and generalize those from quadratic regularization, namely the Hanke-Raus rule and quasi-optimality criterion. A posteriori error estimates are shown for the Hanke-Raus rule, and convergence for both rules is also discussed. Numerical results for both rules are presented to illustrate their applicability.

1 Introduction

We consider the ill-posed problem of determining a solution x to

$$Kx = y^\delta, \quad (1)$$

when only a noisy version y^δ of the exact data y^\dagger is available, which furthermore satisfies an inequality $\|y^\delta - y^\dagger\| \leq \delta$. In our setting $K : X \rightarrow Y$ is a bounded and linear operator mapping from a Banach space X into a Hilbert space Y .

As usual for inverse problems, the numerical solution of problem (1) suffers from ill-posedness. In particular, a small change in the data y^δ can lead to an enormous deviation of the solution x . To combat the inherent instability, regularization has been established as an effective approach since the pioneering work of Tikhonov [35]. The regularization method under consideration is general convex Tikhonov regularization, i.e., for a convex and (weak) lower semi-continuous functional $R : X \rightarrow [0, \infty]$, we seek a minimizer, denoted by x_α^δ , of the functional

$$\mathcal{J}_\alpha(x) = \frac{1}{2} \|Kx - y^\delta\|^2 + \alpha R(x), \quad (2)$$

and takes the minimizer x_α^δ as an approximate solution to the unknown exact solution x^\dagger . Here R is the regularization functional incorporating *a priori*

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information, and α is known as the regularization parameter, determining the tradeoff between the data fitting term and the regularization term.

Tikhonov regularization formulations of this form have attracted considerable interest in recent years, and have found applications in diverse disciplines, e.g., imaging science [33, 12] and signal processing [15, 10]. Because of their immense practical importance, the functional \mathcal{J}_α has been the subject of many recent investigations. Theoretically speaking, since the pioneering work [8], convergence and convergence rates under a variety of conditions have been established [32, 25, 30, 20]. Numerically, several efficient algorithms have also been proposed [11, 21, 38].

But one of the most important questions in applying these techniques to practical problems, i.e., choosing an appropriate regularization parameter α , remains largely underexplored. While the problem of parameter choice has been discussed in depth for the conventional quadratic regularization, see e.g., [18] for theoretical studies and [23, 37] for details on numerical implementation, the case of general convex regularization has scarcely been addressed. As to existing studies on parameter selection for Tikhonov regularization in Banach space, we are aware of Morozov's discrepancy principle [31], which was recently investigated [3, 28]. Some theoretical results, e.g., convergence and convergence rates, were derived. In the latter work, an algorithm for solving the discrepancy equation was also proposed. However, the discrepancy principle requires an estimate of the noise level, which is not always available. Therefore, there is a significant interest in deriving heuristic choice rules which do not require a knowledge of the exact noise level and still allow some theoretical justification. One such rule is due to the authors [26], where existence of a solution and a posteriori error estimates are derived. Another is the balancing principle, recently derived using the model function approach in [13], for a model with L^1 data fitting and quadratic regularization.

In the present study, we shall derive two heuristic choice rules based on error estimates, which are achieved by a refined analysis of regularization process. Error estimate-based heuristic choice rules are well-known for the conventional quadratic regularization [18], but to the best of the authors' knowledge, there is no known rule of this type for general convex variational regularization. The derived rules generalize Hanke-Raus rule and quasi-optimality criterion for quadratic regularization to general convex regularization. Some theoretical justifications, e.g., existence, a posteriori error estimate and convergence, of both rules are provided. Numerical results are presented to validate some theoretical findings and to illustrate the features of both rules.

Notation: The linear operator $K : X \rightarrow Y$ from a Banach space X into a Hilbert space Y is assumed to be bounded; $K^* : Y \rightarrow X^*$ denotes its adjoint operator. We assume that the exact data y^\dagger is attainable, i.e., $y^\dagger \in \text{range } K$, and the noisy data y^δ satisfies $\|y^\dagger - y^\delta\| \leq \delta$. The functional $R : X \rightarrow [0, \infty]$ is assumed to be proper, convex, weakly lower semicontinuous and coercive. This conditions ensure that the functional \mathcal{J}_α defined in (2) possess minimizers (cf. [25]). We shall denote by x_α^δ a minimizer to the functional \mathcal{J}_α , and by x_α a corresponding minimizer for exact data y^\dagger , i.e.,

$$x_\alpha \in \operatorname{argmin} \left\{ \frac{1}{2} \|Kx - y^\dagger\|^2 + \alpha R(x) \right\}.$$

By x^\dagger we denote a minimum- R solution of the equation $Kx = y^\dagger$ (see e.g. [25]). With $\partial R(x)$ we denote the subdifferential of a convex functional R at x [17]. Throughout the paper we assume that the exact solution x^\dagger fulfills the following source condition (see [8]):

$$\exists w : K^*w \in \partial R(x^\dagger). \quad (3)$$

For any $\xi \in \partial R(x)$, we denote the Bregman distance from x to x' with respect to ξ with

$$D_\xi(x', x) = R(x') - R(x) - \langle \xi, x' - x \rangle.$$

We note that the Bregman distance $D_\xi(x', x)$ is always nonnegative, although in general it can vanish for distinct x' and x . Bregman distance provides a natural measure of various errors, and for a detailed discussion, we refer to [9].

2 Estimates for different errors

In the case of regularization in Hilbert spaces, one usually splits the total error, i.e., the distance from x_α^δ to x^\dagger , into the *approximation error* and the *data error*, which refer to the distance from x_α to x^\dagger and that from x_α^δ to x_α , respectively, cf. [18]. This is achieved with the help of a triangle inequality. Then the approximation error and the data error are estimated separately to get an estimate for the total error. Theoretically, the behavior of the approximation error contains information about how difficult it is to approximate the unknown solution x^\dagger and provides hints on what conditions on x^\dagger may be helpful. The behavior of the data error shows how noise influences the accuracy of the reconstruction.

In the case of convex variational regularization one usually estimates the total error directly. One reason is that in this setting the natural distance measure for the errors is the Bregman distance which does not fulfill the triangle inequality. In this section we provide estimates for different terms. This sheds insights in the regularization process and thereby shows that a splitting into approximation and data error is still useful.

Proposition 2.1. *Let x^\dagger fulfill the source condition (3) with $\xi = K^*w$. Then the approximation error and the corresponding discrepancy satisfy*

$$D_\xi(x_\alpha, x^\dagger) \leq \frac{\|w\|^2}{2}\alpha, \quad (4)$$

$$\|Kx_\alpha - y^\dagger\| \leq 2\|w\|\alpha. \quad (5)$$

With the choice $\xi_\alpha = -K^(Kx_\alpha - y^\dagger)/\alpha$, the data error and the corresponding discrepancy satisfy*

$$D_{\xi_\alpha}(x_\alpha^\delta, x_\alpha) \leq \frac{\delta^2}{2\alpha}, \quad (6)$$

$$\|K(x_\alpha^\delta - x_\alpha)\| \leq 2\delta. \quad (7)$$

Proof. Inequalities (4) and (5) have been shown in [8], however, we include a short proof for the sake of completeness. By the minimizing property of x_α and the fact $Kx^\dagger = y^\dagger$ we have

$$\frac{1}{2}\|Kx_\alpha - y^\dagger\|^2 + \alpha R(x_\alpha) \leq \alpha R(x^\dagger).$$

Rearranging the terms and noting $\xi \in \partial R(x^\dagger)$ yields

$$\frac{1}{2}\|Kx_\alpha - y^\dagger\|^2 + \alpha D_\xi(x_\alpha, x^\dagger) \leq -\alpha \langle \xi, x_\alpha - x^\dagger \rangle. \quad (8)$$

By observing the non-negativity of the Bregman distance $D_\xi(x_\alpha, x^\dagger)$ and using $\xi = K^*w$ and Cauchy-Schwarz inequality, we obtain

$$\frac{1}{2}\|Kx_\alpha - y^\dagger\|^2 \leq \alpha \|w\| \|Kx_\alpha - y^\dagger\|$$

which shows estimate (5).

Appealing again to inequality (8) and using $\xi = K^*w$, Cauchy-Schwarz and Young's inequalities, we arrive at

$$\frac{1}{2}\|Kx_\alpha - y^\dagger\|^2 + \alpha D_\xi(x_\alpha, x^\dagger) \leq \frac{\alpha^2 \|w\|^2}{2} + \frac{1}{2}\|Kx_\alpha - y^\dagger\|^2.$$

This establishes estimate (4).

