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Regularization of Ill-Posed Problems: Optimal Parameter Choice in Finite Dimensions*

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We investigate a general class of regularization methods for ill-posed linear operator equations. An optimal a posteriori parameter choice strategy is developed for finite-dimensional approximations. The strategy is illustrated for a number of specific methods. © 1989 Academic Press, Inc.

1. INTRODUCTION

Throughout this paper let X and Y be real Hilbert spaces and let $T: X \to Y$ be a bounded linear compact operator with non-closed range $R(T)$. We are interested in finding the best-approximate solution $T^\dagger y$ of

$$Tx = y, \tag{1.1}$$

i.e., the element of minimal norm minimizing the residual $\|Tx - y\|$. $T^\dagger$ is the "Moore–Penrose inverse" of T and is defined on $D(T^\dagger) = R(T) + R(T)^\perp$. Since we assumed that $R(T)$ is non-closed, $T^\dagger$ is unbounded, so that problem (1.1) is ill-posed. Problem (1.1) includes integral equations of the first kind with non-degenerate L_2-kernels. Usually, (1.1) is solved by regularization methods, i.e., one approximates $T^\dagger y$ by

$$x(\alpha, y_\delta) := U(\alpha, T^*T)\, T^* y_\delta, \tag{1.2}$$

where the function $U(\alpha, \lambda)$ approximates λ^{-1} in an appropriate sense (cf.

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Section 2). The element symbolizes noisy data. We assume that we have approximate data y_δ which satisfy

$$\|Q(y - y_\delta)\| \leqslant \delta, \tag{1.3}$$

where Q is the orthogonal projector onto $\overline{R(T)}$. In [2] an a posteriori parameter selection method has been proposed which is asymptotically optimal and which does not need any information about the exact solution. This method is stated in the infinite-dimensional space X. For numerical computation, however, one has to approximate X by a sequence of finite-dimensional subspaces V_m. A posteriori parameter choice strategies for the finite-dimensional approximation of $T^\dagger y$ using the well-known and effective Tikhonov regularization have been treated in [5, 7] (see also [8]). In [5, 7] convergence rates in terms of the noise level δ and the approximation by finite-dimensional subspaces have been established. However, it has not been proved in these papers that the proposed methods are asymptotically optimal. It is the aim of this paper to prove that our parameter selection method for the finite-dimensional approximation of $T^\dagger y$ is asymptotically optimal (see Section 4). This method includes ordinary and iterated Tikhonov regularization as its most important cases, but also contains a variety of other regularization methods based on spectral theory, like, e.g., Landweber–Fridman iteration (see Section 5). Before we propose our method, we first investigate the "best possible worst-case error" for general approximation methods of the form (1.2), finding the exact behavior of this error.

2. Asymptotic Behavior

In this section we consider general regularization methods of the form (1.2) and we establish upper and lower bounds for the "best possible worst case error" as defined in [2]. We make the following assumptions about the function $U(\alpha, \lambda)$.

Assumption 2.1. Suppose U: $R^+ \times R_0^+ \to R$ is continuous and assume that for all $\lambda > 0$,

$$U(0, \lambda) = \lim_{\alpha \to 0} U(\alpha, \lambda) = \lambda^{-1} \neq \lim_{\alpha \to \infty} U(\alpha, \lambda) < \infty \tag{2.1}$$

and that

$$|\lambda U(\alpha, \lambda)| \leqslant C \tag{2.2}$$

for all $\alpha > 0$, $\lambda \geqslant 0$, and some constant C. Moreover, we assume that there exist $\bar{\lambda} > 0$ and $\bar{\alpha} > 0$ such that

$$0 < U(\cdot, \lambda) \text{ is decreasing on } (0, \bar{\alpha}] \text{ for all } \lambda \in [0, \bar{\lambda}] \tag{2.3}$$

and

$$(\lambda U(\cdot, \lambda) - 1)^2 \text{ is increasing on } (0, \bar{\alpha}] \text{ for all } \lambda > 0. \tag{2.4}$$

Note that (2.3) and (2.4) imply

$$\lambda U(\alpha, \lambda) \leqslant 1 \text{ for } \alpha \in [0, \bar{\alpha}] \text{ and } \lambda \in [0, \bar{\lambda}]. \tag{2.5}$$

Assumption (2.1) is not really very restrictive: (2.1) and (2.2) are always used in the context of regularization (cf. [6]); the other assumptions are satisfied for a wide variety of regularization methods (cf. Section 5). Note that it would suffice to define $U(\alpha, \cdot)$ only for $\lambda \in [0, \|T\|^2]$, since only its behavior on $\sigma(TT^*)$, the spectrum of TT^*, matters. In this paper we restrict our attention to compact operators T, although the following results are also true for bounded linear operators T with slight modifications of the proofs.

For $y \in D(T^\dagger)$, the best possible worst case error is defined by

$$\tilde{\psi}(y, \delta) := \sup\{\inf\{\|x(\alpha, y_\delta) - T^\dagger y\| / \alpha > 0\} / \|Q(y - y_\delta)\| \leqslant \delta\}, \tag{2.6}$$

where Q is the orthogonal projector onto $\overline{R(T)}$. We also define the "ideal data error" by

$$\phi(\alpha, y) := \|x(\alpha, y) - T^\dagger y\|. \tag{2.7}$$

Finally, define the function $h(\alpha)$ (cf. also [2]) by

$$h(\alpha) := \sup\{\lambda U(\alpha, \lambda)^2 / \lambda \in \sigma(TT^*)\}. \tag{2.8}$$

We show in the next theorem that, under Assumption 2.1, the convergence behaviors of $\tilde{\psi}(y, \delta)$ and

$$\psi(y, \delta) := \inf\{(\phi(\alpha, y)^2 + \delta^2 h(\alpha))^{1/2} / \alpha > 0\} \tag{2.9}$$

are the same as $\delta \to 0$.

THEOREM 2.2. *Suppose $y \in D(T^\dagger)$, with $Qy \neq 0$, and let Assumption 2.1 be satisfied. Moreover, suppose that there is a $\lambda \in \sigma(TT^*)$ with $0 < \lambda \leqslant \bar{\lambda}$ ($\bar{\lambda}$ as in Assumption 2.1). Then*

$$\tfrac{1}{2}\psi(y, \delta)^2 \leqslant \tilde{\psi}(y, \delta)^2 \leqslant 2\psi(y, \delta)^2 \tag{2.10}$$

for δ sufficiently small.

Proof. First we show that the estimate on the right-hand side holds for all $\delta > 0$. Let $\{F_\lambda\}$ be the spectral family of TT^*. Then we have for all y_δ with $\|Q(y - y_\delta)\| \leq \delta$

$$\begin{aligned}\|x(\alpha, y_\delta) - T^\dagger y\|^2 &\leq (\|x(\alpha, y) - T^\dagger y\| + \|x(\alpha, y) - x(\alpha, y_\delta)\|)^2 \\ &\leq 2(\|x(\alpha, y) - T^\dagger y\|^2 + \|x(\alpha, y) - x(\alpha, y_\delta)\|^2) \\ &= 2\left(\|x(\alpha, y) - T^\dagger y\|^2 + \int_0^\infty \lambda U(\alpha, \lambda)^2 \, d\|F_\lambda Q(y - y_\delta)\|^2\right).\end{aligned}$$

The estimate now follows from (2.7), (2.8), (2.9), and well-known spectral theoretical results.

Concerning the other estimate, let λ_i be an eigenvalue of TT^* in $(0, \bar{\lambda}]$ with associated norm-one eigenvector u_i and define y_δ^i by

$$y_\delta^i = Qy - \delta \operatorname{sgn}(Qy, u_i)\, u_i. \tag{2.11}$$

Then for all $\alpha \in (0, \bar{\alpha}]$ ($\bar{\alpha}$ as in Assumption 2.1),

$$\begin{aligned}&(x(\alpha, y) - T^\dagger y, x(\alpha, y_\delta^i) - x(\alpha, y)) \\ &\quad = ((U(\alpha, TT^*)\, TT^* - I)\, Qy, U(\alpha, TT^*)\, Q(y_\delta^i - y)) \\ &\quad = (U(\alpha, \lambda_i)\, \lambda_i - 1)\, U(\alpha, \lambda_i)(-\delta) \operatorname{sgn}(Qy, u_i) \cdot (Qy, u_i) \geq 0\end{aligned}$$

and

$$\|x(\alpha, y) - x(\alpha, y_\delta^i)\|^2 = \lambda_i U(\alpha, \lambda_i)^2 \delta^2.$$