Next we use the minimizing property of x_α^δ to get

$$\frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 + \alpha D_{\xi_\alpha}(x_\alpha^\delta, x_\alpha) \leq \frac{1}{2}\|Kx_\alpha - y^\delta\|^2 - \alpha \langle \xi_\alpha, x_\alpha^\delta - x_\alpha \rangle.$$

From the optimality of x_α , we have $\xi_\alpha = -K^*(Kx_\alpha - y^\dagger)/\alpha \in \partial R(x_\alpha)$. Plugging in ξ_α and rearranging the formula gives

$$\begin{aligned} \frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 + \alpha D_{\xi_\alpha}(x_\alpha^\delta, x_\alpha) &\leq \frac{1}{2}\|Kx_\alpha - y^\delta\|^2 + \langle Kx_\alpha - y^\dagger, K(x_\alpha^\delta - x_\alpha) \rangle \\ &= \frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 - \frac{1}{2}\|K(x_\alpha^\delta - x_\alpha)\|^2 \\ &\quad - \langle y^\dagger - y^\delta, K(x_\alpha^\delta - x_\alpha) \rangle, \end{aligned}$$

i.e.,

$$\frac{1}{2}\|K(x_\alpha^\delta - x_\alpha)\|^2 + \alpha D_\xi(x_\alpha^\delta, x_\alpha) \leq -\langle y^\dagger - y^\delta, K(x_\alpha^\delta - x_\alpha) \rangle. \quad (9)$$

Now the non-negativity of the Bregman distance and Cauchy-Schwarz inequality yields estimate (7). Next by virtue of inequality (9) and Cauchy-Schwarz and Young's inequalities, we obtain

$$\frac{1}{2}\|K(x_\alpha^\delta - x_\alpha)\|^2 + \alpha D_\xi(x_\alpha^\delta, x_\alpha) \leq \delta \|K(x_\alpha^\delta - x_\alpha)\| \leq \frac{\delta^2}{2} + \frac{1}{2}\|K(x_\alpha^\delta - x_\alpha)\|^2$$

which concludes the proof. \square

From [8] we cite the following result.

Proposition 2.2 (Estimate for the total error). *If the source condition (3) holds with $\xi = K^*w \in \partial R(x^\dagger)$, then we have*

$$D_\xi(x_\alpha^\delta, x^\dagger) \leq \frac{1}{2} \left(\frac{\delta}{\sqrt{\alpha}} + \sqrt{\alpha} \|w\| \right)^2, \quad (10)$$

$$\|Kx_\alpha^\delta - y^\delta\| \leq \delta + 2\alpha \|w\|. \quad (11)$$

Although the Bregman distance does in general not fulfill the triangle inequality we see that the total error $D(x_\alpha^\delta, x^\dagger)$ behaves like the sum of the approximation error $D(x_\alpha, x^\dagger)$ and the data error $D(x_\alpha^\delta, x_\alpha)$. Indeed there holds for $a, b \geq 0$ that $(a+b)^2/2 \leq a^2 + b^2 \leq (a+b)^2$ and hence, we see that the estimate (10) behaves like the sum of the estimates (4) and (6).

The connection between the total error in the Bregman distance and the approximation and data errors can be made a bit more precise. To this end, we utilize the following lemma which is an immediate consequence of the definition of the Bregman distance:

Lemma 2.3. *Let $\xi \in \partial R(x^\dagger)$ and $\zeta \in \partial R(x)$. Then there holds for any x' that*

$$D_\xi(x', x^\dagger) = D_\zeta(x', x) + D_\xi(x, x^\dagger) + \langle \xi - \zeta, x - x' \rangle.$$

The next result is a consequence of Lemma 2.3, and will be used frequently.

Corollary 2.4. *Let the source condition (3) be fulfilled. Then with the obvious choices of the respective subgradients, there holds*

$$\left| D(x_\alpha^\delta, x^\dagger) - (D(x_\alpha^\delta, x_\alpha) + D(x_\alpha, x^\dagger)) \right| \leq 6\|w\|\delta.$$

Proof. Taking $x = x_\alpha$, $x' = x_\alpha^\delta$, $\xi = K^*w$ and $\xi_\alpha = -K^*(Kx_\alpha - y^\dagger)/\alpha$ in Lemma 2.3 gives

$$D(x_\alpha^\delta, x^\dagger) = D(x_\alpha^\delta, x_\alpha) + D(x_\alpha, x^\dagger) + \langle w + (Kx_\alpha - y^\dagger)/\alpha, K(x_\alpha - x_\alpha^\delta) \rangle,$$

which together with inequalities (5) and (7) gives

$$\begin{aligned} |\langle w + (Kx_\alpha - y^\dagger)/\alpha, K(x_\alpha - x_\alpha^\delta) \rangle| &\leq (\|w\| + \|Kx_\alpha - y^\dagger\|/\alpha) \|K(x_\alpha^\delta - x_\alpha)\| \\ &\leq 6\|w\|\delta. \end{aligned}$$

This concludes the proof. \square

Hence, the total error differs from the sum of approximation and data errors only by a term of magnitude δ . In general, the difference can be either positive or negative and both cases are observed in numerical experiments.

We shall need the following result on the function $\alpha \mapsto \|Kx_\alpha^\delta - y^\delta\|$.

Lemma 2.5. *The function $\alpha \mapsto \|Kx_\alpha^\delta - y^\delta\|$ is monotonically increasing and uniformly bounded. Moreover, if \mathcal{J}_α has a unique minimizer, then it is also continuous at α .*

Proof. Let \tilde{x} be an R -minimizing element in X . By the minimizing property of x_α^δ , we have

$$\frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 + \alpha R(x_\alpha^\delta) \leq \frac{1}{2}\|K\tilde{x} - y^\delta\|^2 + \alpha R(\tilde{x}),$$

and thus $0 \leq \|Kx_\alpha^\delta - y^\delta\| \leq \|K\tilde{x} - y^\delta\| < +\infty$, and is uniformly bounded. The proof of the remaining assertion can be found in [3, 28]. \square

The last result in this section gives an estimate for the distance between two regularized solutions for the same data but different regularization parameters. This estimate underlies the quasi-optimality principle in Section 4.

Proposition 2.6. *For $q \in]0, 1[$ and $\xi_\alpha^\delta = -K^*(Kx_\alpha^\delta - y^\delta)/\alpha$ there holds*

$$D_{\xi_\alpha^\delta}(x_{q\alpha}^\delta, x_\alpha^\delta) \leq \frac{(1-q)^2 \|Kx_\alpha^\delta - y^\delta\|^2}{2\alpha q}. \quad (12)$$

Moreover, if the source condition (3) is fulfilled, then

$$\|K(x_{q\alpha}^\delta - x_\alpha^\delta)\| \leq 2(1-q)(\delta + 2\alpha\|w\|). \quad (13)$$

Proof. The minimizing property of $x_{q\alpha}^\delta$ implies

$$\frac{1}{2}\|Kx_{q\alpha}^\delta - y^\delta\|^2 + q\alpha R(x_{q\alpha}^\delta) \leq \frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 + q\alpha R(x_\alpha^\delta).$$

Rearranging the terms gives

$$\frac{1}{2}\|Kx_{q\alpha}^\delta - y^\delta\|^2 + q\alpha D_{\xi_\alpha^\delta}(x_{q\alpha}^\delta, x_\alpha^\delta) \leq \frac{1}{2}\|Kx_\alpha^\delta - y^\delta\|^2 + q\langle Kx_\alpha^\delta - y^\delta, K(x_{q\alpha}^\delta - x_\alpha^\delta) \rangle,$$

which leads to

$$q\alpha D_{\xi_\alpha^\delta}(x_{q\alpha}^\delta, x_\alpha^\delta) \leq -(1-q)\langle Kx_\alpha^\delta - y^\delta, K(x_{q\alpha}^\delta - x_\alpha^\delta) \rangle - \frac{1}{2}\|K(x_{q\alpha}^\delta - x_\alpha^\delta)\|^2.$$

Appealing again to Cauchy-Schwarz and Young's inequalities gives (12). Using Cauchy-Schwarz inequality in

$$\frac{1}{2}\|K(x_{q\alpha}^\delta - x_\alpha^\delta)\|^2 \leq -(1-q)\langle Kx_\alpha^\delta - y^\delta, K(x_{q\alpha}^\delta - x_\alpha^\delta) \rangle,$$

and noting estimate (11) shows the remaining assertion. \square

3 A parameter choice á la Hanke-Raus

In this section, we investigate a first heuristic parameter choice rule based on error estimate, which resembles a rule due to Hanke and Raus [22]. Although it is known that heuristic rules can never lead to regularization methods in the context of the classical worst-case scenario unless the problem is well-posed [1], they have proven applicable and useful in practice [23]. Recent results [29] show that weak assumptions on the true data y^\dagger as well as the noisy data y^δ , hence leaving the worst-case scenario analysis, lead to provable error estimates. We shall establish a posteriori error estimates as well as convergence for the rule.

3.1 Motivation

We see from Proposition 2.2 that the estimate for the total error differs from that for the squared residual by a factor of $1/\alpha$:

$$\begin{aligned} \frac{\|Kx_\alpha^\delta - y^\delta\|^2}{\alpha} &\leq \frac{(\delta + 2\alpha\|w\|)^2}{\alpha} = \left(\frac{\delta}{\sqrt{\alpha}} + 2\sqrt{\alpha}\|w\|\right)^2 \\ &\approx \frac{1}{2}\left(\frac{\delta}{\sqrt{\alpha}} + \sqrt{\alpha}\|w\|\right)^2 \geq D(x_\alpha^\delta, x^\dagger). \end{aligned}$$

Since the value $\|Kx_\alpha^\delta - y^\delta\|^2/\alpha$ can be evaluated a posteriori without resorting to any knowledge of the exact noise level δ , we propose to use it as an estimate of the total error and to choose an appropriate regularization parameter α by minimizing the function

$$\phi(\alpha) = \frac{\|Kx_\alpha^\delta - y^\delta\|^2}{\alpha}. \quad (14)$$

This resembles the parameter choice due to Hanke and Raus [22] for classical Tikhonov regularization as well as several iterative regularization methods.

In view of Lemma 2.5 we see that $\lim_{\alpha \rightarrow +\infty} \phi(\alpha) = 0$. Similarly, in case of a unique minimizer to the functional \mathcal{J}_α for any $\alpha > 0$, the optimization problem of minimizing ϕ over any bounded and closed interval of the positive semi-axis \mathbf{R}_+ is well-defined.

3.2 A posteriori error estimates

In this part, we derive a posteriori error estimates for the Hanke-Raus rule to offer partial theoretical justification. We shall treat two cases of uniformly convex R and the particular case $R(x) = \|x\|_{\ell^1}$ separately.

Theorem 3.1. *Let the source condition (3) be fulfilled. Let ϕ be defined by (14) and α^* defined as*

$$\alpha^* \in \underset{\alpha \in [0, \|K\|^2]}{\operatorname{argmin}} \phi(\alpha). \quad (15)$$

If furthermore $\delta^* := \|Kx_{\alpha^*}^\delta - y^\delta\| \neq 0$ then there exists a constant $C > 0$ such that

$$D(x_{\alpha^*}^\delta, x^\dagger) \leq C \left(1 + \left(\frac{\delta}{\delta^*}\right)^2\right) \max(\delta, \delta^*).$$

Proof. We have from Corollary 2.4

$$D(x_\alpha^\delta, x^\dagger) \leq D(x_\alpha, x^\dagger) + D(x_\alpha^\delta, x_\alpha) + 6\|w\|\delta.$$

It suffices to estimate the two Bregman distance terms. First we estimate the approximation error $D(x_{\alpha^*}, x^\dagger)$ for $\alpha = \alpha^*$. By inequalities (13) and (11), we obtain

$$\begin{aligned} D(x_{\alpha^*}, x^\dagger) &\leq \|w\| \|Kx_{\alpha^*} - y^\dagger\| \\ &\leq \|w\| (\|K(x_{\alpha^*} - x_{\alpha^*}^\delta)\| + \|Kx_{\alpha^*}^\delta - y^\delta\| + \delta) \\ &\leq \|w\| (2\delta + \delta^* + \delta) \leq 4\|w\| \max(\delta, \delta^*). \end{aligned}$$

Next we estimate the data error $D(x_{\alpha^*}^\delta, x_{\alpha^*})$. Using inequality (6), we get

$$D(x_{\alpha^*}^\delta, x_{\alpha^*}) \leq \frac{\delta^2}{2\alpha^*} = \left(\frac{\delta}{\delta^*}\right)^2 \frac{\|Kx_{\alpha^*}^\delta - y^\delta\|^2}{2\alpha^*}. \quad (16)$$

By the definition of α^* , we only increase the right hand side if we replace α^* by any other $\bar{\alpha} \in [0, \|K\|^2]$. We use $\bar{\alpha} = \bar{c}\delta$ with $\bar{c} = \min(1, \delta^{-1})\|K\|^2$ and deduce from inequality (11) that

$$\|Kx_{\bar{\alpha}}^\delta - y^\delta\| \leq (1 + 2\bar{c}\|w\|)\delta.$$

Replacing α^* by $\bar{\alpha}$ in inequality (16), we have

$$D(x_{\alpha^*}^\delta, x_{\alpha^*}) \leq \left(\frac{\delta}{\delta^*}\right)^2 \frac{\|Kx_{\bar{\alpha}}^\delta - y^\delta\|^2}{2\bar{\alpha}} \leq \left(\frac{\delta}{\delta^*}\right)^2 \frac{(1 + 2\bar{c}\|w\|)^2 \delta}{2\bar{c}}.$$

By combining the above two estimates, we finally arrive at

$$\begin{aligned} D(x_{\alpha^*}^\delta, x^\dagger) &\leq 4\|w\| \max(\delta, \delta^*) + \left(\frac{\delta}{\delta^*}\right)^2 \frac{(1 + 2\bar{c}\|w\|)^2}{2\bar{c}} \delta + 6\|w\|\delta \\ &\leq C \left(1 + \left(\frac{\delta}{\delta^*}\right)^2\right) \max(\delta, \delta^*) \end{aligned}$$

with $C = \max(10\|w\|, (1 + 2\bar{c}\|w\|)^2/(2\bar{c}))$ as desired. \square

The preceding result estimates the error in terms of the Bregman distance. In the case of p -convex regularization terms R (see e.g., [4]), this also provides error estimates in norm, i.e., $\|x_{\alpha^*}^\delta - x^\dagger\|$. However, the interesting case of ℓ^1

regularization, i.e., $X = \ell^2$ and $R(x) = \|x\|_{\ell^1} = \sum_k |x_k|$ is not covered. In this case the Bregman distance is not even positive definite, i.e., $D(x', x)$ may vanish for distinct x' and x . However, by using techniques from [30, 20], we are still able to prove an analogous error estimate for this case. To this end, we recall the following result [20].

Lemma 3.2. *Let $X = \ell^2$ and $R(x) = \sum_k |x_k|$. Assume that the solution x^\dagger is finitely supported and satisfies the source condition (3). Moreover, assume that the operator K satisfies the finite basis injectivity property, that is, for any finitely support u and v , there holds that $Ku = Kv$ implies $u = v$. Then there exist two positive constants c_1 and c_2 such that*

$$\|x - x^\dagger\|_{\ell^1} \leq c_1[R(x) - R(x^\dagger)] + c_2\|K(x - x^\dagger)\|.$$

We are now ready to transfer Theorem 3.1 to the case $R(x) = \|x\|_{\ell^1}$.

Theorem 3.3. *Assume that the conditions in Lemma 3.2 are satisfied. Let α^* be chose according to (16). If furthermore $\delta^* := \|Kx_{\alpha^*}^\delta - y^\delta\| \neq 0$ then there exists a constant $C > 0$ such that*

$$\|x^\dagger - x_{\alpha^*}^\delta\|_{\ell^1} \leq C(1 + (\frac{\delta}{\delta^*})^2)\max(\delta^*, \delta).$$

Proof. By Lemma 3.2, the definition of Bregman distance $D(x, x^\dagger)$ and the source condition (3), we have

$$\begin{aligned} \|x - x^\dagger\|_{\ell^1} &\leq c_1[R(x) - R(x^\dagger)] + c_2\|K(x - x^\dagger)\| \\ &= c_1D(x, x^\dagger) + c_1\langle \xi, x - x^\dagger \rangle + c_2\|K(x - x^\dagger)\| \\ &= c_1D(x, x^\dagger) + c_1\langle w, K(x - x^\dagger) \rangle + c_2\|K(x - x^\dagger)\| \\ &\leq c_1D(x, x^\dagger) + (c_1\|w\| + c_2)\|K(x - x^\dagger)\| \end{aligned}$$

by Cauchy-Schwarz inequality. Now by virtue of Corollary 2.4 we have

$$\|x_{\alpha^*}^\delta - x^\dagger\|_{\ell^1} \leq c_1(D(x_{\alpha^*}^\delta, x_{\alpha^*}^\delta) + D(x_{\alpha^*}^\delta, x^\dagger) + 6\|w\|\delta) + (c_1\|w\| + c_2)\|K(x_{\alpha^*}^\delta - x^\dagger)\|.$$

Next we bound each term on the right hand side. First observe

$$\begin{aligned} \|K(x_{\alpha^*}^\delta - x^\dagger)\| &\leq \|Kx_{\alpha^*}^\delta - y^\delta\| + \|y^\delta - Kx^\dagger\| \\ &\leq \delta^* + \delta \leq 2\max(\delta, \delta^*). \end{aligned}$$

Then, for the approximation error $D(x_{\alpha^*}^\delta, x^\dagger)$, we obtain as before

$$\begin{aligned} D(x_{\alpha^*}^\delta, x^\dagger) &\leq \|w\|\|Kx_{\alpha^*}^\delta - y^\delta\| \\ &\leq \|w\|(\|K(x_{\alpha^*}^\delta - x_{\alpha^*}^\delta)\| + \|Kx_{\alpha^*}^\delta - y^\delta\| + \delta) \\ &\leq \|w\|(2\delta + \delta^* + \delta) \leq 4\|w\|\max(\delta, \delta^*). \end{aligned}$$

Finally, for the data error $D(x_{\alpha^*}^\delta, x_{\alpha^*}^\delta)$, we obtain from inequality (6) and the definition of α^*

$$D(x_{\alpha^*}^\delta, x_{\alpha^*}^\delta) \leq \frac{\delta^2}{2\alpha^*} = \left(\frac{\delta}{\delta^*}\right)^2 \frac{\|Kx_{\alpha^*}^\delta - y^\delta\|^2}{2\alpha^*}. \quad (17)$$

By the minimizing property of α^* , replacing α^* by any other $\bar{\alpha} \in [0, \|K\|^2]$ only increases the right hand side. Setting $\bar{\alpha} = c_3\delta \in [0, \|K\|^2]$, then $\|Kx_{\bar{\alpha}}^\delta - y^\delta\|^2 \leq c_4\delta$ (cf. [20]), which consequently gives

$$D(x_{\alpha^*}^\delta, x_{\alpha^*}) \leq \left(\frac{\delta}{\delta^*}\right)^2 \frac{c_4^2}{2c_3} \delta \leq \frac{c_4^2}{2c_3} \left(\frac{\delta}{\delta^*}\right)^2 \max(\delta, \delta^*).$$

Combining these three estimates we arrive at the desired inequality with $C = \max(12c_1\|w\| + 2c_2, \frac{c_1c_4^2}{2c_3})$. \square

As long as the discrepancy δ^* is of order δ , Theorems 3.1 and 3.3 imply that the approximation $x_{\alpha^*}^\delta$ with α^* chosen by the rule (14) converges to the exact solution x^\dagger at the same rate as a priori parameter choice rules under identical source conditions [20]. On the other hand, if δ^* does not decrease as quickly as δ , then the convergence would be suboptimal. More dangerous is the case that δ^* decreases more quickly. Then the prefactor δ/δ^* blows up, and the approximation may diverge. Therefore, the value of δ^* should always be monitored as an a posteriori criterion: The computed approximation should be discarded if δ^* is deemed too small.