Hence,

$$\begin{aligned}\|x(\alpha, y_\delta^i) - T^\dagger y\|^2 &= \|x(\alpha, y) - T^\dagger y\|^2 + \|x(\alpha, y) - x(\alpha, y_\delta^i)\|^2 \\ &\quad + 2(x(\alpha, y) - T^\dagger y, x(\alpha, y_\delta^i) - x(\alpha, y)) \\ &\geq \phi(\alpha, y)^2 + \delta^2 \lambda_i U(\alpha, \lambda_i)^2\end{aligned} \tag{2.12}$$

for all $\alpha \in (0, \bar{\alpha}]$ and $\lambda_i \in (0, \bar{\lambda}] \cap \sigma(TT^*)$. Now define $z(\alpha, \delta)$ by

$$z(\alpha, \delta) := \phi(\alpha, y)^2 - \delta^2 h(\alpha). \tag{2.13}$$

Then Assumption 2.1 implies that z is continuous,

$$\lim_{\alpha \to 0} z(\alpha, \delta) < 0, \qquad \text{and} \qquad \lim_{\alpha \to \infty} z(\alpha, \delta) > 0$$

for sufficiently small positive δ. Therefore, there exists a $\delta_1 > 0$ such that for each $\delta \in (0, \delta_1]$ there is an $\alpha(\delta) > 0$ with $z(\alpha(\delta), \delta) = 0$, or equivalently

$$\phi(\alpha(\delta), y)^2 = \delta^2 h(\alpha(\delta)). \tag{2.14}$$

Moreover, $\alpha(\delta) \to 0$ as $\delta \to 0$. On the other hand, Assumption 2.1 also implies that for α sufficiently small, $h(\alpha) = \lambda_i U(\alpha, \lambda_i)^2$ for some $\lambda_i \in (0, \bar{\lambda}] \cap \sigma(TT^*)$. Hence, there is a positive $\delta_2 \leqslant \delta_1$ such that for all positive $\delta < \delta_2$, $\alpha(\delta) \leqslant \bar{\alpha}$, and

$$h(\alpha(\delta)) = \lambda_i U(\alpha(\delta), \lambda_i)^2 \tag{2.15}$$

for some $\lambda_i = \lambda_i(\delta) \in (0, \bar{\lambda}] \cap \sigma(TT^*)$. Now let λ_i be such that (2.15) holds. Then by (2.4)

$$\phi(\alpha, y)^2 + \delta^2 \lambda_i U(\alpha, \lambda_i)^2 \geqslant \phi(\alpha(\delta), y)^2 \tag{2.16}$$

for all $\alpha \in [\alpha(\delta), \bar{\alpha}]$ and by (2.3)

$$\phi(\alpha, y)^2 + \delta^2 \lambda_i U(\alpha, \lambda_i)^2 \geqslant \delta^2 \lambda_i U(\alpha(\delta), \lambda_i)^2 \tag{2.17}$$

for all $\alpha \in (0, \alpha(\delta)]$. Now (2.12) and (2.14)–(2.17) imply that

$$\begin{aligned} \|x(\alpha, y_\delta^i) - T^\dagger y\|^2 &\geqslant \min\{\phi(\alpha(\delta), y)^2, \delta^2 \lambda_i U(\alpha(\delta), \lambda_i)^2\} \\ &= \tfrac{1}{2}(\phi(\alpha(\delta), y)^2 + \delta^2 (h(\alpha(\delta))) \\ &\geqslant \tfrac{1}{2} \bar{\psi}(y, \delta)^2 \end{aligned} \tag{2.18}$$

for all $\alpha \in (0, \bar{\alpha}]$ and $\delta \in (0, \delta_2]$. Since $\bar{\psi}(y, \delta) \to 0$ as $\delta \to 0$, it is easy to see that

$$\inf\{\|x(\alpha, y_\delta) - T^\dagger y\| / \alpha > 0\} = \inf\{\|x(\alpha, y_\delta) - T^\dagger y\| / \alpha \in (0, \bar{\alpha}]\}$$

for all y_δ with $\|Q(y - y_\delta)\| \leqslant \delta$ and δ sufficiently small. Hence (2.18) and (2.6) imply that there is a positive $\delta_3 \leqslant \delta_2$ such that for $\delta \in (0, \delta_3]$

$$\tilde{\psi}^2(y, \delta) \geqslant \frac{1}{2} \bar{\psi}(y, \delta)^2. \quad \blacksquare$$

If $\alpha(\delta)$ is some parameter choice strategy, then we say (compare [2]) the convergence rate for this strategy is *optimal* if

$$\psi(y, \delta) = 0(\tilde{\psi}(y, \delta)) \qquad \text{as} \quad \delta \to 0, \tag{2.19}$$

where

$$\psi(y, \delta) := \sup\{\|x(\alpha(\delta), y_\delta) - T^\dagger y\| / \|Q(y - y_\delta)\| \leqslant \delta\}, \tag{2.20}$$

and is *quasi-optimal*, if (2.19) holds for some sequence $\delta_k \to 0$ as $k \to \infty$. Theorem 2.2 shows that (2.19) is equivalent to $\psi(y, \delta)) = 0(\bar{\psi}(y, \delta))$ as $\delta \to 0$. In [2] an a posteriori parameter choice strategy has been proposed which always leads to quasi-optimal convergence rates and which gives optimal rates under a certain (not too restrictive) condition on the spectrum $\sigma(TT^*)$.

In Section 4, we propose an a posteriori parameter choice for regularization in finite-dimensional subspaces of the Hilbert space X which is quite similar to the strategy in [2]. We will also prove quasi-optimality of our strategy and optimality under a similar condition on the eigenvalues of TT^* as in [2].

3. The Finite-Dimensional Approach

For numerical computation one must approximate the infinite-dimensional Hilbert space X by a sequence of finite-dimensional subspaces $\{V_m\}$. We use here the same approach as in [7], since it has some numerical advantages over the usual finite-dimensional approach (see [7]).

Let $W_1 \subset W_2 \subset \cdots \subset W_m \subset \cdots$ be a sequence of finite-dimensional subspaces of $N(T^*)^\perp = \overline{R(T)}$ and let $V_m := T^* W_m$. We denote the orthogonal projectors onto W_m and V_m by Q_m and P_m, respectively. It is wellknown that for $y \in D(T^\dagger)$ (cf. [6]),

$$T_m^\dagger y = P_m T^\dagger y, \qquad \text{where} \quad T_m := Q_m T, \tag{3.1}$$

and hence $T_m^\dagger y$ is the best approximation to $T^\dagger y$ by elements in V_m. Therefore, it seems to be unnecessary to regularize the finite-dimensional problem

$$T_m x = Q_m y. \tag{3.2}$$

But it is also well known (cf. [1]) that

$$\| T_m^\dagger y - T_m^\dagger y_\delta \| \leq \| Q_m(y - y_\delta) \| / \sqrt{\lambda_n^m}, \tag{3.3}$$

where λ_n^m is the smallest positive eigenvalue of $T_m T_m^*$; $n = n(m)$ is the dimension of W_m. If λ_n^m is very small, then the problem of solving (3.2) with noisy data is severely ill-conditioned. It has been shown in [7] that combining projection with Tikhonov regularization is much more effective than merely projection alone.

In the following we combine projection with a general regularization method. That is, we approximate $T^\dagger y$ by

$$x(m, \alpha, y_\delta) := U(\alpha, T_m^* T_m)\, T_m^* y_\delta. \tag{3.4}$$

where $U(\cdot, \cdot)$ satisfies Assumption 2.1 (cf. [4] where weaker results are obtained under different assumptions on $U(\cdot, \cdot)$). To guarantee convergence of $x(m, \alpha, y)$ to $T^\dagger y$ as $\alpha \to 0$ and $m \to \infty$ we need some further conditions on $U(\cdot, \cdot)$ which, like Assumption 2.1, are also satisfied for a wide class of methods.