3.3 Convergence

By stipulating additional conditions on the data y^δ as in reference [22], however, we can get rid of the prefactor $\frac{\delta}{\delta^*}$ in the estimates and even obtain convergence of the method. To show this, we denote by Q the orthogonal projection onto the orthogonal complement of the closure of range K .

Corollary 3.4. *If for the noisy data y^δ , there exists some $\varepsilon > 0$ such that*

$$\|Q(y^\dagger - y^\delta)\| \geq \varepsilon\|y^\dagger - y^\delta\|,$$

then α^ according to (15) is positive. Moreover, under the conditions of Theorem 3.1, there holds*

$$D(x_{\alpha^*}^\delta, x^\dagger) \leq C \left(1 + \frac{1}{\varepsilon^2}\right) \max(\delta, \delta^*),$$

and under the conditions of Theorem 3.3, there holds

$$\|x_{\alpha^*}^\delta - x^\dagger\| \leq C \left(1 + \frac{1}{\varepsilon^2}\right) \max(\delta, \delta^*),$$

Proof. We observe

$$\|Kx_{\alpha^*}^\delta - y^\delta\| \geq \|Q(Kx_{\alpha^*}^\delta - y^\delta)\| = \|Qy^\delta\| = \|Q(y^\delta - y^\dagger)\| \geq \varepsilon\|y^\delta - y^\dagger\|. \quad (18)$$

This shows $\delta^* \geq \varepsilon\delta$ and especially that $\phi(\alpha) \rightarrow +\infty$ as $\alpha \rightarrow 0$. Consequently, there exists a positive α^* minimizing $\phi(\alpha)$ over $[0, \|K\|^2]$. The remaining assertion follows from the preceding estimate and the respective error estimate. \square

The next theorem shows the convergence of the rule under the condition that $\|Q(y^\dagger - y^\delta)\| \geq \varepsilon\|y^\dagger - y^\delta\|$ holds uniformly for the data y^δ as δ tends to zero.

Theorem 3.5. *Assume that the functional \mathcal{J}_α is coercive and has a unique minimizer. Furthermore, in the situation of Theorem 3.1 let the assumption of Corollary 3.4 be fulfilled uniformly, i.e., there exists an $\epsilon > 0$ such that for every $\delta > 0$, the following inequality holds*

$$\|Q(y^\dagger - y^\delta)\| \geq \epsilon \|y^\dagger - y^\delta\|. \quad (19)$$

Then there holds

$$D(x_{\alpha^*(y^\delta)}^\delta, x^\dagger) \rightarrow 0 \quad \text{for } \delta \rightarrow 0.$$

Proof. By the definition of α^* , we observe that the sequence $(\alpha^* \equiv \alpha^*(y^\delta))_{\delta \geq 0}$ is uniformly bounded and hence, there exists an accumulation point $\bar{\alpha}$. We distinguish the two cases $\bar{\alpha} = 0$ and $\bar{\alpha} > 0$.

We first consider the case $\bar{\alpha} = 0$. By Corollary 2.4, we split the error

$$D(x_{\alpha^*}^\delta, x^\dagger) \leq D(x_{\alpha^*}^\delta, x_{\alpha^*}) + D(x_{\alpha^*}, x^\dagger) + 6\|w\|\delta, \quad (20)$$

and estimate the data and approximation errors separately.

For the data error $D(x_{\alpha^*}^\delta, x_{\alpha^*})$, we deduce from inequality (18) and assumption (19) that

$$D(x_{\alpha^*}^\delta, x_{\alpha^*}) \leq \frac{\delta^2}{2\alpha^*} \leq \frac{\|Kx_{\alpha^*}^\delta - y^\delta\|^2}{2\epsilon^2\alpha^*} = \frac{\phi(\alpha^*)}{2\epsilon^2}.$$

Therefore, it suffices to show that $\phi(\alpha^*)$ goes to zero as $\delta \rightarrow 0$. By Proposition 2.2, there holds for every $\alpha \in [0, \|K\|^2]$ that

$$\phi(\alpha^*) \leq \phi(\alpha) \leq \left(\frac{\delta}{\sqrt{\alpha}} + 2\|w\|\sqrt{\alpha} \right)^2.$$

Hence, we may choose $\alpha(\delta)$ in the usual way such that $\alpha(\delta) \rightarrow 0$ and $\delta^2/\alpha(\delta) \rightarrow 0$ for $\delta \rightarrow 0$. This shows $\phi(\alpha^*) \rightarrow 0$ for $\delta \rightarrow 0$.

For the approximation error $D(x_{\alpha^*}, x^\dagger)$, we deduce from the fact that $\bar{\alpha} = 0$ and estimate (4) that

$$D(x_{\alpha^*}, x^\dagger) \leq \frac{\alpha^*\|w\|^2}{2} \rightarrow \frac{\bar{\alpha}\|w\|^2}{2} = 0 \quad \text{for } \delta \rightarrow 0.$$

Hence, all three terms on the right hand side of inequality (20) tend to zero for $\delta \rightarrow 0$ as desired.

Next we consider the remaining case $\bar{\alpha} > 0$. we use $\alpha^* \leq \|K\|^2$ to get

$$\phi(\alpha^*) \geq \frac{\|Kx_{\alpha^*}^\delta - y^\delta\|^2}{\|K\|^2} \geq 0.$$

Since $\phi(\alpha^*)$ goes to zero for $\delta \rightarrow 0$ we deduce that $\|Kx_{\alpha^*}^\delta - y^\delta\|$ tends to zero as well. Next by the minimizing property of $x_{\alpha^*}^\delta$, we have

$$\frac{1}{2}\|Kx_{\alpha^*}^\delta - y^\delta\|^2 + \alpha^*R(x_{\alpha^*}^\delta) \leq \frac{1}{2}\|Kx^\dagger - y^\delta\|^2 + \alpha^*R(x^\dagger).$$

Therefore, both sequences $(\|Kx_{\alpha^*}^\delta - y^\delta\|)_\delta$ and $(R(x_{\alpha^*}^\delta))_\delta$ are uniformly bounded by the assumption $\bar{\alpha} > 0$. By the coercivity of the functional \mathcal{J}_α , the sequence $(x_{\alpha^*}^\delta)_\delta$ is uniformly bounded, and thus there exists a subsequence, possibly

after relabeling as $(x_{\alpha^*}^\delta)_\delta$, that converges weakly to some \hat{x} . By the weak lower semicontinuity of the norm and the functional R , we have

$$\|K\hat{x} - y^\dagger\| \leq \liminf_{\delta \rightarrow 0} \|Kx_{\alpha^*}^\delta - y^\delta\| = 0, \quad R(\hat{x}) \leq \liminf_{\delta \rightarrow 0} R(x_{\alpha^*}^\delta). \quad (21)$$

Consequently, for any x

$$\begin{aligned} \frac{1}{2}\|K\hat{x} - y^\dagger\|^2 + \bar{\alpha}R(\hat{x}) &\leq \liminf_{\delta \rightarrow 0} \frac{1}{2}\|Kx_{\alpha^*}^\delta - y^\delta\|^2 + \liminf_{\delta \rightarrow 0} \alpha^*R(x_{\alpha^*}^\delta) \\ &\leq \liminf_{\delta \rightarrow 0} \left\{ \frac{1}{2}\|Kx_{\alpha^*}^\delta - y^\delta\|^2 + \alpha^*R(x_{\alpha^*}^\delta) \right\} \\ &\leq \liminf_{\delta \rightarrow 0} \left\{ \frac{1}{2}\|Kx - y^\delta\|^2 + \alpha^*R(x) \right\} \\ &= \frac{1}{2}\|Kx - y^\dagger\|^2 + \bar{\alpha}R(x). \end{aligned} \quad (22)$$

Hence \hat{x} is a minimizer of the functional $\mathcal{J}_{\bar{\alpha}}$, and by the uniqueness of the minimizer, $\hat{x} = x_{\bar{\alpha}}$. Since this holds for every subsequence, the whole sequence converges weakly. Moreover, by the weak lower semicontinuity, we have

$$R(x_{\alpha^*}^\delta) \rightarrow R(x_{\bar{\alpha}}). \quad (23)$$

Next we show that $x_{\bar{\alpha}}$ is an R -minimizing solution to the equation $Kx = y^\dagger$. However, this follows directly from inequality (21) that $\|Kx_{\bar{\alpha}} - y^\dagger\| = 0$, and from inequality (22)

$$R(x_{\bar{\alpha}}) \leq R(x) \quad \forall x,$$

which in particular by choosing x in the set of R -minimizing solutions shows the claim. Now we deduce that

$$\lim_{\delta \rightarrow 0} D(x_{\alpha^*}^\delta, x^\dagger) = \lim_{\delta \rightarrow 0} \left(R(x_{\alpha^*}^\delta) - R(x^\dagger) - \langle \xi, x_{\alpha^*}^\delta(y^\delta) - x^\dagger \rangle \right) = 0.$$

by observing identity (23) and the weak convergence of the sequence $(x_{\alpha^*}^\delta(y^\delta))_\delta$ to x^\dagger . This concludes the proof of the theorem. \square

Remark 3.6. *In Theorem 3.5, the uniqueness assumption on the functional \mathcal{J}_α can be relaxed as equation (23) holds for each weakly convergent subsequence. We have utilized the uniqueness of R -minimizing solution, which may also be dropped by restating the result as: then there exists some R -minimizing solution x^\dagger , such that*

$$D(x_{\alpha^*}^\delta, x^\dagger) \rightarrow 0 \quad \text{for } \delta \rightarrow 0.$$

In our context we are able to further weaken the assumption (19) on the noise.

Corollary 3.7. *If there exists an $\epsilon \in]0, 1[$ such that for all $z \in \overline{K(\text{dom } \partial R)}$ the following inequality holds*

$$\langle y^\delta - y^\dagger, z \rangle \leq (1 - \epsilon) \|y^\delta - y^\dagger\| \|z\|.$$

then the minimizer α^ to $\phi(\alpha)$ is positive. Moreover, under the conditions of Theorem 3.1, there holds*

$$D(x_{\alpha^*}^\delta, x^\dagger) \leq C \left(1 + \frac{1}{1 - (1 - \epsilon)^2} \right) \max(\delta, \delta^*),$$

and under the conditions of Theorem 3.3, there holds

$$\|x_{\alpha^*}^\delta - x^\dagger\| \leq C \left(1 + \frac{1}{1 - (1 - \epsilon)^2}\right) \max(\delta, \delta^*),$$

Proof. By observing the fact that both x_α^δ and x^\dagger are in $\text{dom } \partial R$ and the assumption on the noise $y^\dagger - y^\delta$, we derive

$$\begin{aligned} \|Kx_\alpha^\delta - y^\delta\|^2 &= \|K(x_\alpha^\delta - x^\dagger) - (y^\delta - y^\dagger)\|^2 \\ &= \|K(x_\alpha^\delta - x^\dagger)\|^2 - 2\langle K(x_\alpha^\delta - x^\dagger), y^\delta - y^\dagger \rangle + \|y^\delta - y^\dagger\|^2 \\ &\geq \|K(x_\alpha^\delta - x^\dagger)\|^2 - 2(1 - \epsilon)\|K(x_\alpha^\delta - x^\dagger)\|\|y^\delta - y^\dagger\| + \|y^\delta - y^\dagger\|^2 \\ &= (\|K(x_\alpha^\delta - x^\dagger)\| - (1 - \epsilon)\|y^\delta - y^\dagger\|)^2 + (1 - (1 - \epsilon)^2)\|y^\delta - y^\dagger\|^2 \\ &\geq (1 - (1 - \epsilon)^2)\delta^2. \end{aligned}$$

This in particular implies $(\delta^*)^2 \geq (1 - (1 - \epsilon)^2)\delta^2$ and consequently that $\phi(\alpha) \rightarrow +\infty$ as $\alpha \rightarrow 0$. Therefore, there exists a positive α^* minimizing $\phi(\alpha)$ over $[0, \|K\|^2]$. The remaining assertion follows similar to the proof of Theorem 3.5. \square

Remark 3.8 (Comparing the assumptions on the noise). *In Corollary 3.4 or Theorem 3.5 we assumed*

$$\exists \epsilon \in]0, 1[\forall \delta > 0 : \|Q(y^\dagger - y^\delta)\| \geq \epsilon \|y^\dagger - y^\delta\|$$

which is, with P denoting the orthogonal projector onto $\overline{\text{range } K}$, equivalent to

$$\exists \epsilon' >]0, 1[\forall \delta > 0 : \|P(y^\dagger - y^\delta)\| \leq \epsilon' \|y^\dagger - y^\delta\|. \quad (24)$$

In Corollary 3.7 we assumed

$$\exists \epsilon'' \in]0, 1[\forall \delta > 0 \forall z \in \overline{K(\text{dom } \partial R)} : \langle y^\delta - y^\dagger, z \rangle \leq \epsilon'' \|y^\delta - y^\dagger\| \|z\|. \quad (25)$$

In the case $\text{dom } \partial R = X$ we conclude from this assumption that (24) holds with $\epsilon' = \sqrt{1 - \epsilon''}$. Hence, in this case (25) implies (24). However, if $\text{dom } \partial R$ is strictly contained in X condition (25) may be considerably weaker.

4 The quasi-optimality principle

In this part, we derive another error-estimate based heuristic choice rule, i.e., the quasi-optimality principle, and discuss its convergence properties. The motivation of the principle is as follows: By Proposition 2.6 for any $q \in]0, 1[$, there holds

$$D(x_{q\alpha}^\delta, x_\alpha^\delta) \leq \frac{(1 - q)^2}{2q} \phi(\alpha).$$

In particular, for a geometrically decreasing sequence of regularization parameters, the Bregman distances of two consecutive regularized solutions are bounded from above by a constant times the estimator ϕ . This suggests itself a parameter choice rule which resembles the classical quasi-optimality criterion [35, 34]. More precisely, for given data y^δ and $q \in]0, 1[$ we define a *quasi-optimality sequence* as

$$\mu_k = D(x_{q^k}^\delta, x_{q^{k-1}}^\delta).$$

The quasi-optimality principle consists of choosing the regularization parameter $\alpha^{q_0} = q^k$ such that μ_k is minimal over a given range $k \geq k_0$.

Remark 4.1. *The classical quasi-optimality principle as e.g., stated in [35, 34], chooses α^{qo} such that the quantity $\|\alpha \frac{dx^\delta}{d\alpha}\|$ is minimal. In our setting this approach seems not applicable since the mapping $\alpha \mapsto x_\alpha^\delta$ is in general not differentiable. For instance, in the case of ℓ^1 regularization, the solution path, i.e., x_α^δ with respect to α , is piecewise linear [16]. Hence we resort to the discrete version which is also used in [2].*

We shall follow closely the lines of reference [19] and start with some basic observations of the quasi-optimality sequence. The quasi-optimality sequence for the exact data will be denoted by

$$\mu_k^\dagger = D(x_{q^k}, x_{q^{k-1}}).$$

Lemma 4.2. *Let the source condition (3) be satisfied. Then the quasi-optimality sequences $(\mu_k)_k$ and $(\mu_k^\dagger)_k$ fulfill*

1. $\lim_{k \rightarrow -\infty} \mu_k = 0$,
2. $\lim_{k \rightarrow -\infty} \mu_k^\dagger = 0$ and $\lim_{k \rightarrow \infty} \mu_k^\dagger = 0$.

Proof. Appealing to estimate (13), we have

$$\mu_k \leq \frac{(1-q)^2}{2q} \frac{\|Kx_{q^{k-1}}^\delta - y^\delta\|^2}{q^{k-1}}.$$

Since the sequence $\left(\|Kx_{q^{k-1}}^\delta - y^\delta\|\right)_k$ stays bounded for $k \rightarrow -\infty$, see Lemma 2.5, the first claim follows directly. Setting $\delta = 0$ in the above argumentation shows the first statement of Claim 2. Now we use inequality (5) and estimate

$$\mu_k^\dagger \leq \frac{(1-q)^2}{2} \frac{\|Kx_{q^{k-1}} - y^\dagger\|^2}{q^k} \leq 2(1-q)^2 \|w\|^2 q^{k-2}.$$

This shows the second statement of Claim 2. \square

Now we show that the quasi-optimality sequences for exact and noisy data approximate each other for vanishing noise level.

Lemma 4.3. *Let the source condition (3) be satisfied. Then for any $k_1 \in \mathbf{Z}$, there holds*

$$\lim_{\delta \rightarrow 0} \sup_{k \leq k_1} |\mu_k - \mu_k^\dagger| = 0.$$

Proof. We will use the abbreviations $x_k^\delta = x_{q^k}^\delta$, $x_k = x_{q^k}$, $\xi_k^\delta = -K^*(Kx_k^\delta - y^\delta)$ and $\xi_k = -K^*(Kx_k - y)$ to simplify the notation. By the definition of μ_k and μ_k^\dagger , we have

$$\begin{aligned} |\mu_k - \mu_k^\dagger| &= |D(x_k^\delta, x_{k-1}^\delta) - D(x_k, x_{k-1})| \\ &= |R(x_k^\delta) - R(x_{k-1}^\delta) - \langle \xi_{k-1}^\delta, x_k^\delta - x_{k-1}^\delta \rangle \\ &\quad - R(x_k) + R(x_{k-1}) + \langle \xi_{k-1}, x_k - x_{k-1} \rangle| \\ &= |D(x_k^\delta, x_k) - D(x_{k-1}^\delta, x_{k-1}) \\ &\quad + \langle \xi_{k-1} - \xi_{k-1}^\delta, x_k^\delta - x_{k-1}^\delta \rangle + \langle \xi_k - \xi_{k-1}, x_k^\delta - x_k \rangle|. \end{aligned}$$

Now we estimate all four terms separately. Using inequality (6) we can bound the first two terms by

$$D(x_k^\delta, x_k) \leq \frac{\delta^2}{2q^k}, \quad D(x_{k-1}^\delta, x_{k-1}) \leq \frac{\delta^2}{2q^{k-1}}.$$

For the third term, we get from estimates (7) and (13)

$$\begin{aligned} \langle \xi_{k-1} - \xi_{k-1}^\delta, x_k^\delta - x_{k-1}^\delta \rangle &= \langle K(x_{k-1} - x_{k-1}^\delta) + (y^\delta - y^\dagger), K(x_k^\delta - x_{k-1}^\delta) \rangle / q^{k-1} \\ &\leq (\|K(x_{k-1} - x_{k-1}^\delta)\| + \delta) \|K(x_k^\delta - x_{k-1}^\delta)\| / q^{k-1} \\ &\leq 6\delta(1-q)(\delta + 2q^k\|w\|) / q^{k-1}. \end{aligned}$$

Similarly, we can estimate the last term by

$$\langle \xi_k - \xi_{k-1}, x_k^\delta - x_k \rangle \leq 8\delta(1-q)\|w\|/q.$$

Hence, all four terms are bounded for $k \leq k_1$ and decrease to zero as $\delta \rightarrow 0$. This proves the claim. \square

In general, the quasi-optimality sequences $(\mu_k)_k$ and $(\mu_k^\dagger)_k$ can vanish for finite indices k . Fortunately, their positivity can be guaranteed for a class of functionals R .

Lemma 4.4. *Let the functional R be p -convex, $R(x) = 0$ only for $x = 0$ and satisfy that for any x the value $\langle \xi, x \rangle$ is independent of the choice of $\xi \in \partial R(x)$. If the data y^\dagger (resp. y^δ) admits nonzero α^* for which $x_{\alpha^*} \neq 0$, then $\mu_k^\dagger > 0$ (resp. $\mu_k > 0$) for all $k \geq \lceil \ln \alpha^* / \ln q \rceil$.*

Proof. By the optimality condition for x_α , we have

$$-K^*(Kx_\alpha - y^\dagger) \in \alpha \partial R(x_\alpha).$$

By assumption, the value $\langle \xi_\alpha, x_\alpha \rangle$ is independent of the choice of $\xi_\alpha \in \partial R(x_\alpha)$ and hence, taking duality pairing with x_α gives for any $\xi_\alpha \in \partial R(x_\alpha)$

$$\langle Kx_\alpha, Kx_\alpha - y^\dagger \rangle + \alpha \langle \xi_\alpha, x_\alpha \rangle = 0.$$

For non-zero x_α we have that $\langle \xi_\alpha, x_\alpha \rangle$ is non-zero and hence, we get

$$\alpha = \frac{\langle Kx_\alpha, Kx_\alpha - y^\dagger \rangle}{\langle \xi_\alpha, x_\alpha \rangle} \quad (26)$$

Next by the assumption that the data y^\dagger admits nonzero α^* for which $x_{\alpha^*} \neq 0$, then for any $\alpha < \alpha^*$, 0 cannot be a minimizer of the Tikhonov functional. To see this, we assume that 0 is a minimizer, i.e.,

$$\frac{1}{2}\|y^\dagger\|^2 = \frac{1}{2}\|K0 - y^\dagger\|^2 + \alpha R(0) < \frac{1}{2}\|Kx_{\alpha^*} - y^\dagger\|^2 + \alpha^* R(x_{\alpha^*}),$$

by the strict positivity of R for nonzero x . This contradicts the minimality of x_{α^*} . Now let $\alpha_1, \alpha_2 < \alpha^*$ be distinct. Then both sets $\{x_{\alpha_1}\}$ and $\{x_{\alpha_2}\}$ contain no zero element. Next we show that the two sets are disjoint. Assume that $\{x_{\alpha_1}\}$ and $\{x_{\alpha_2}\}$ intersects nontrivially, i.e., there exists some nonzero \tilde{x} such

that $\tilde{x} \in \{x_{\alpha_1}\} \cap \{x_{\alpha_2}\}$. Then by equation (26) and choosing any $\tilde{\xi} \in \partial R(\tilde{x})$, we have

$$\alpha_1 = \frac{\langle K\tilde{x}, K\tilde{x} - y^\dagger \rangle}{\langle \tilde{\xi}, \tilde{x} \rangle} = \alpha_2,$$

which is in contradiction with the distinctness of α_1 and α_2 . Therefore, for distinct $\alpha_1, \alpha_2 < \alpha^*$, the sets $\{x_{\alpha_1}\}$ and $\{x_{\alpha_2}\}$ are disjointed. Consequently, we have

$$\|x_{\alpha_1} - x_{\alpha_2}\| > 0.$$

Now by the p -convexity of R , we deduce for $q^k \leq \alpha^*$ that

$$\mu_k^\dagger = D(x_{q^k}, x_{q^{k-1}}) \geq C\|x_{q^k} - x_{q^{k-1}}\|^p > 0,$$

which shows the assertion for μ_k^\dagger . The claim for μ_k can be shown similarly. \square

Remark 4.5. *The assumptions on R in Lemma 4.4 are satisfied for many commonly used regularization functionals, e.g., $\|x\|_{\ell^p}$, $\|x\|_{L^p}$ with $p > 1$ and the elastic-net functional [27]. However, the special case of $\|x\|_{\ell^1}$ is not covered. Indeed, the ℓ^1 minimization can retrieve the support of the exact solution for sufficiently small noise level δ and α , see [36]. Consequently, both μ_k and μ_k^\dagger vanish for sufficiently large k , due to the lack of p -convexity. The bound α^* depends on $y(y^\delta)$, and for nonvanishing $y(y^\delta)$ can be either positive or $+\infty$, see [28] for some discussions. The choice of k_0 should be related to α^* such that μ_{k_0} ($\mu_{k_0}^\dagger$) is nonzero.*

By combining the above two lemmas, we have the following important corollary, which will play a key role in establishing the convergence result.

Corollary 4.6. *Under the conditions of Lemma 4.4, the parameter α^{qo} chosen by the quasi-optimality principle satisfies that for any sequence $\delta_n \rightarrow 0$ there holds that $\alpha^{\text{qo}} \rightarrow 0$.*

Proof. By definition it holds that $\alpha^{\text{qo}} = q^{k^*}$ where k^* is such that the sequence μ_k is minimal.

Observe that $\mu_k \leq \mu_k^\dagger + |\mu_k - \mu_k^\dagger|$. Now, let $\epsilon > 0$. Due to Lemma 4.2 there holds that $\mu_k^\dagger \rightarrow 0$ for $k \rightarrow \infty$ and hence, there exists an integer \underline{k} such that $\mu_{\underline{k}}^\dagger \leq \epsilon/2$. Moreover, due to Lemma 4.3, for any k_1 there is $\bar{\delta} > 0$ such that $|\mu_k - \mu_k^\dagger| \leq \epsilon/2$ for all $k \leq k_1$, in particular with \underline{k} . Hence $\mu_k \leq \mu_k^\dagger + |\mu_k^\dagger - \mu_k| < \epsilon$ for the same value of \underline{k} .

By Lemma 4.4, for any finite integer k_1 , the set $\{\mu_k^\dagger\}_{k=k_0}^{k_1}$ is finite and positive, and thus there exists a constant $\sigma > 0$ such that $\mu_k^\dagger > \sigma$ for $k = k_0, \dots, k_1$. Lemma 4.3 indicates that μ_k is larger than $\sigma/2$ for $k = k_0, \dots, k_1$ and sufficiently small δ . Thus the sequence $(\alpha^{\text{qo}})_{\delta_n}$ can contain terms on $\{q^k\}_{k=k_0}^{k_1}$ only if δ is not too small, since μ_k goes to zero as δ tends to zero. Since k_1 is chosen arbitrarily, this implies the desired assertion. \square

As remarked earlier, it is in general impossible to show the convergence of $x_\alpha^\delta \rightarrow x^\dagger$ for a heuristic parameter choice in the context of worst-case scenario analysis. For the quasi-optimality principle, Glasko et al [19] defined the notion of auto-regularizable set as a condition on the exact as well as noisy data. In

the case of the continuous quasi-optimality principle this is the set of y^δ such that

$$\frac{\|\alpha \frac{dx_\alpha^\delta}{d\alpha} - \alpha \frac{dx_\alpha}{d\alpha}\|}{\|x_\alpha^\delta - x_\alpha\|} \geq q > 0$$

holds uniformly in α and δ . This abstract condition on the exact data has been replaced by a condition on the noise in [2].

In our setting, the following sets are helpful for proving convergence.

Definition 4.7. For $r > 0$, $q \in]0, 1[$, $K : X \rightarrow Y$ and $y^\dagger \in \text{range } K$ we define the sets

$$\mathcal{D}_r = \{y^\delta \in Y \mid \forall k : |D(x_{q^k}^\delta, x_{q^{k-1}}^\delta) - D(x_{q^k}, x_{q^{k-1}})| \geq rD(x_{q^k}^\delta, x_{q^k})\}.$$

The condition $y^\delta \in \mathcal{D}_r$ can be regarded as a discrete analogue of the above-mentioned auto-regularizable condition. With the set \mathcal{D}_r at hand, we can now show another result on the asymptotic behavior of the quasi-optimality sequence. The condition is that the noisy data belongs to some set \mathcal{D}_r .

Lemma 4.8. Let $y^\delta \in \mathcal{D}_r$ for some $r > 0$ and assume that $R(x_\alpha^\delta) \rightarrow \infty$ for $\alpha \rightarrow 0$. Then $\mu_k \rightarrow \infty$ for $k \rightarrow \infty$.

Proof. We observe that

$$rD(x_{q^k}^\delta, x_{q^k}) \leq |D(x_{q^k}^\delta, x_{q^{k-1}}^\delta) - D(x_{q^k}, x_{q^{k-1}})| = |\mu_k - \mu_k^\dagger|. \quad (27)$$

By the definition of the Bregman distance, (5) and (7) we have for $\xi_\alpha = -K^*(Kx_\alpha - y^\dagger)/\alpha$ that

$$\begin{aligned} D_{\xi_\alpha}(x_\alpha^\delta, x_\alpha) &= R(x_\alpha^\delta) - R(x_\alpha) - \langle \xi_\alpha, x_\alpha^\delta - x_\alpha \rangle \\ &= R(x_\alpha^\delta) - R(x_\alpha) + \frac{1}{\alpha} \langle Kx_\alpha - y^\dagger, K(x_\alpha^\delta - x_\alpha) \rangle \\ &\geq R(x_\alpha^\delta) - R(x_\alpha) + 4\|w\|\delta. \end{aligned}$$

Since $R(x_\alpha)$ is bounded for $\alpha \rightarrow 0$ we see that by assumption that $D_{\xi_\alpha}(x_\alpha^\delta, x_\alpha) \rightarrow \infty$ for $\alpha \rightarrow 0$. This means that for $k \rightarrow \infty$ there holds that $D(x_{q^k}^\delta, x_{q^k}) \rightarrow \infty$ and since $\mu_k^\dagger \rightarrow 0$, the claim follows from (27). \square

Now we are in position to show the main result of this section, i.e., convergence for the quasi-optimality principle.

Theorem 4.9. Let $(\delta_n)_n$, $\delta_n > 0$, be a sequence converging to zero such that $y^{\delta_n} \rightarrow y^\dagger \in \text{range } K$ and $y^{\delta_n} \in \mathcal{D}_r$ for some $r > 0$. Let $(\alpha_n^{\text{qo}} = \alpha_n^{\text{qo}}(y^{\delta_n}))_n$ be the sequence of regularization parameters chosen by the quasi-optimality principle. Then

$$\lim_{n \rightarrow \infty} D(x_{\alpha_n^{\text{qo}}}^{\delta_n}, x^\dagger) = 0.$$

Proof. Denote α_n^{qo} by q^{k_n} . Then by using Corollary 2.4, we derive

$$\begin{aligned} D(x_{q^{k_n}}^{\delta_n}, x^\dagger) &\leq D(x_{q^{k_n}}^{\delta_n}, x_{q^{k_n}}) + D(x_{q^{k_n}}, x^\dagger) + 6\|w\|\delta_n \\ &\leq \frac{1}{r} |D(x_{q^{k_n}}^{\delta_n}, x_{q^{k_n-1}}^{\delta_n}) - D(x_{q^{k_n}}, x_{q^{k_n-1}})| + D(x_{q^{k_n}}, x^\dagger) + 6\|w\|\delta_n \\ &= \frac{1}{r} |\mu_{k_n} - \mu_{k_n}^\dagger| + D(x_{q^{k_n}}, x^\dagger) + 6\|w\|\delta_n. \end{aligned}$$

Now all three terms on the right hand side tend to zero for $n \rightarrow \infty$ (the first due to Lemma 4.3 and the second due to $q^{k_n} = \alpha_n^{\text{qo}} \rightarrow 0$ by Corollary 4.6). \square

This theorem shows that it is possible that the quasi-optimality principle leads to convergence in the setting of convex variational regularization. However, the important question on how the sets \mathcal{D}_r look like, and especially, under what circumstance they are non-empty, remains open. In [19, 2] the authors use spectral theory to investigate this issue – a tool which is unfortunately unavailable in our general setting.

5 Numerical experiments

We conducted several experiments to illustrate our theoretical findings.

5.1 Experiment 1: Accuracy of the estimates

In the first experiment we show sharpness of the estimates of the approximation, data and total errors. Especially we illustrate how the function ϕ from the Hanke-Raus rule approximates the total error.

The setting is as follows: We consider a deconvolution problem with sparsity constraints. In particular, the space X is a sequence space ℓ^2 and Y is the Hilbert space $L^2[0, 1]$. The operator under consideration is $K = AB : \ell^2 \rightarrow L^2[0, 1]$ where $A : L^2[0, 1] \rightarrow L^2[0, 1]$ is a circular convolution operator which convolves with a characteristic function of an interval of width 0.2 and $B : \ell^2 \rightarrow L^2[0, 1]$ is a Haar wavelet synthesis operator. Hence, the operator K takes a square summable sequence x , uses it as the expansion coefficients with respect to an orthonormal Haar wavelet basis and afterwards performs a circular convolution. The regularization function R is the $\|\cdot\|_{\ell^p}$ norm, i.e.,

$$R(x) = \sum_k |x_k|^p$$

which has, for $p > 1$, a single valued subgradient $\partial R(x) = \{p \operatorname{sign}(x)|x|^{p-1}\}$. In particular we have chosen $p = 1.2$ to promote sparsity of the minimizers (cf. [14]) and to get a p -convex functional simultaneously. To construct a solution x^\dagger fulfilling the source condition (3), we started with a function $w \in L^2[0, 1]$ and set $\xi = K^*w$. Then x^\dagger was defined as

$$x_k^\dagger = \operatorname{sign}(\xi_k)|\xi_k/p|^{1/(p-1)}.$$

We discretized the problem to 512 wavelet coefficients. Figure 1 shows the chosen $w \in L^2[0, 1]$, the function $Bx^\dagger \in L^2[0, 1]$ and the exact data $y^\dagger = ABx^\dagger \in L^2[0, 1]$. Both vectors ξ and x^\dagger consist of 165 non-zero coefficients, however, their plots are noninformative.

For a fixed noise level $\delta = 0.02$, we generated noisy data y^δ such that $\|y^\dagger - y^\delta\| = \delta$. Then we calculated minimizers x_α^δ and x_α of the Tikhonov functional with data y^δ and y^\dagger , respectively, for different values of α with the combined iterative hard- and soft-thresholding from [7] (see [5] for the iterative hard-thresholding algorithm and [14, 6] for the iterative soft-thresholding algorithm, the code is available at http://www-public.tu-bs.de:8080/~dirloren/progs/iter_thresh.m). We calculated the different errors and the function ϕ from the Hanke-Raus rule and show them in Figure 2. We observe that the function ϕ captures the behavior of the total error very well. Moreover, the sum of the

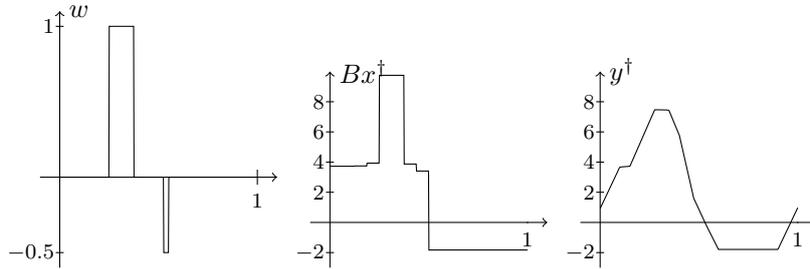


Figure 1: Experiment 1: Left: w from the source condition. Middle: Bx^\dagger . Right: y^\dagger .

approximation and data errors is close to the total error. Surprisingly, the estimate from Proposition 2.2 is even closer to the function ϕ than the total error itself—a result which is not backed up by theory by now.

Remark 5.1. *The obtained results have been observed to be robust with respect to different noise realizations and different w (if the obtained sparsity of the corresponding x^\dagger is comparable).*

5.2 Experiment 2: The Hanke-Raus rule

In this experiment we illustrate the performance of the Hanke-Raus rule. We use the same set up as in the first experiment, i.e., the same x^\dagger and K . For a range of δ we generated noisy data y^δ and calculated the regularization parameter α^{HR} with the Hanke-Raus rule of Section 3 in a brute-force manner: we tested values for α on a logarithmically uniform grid. As the exact solution x^\dagger is known in this case, we also calculated the optimal regularization parameter α^{opt} , i.e., the parameter α for which the error $D(x_\alpha^\delta, x^\dagger)$ is smallest, see Figure 3 for the results. It is observed that the Hanke-Raus parameter follows the optimal parameter closely in this example and accordingly the error of the Hanke-Raus rule is close to the optimal error.

5.3 Experiment 3: The quasi-optimality principle

This time the operator K , the data x^\dagger and the regularization function R is again similar to Experiments 1 and 2. Here we analyze how the quasi-optimality principle from Section 4 performs in practice. We chose $\alpha_0 = 100 \cdot \delta$ and $q = 0.8$. Then we calculated minimizers $x_{q^k \alpha_0}^\delta$ for several values of k and chose $\alpha^{q_0} = q^k \alpha_0$ as the one which minimized $D(x_{q^k \alpha_0}^\delta, x_{q^{k-1} \alpha_0}^\delta)$. Again, we also calculated the optimal value α^{opt} of the regularization parameter and the corresponding errors, see Figure 4 for the results. Again we observed that this choice follows the optimal regularization parameter closely and can produce accurate solutions.

5.4 Experiment 4: Deblurring with elastic net

In this experiment we used a standard problem from the Regularization Tools toolbox by P.C. Hansen [24], namely the `blur` problem. We used the param-

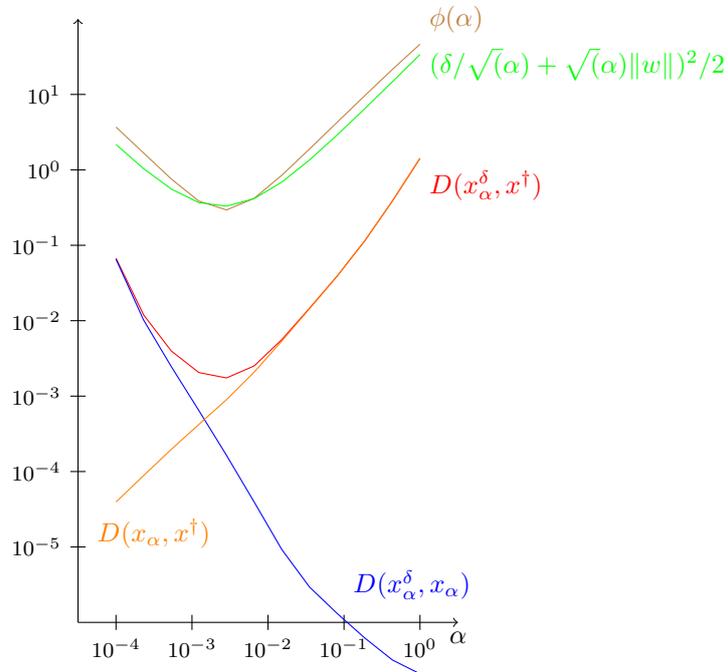


Figure 2: Experiment 1: Illustration of the different errors in log-log scale.

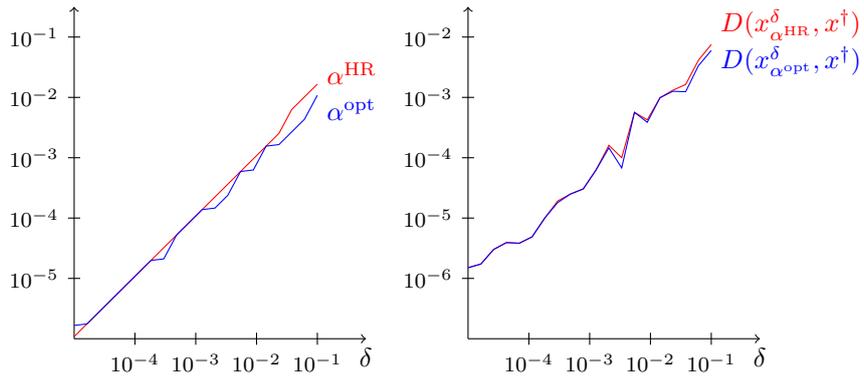


Figure 3: Experiment 2: Left: The regularization parameter by the Hanke-Raus rule and the optimal parameter in dependence of δ . Right: The corresponding errors.

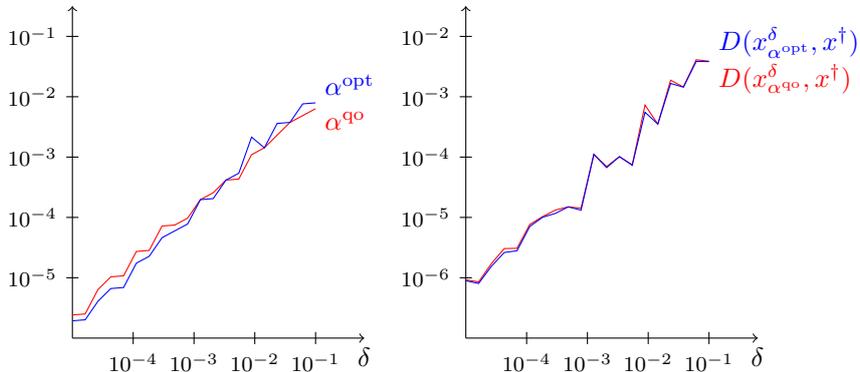


Figure 4: Experiment 3: Left: The regularization parameter by the quasi-optimality criterion and the optimal parameter in dependence of δ . Right: The corresponding errors.

Table 1: Results for experiment 4.

	α	$D(x_{\alpha}^{\delta}, x^{\dagger})$	$\ x_{\alpha}^{\delta} - x^{\dagger}\ _2$
smallest Bregman distance	1.10e-02	5.54e-02	1.02e+01
smallest norm	3.20e-03	7.39e-02	7.36e+00
Hanke-Raus	2.61e-03	9.03e-02	7.47e+00
quasi-optimality	3.02e-03	7.51e-02	7.38e+00
discrepancy	9.29e-04	7.16e-01	1.01e+01

eters $N=50$, $\text{band}=5$, $\text{sigma}=1.2$ and employed the so-called elastic-net regularization [39, 27], that is a penalty term

$$R(x) = \|x\|_1 + \frac{\eta}{2} \|x\|_2^2.$$

On the one hand, this weighted sum of the one- and the two-norm can be seen as a stabilization for one-norm regularization and on the other hand, it leads to a kind of grouping effect, see also [39, 27].

We generated a noisy image y^{δ} (with $\delta = 0.1$) and fixed $\eta = 10^{-3}$. We used a regularized semismooth Newton method (proposed in [21] for the case $\eta = 0$ and generalized to $\eta > 0$ in [27]). Then we calculated solutions for a range of α and determined the regularization parameters according to the Hanke-Raus rule and the quasi-optimality criterion. Moreover, we calculated the parameter according to the discrepancy principle [31] (to compare with a non-heuristic a-posteriori rule) and the optimal regularization parameter with respect to the norm and the Bregman distance. We report the results in Table 1 and Figure 5.

We observe that all rules produce reasonable results and perform comparably in terms of visual inspection. However, the numbers say a little bit more: The discrepancy principle chooses a parameter which is a bit too small and leads to larger errors both in terms of the Bregman distance and the norm. The Hanke-Raus rule and the quasi-optimality principle choose comparable parameters while the quasi-optimality principle performs slightly better. Moreover, the errors by the two proposed rules agree excellently with the optimal one both in

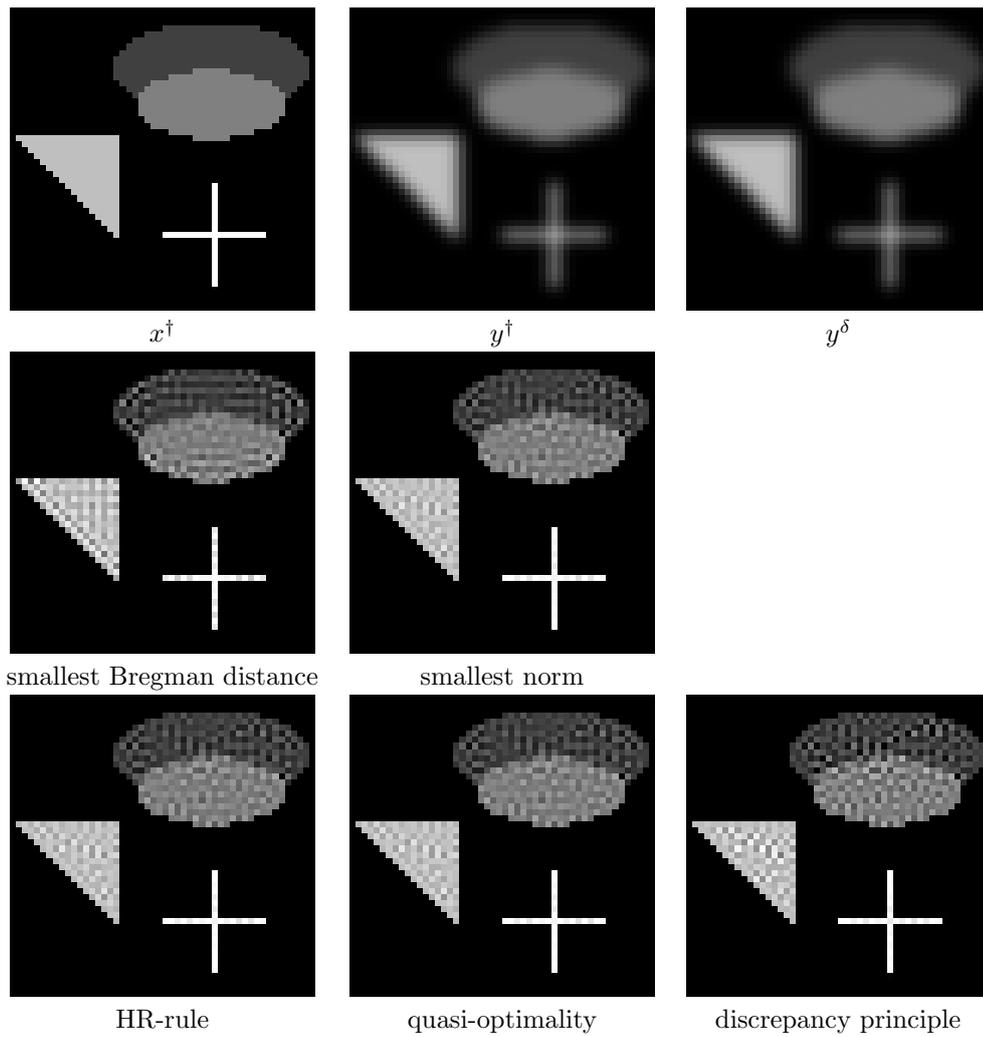


Figure 5: Results for the blur problem for the Hanke-Raus rule and the quasi-optimality criterion.

terms the Bregman distance and norm.

6 Conclusion

We have derived two error estimate-based heuristic parameter choice rules for general convex variational regularization on the basis of a refined analysis of the regularization process. These rules reproduce the Hanke-Raus rule and the quasi-optimality criterion for the conventional quadratic regularization. A posteriori error estimates have been derived for the Hanke-Raus rule using the Bregman distance. The convergence of both rules are discussed by imposing conditions on the noisy data. Numerical results have verified some theoretical findings and showed the effectiveness of these rules. An important future research problem is to develop efficient algorithms to numerically realize these rules. This is nontrivial because the functionals under consideration are often nonsmooth and there exists only an implicit relation between the solution x_α^δ and the regularization parameter α .

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