ASSUMPTION 3.1. In addition to Assumption 2.1, suppose that (2.1) holds uniformly for $\lambda \geqslant \bar{\lambda}$ and that

$$\sup\{(\lambda U(\alpha, \lambda) - 1)^2 \lambda / \lambda \geqslant 0\} \to 0 \qquad \text{as} \quad \alpha \to 0. \tag{3.5}$$

Note that in (3.5) $\lambda \geqslant 0$ can be replaced by $0 \leqslant \lambda \leqslant \|T\|^2$, since $\|T_m\|^2 \leqslant \|T\|^2$ and only the behavior of $U(\alpha, \cdot)$ on the sets $\sigma(T_m T_m^*)$ matters.

THEOREM 3.2. *Let $x(m, \alpha, y)$ be defined as in* (3.4) *with y_δ replaced by y and suppose Assumption* 3.1 *holds. Then for any sequence $\alpha_m \to 0$ as $m \to \infty$, we have*

$$\lim_{m \to \infty} x(m, \alpha_m, y) = T^\dagger y.$$

Proof. Let $\{E_\lambda^m\}$ be the spectra family for $T_m^* T_m$ and suppose $\alpha_m \to 0$ as $m \to \infty$. Then (2.5) implies that for m sufficiently large

$$\begin{aligned} \|x(m, \alpha_m, y)\|^2 &= \int_0^\infty \lambda^2 U(\alpha_m, \lambda)^2 \, d\|E_\lambda^m T^\dagger y\|^2 \\ &\leqslant \|P_m T^\dagger y\|^2 + \int_{\bar{\lambda}}^\infty (\lambda^2 U(\alpha_m, \lambda)^2 - 1) \, d\|E_\lambda^m T^\dagger y\|^2 \\ &\leqslant \|T^\dagger y\|^2 (1 + \sup\{|\lambda^2 U(\alpha_m, \lambda)^2 - 1| / \lambda \in [\bar{\lambda}, \|T\|^2]\}). \end{aligned}$$

Now, since (2.1) holds uniformly for $\lambda \geqslant \bar{\lambda}$ and

$$\begin{aligned} |\lambda^2 U(\alpha_m, \lambda)^2 - 1| &= |\lambda U(\alpha_m, \lambda) + 1| \, |(\lambda U(\alpha_m, \lambda) - 1| \\ &\leqslant (C+1) \|T\|^2 \, |U(\alpha_m, \lambda) - \lambda^{-1}| \end{aligned}$$

for $\lambda \leqslant \|T\|^2$, we obtain

$$\limsup_{m \to \infty} \|x(m, \alpha_m, y)\| \leqslant \|T^\dagger y\|. \tag{3.6}$$

Now let $\{\alpha_l\}$ be an arbitrary subsequence of $\{\alpha_m\}$. Then by (3.6) $\{\alpha_l\}$ has a subsequence $\{\alpha_k\}$ with

$$x(k, \alpha_k, y) \rightharpoonup u \qquad \text{as} \quad k \to \infty \tag{3.7}$$

for some u, where $\|u\| \leqslant \|T^\dagger y\|$ and "$\rightharpoonup$" denotes weak convergence. Now let z be an arbitrary element of Y. Then

$$\begin{aligned} &\|(T_k x(k, \alpha_k, y) - Tu, z)\| \\ &\quad \leqslant \|T\| \, \|x(k, \alpha_k, y)\| \, \|(I - Q_k) Qz\| + |(x(k, \alpha_k, y) - u, T^* z)| \\ &\quad \to 0 \qquad \text{as} \quad k \to \infty, \text{ by (3.6) and (3.7).} \end{aligned}$$

Hence,

$$T_k x(k, \alpha_k, y) \rightharpoonup Tu. \tag{3.8}$$

On the other hand,

$$\|T_k x(k, \alpha_k, y) - Qy\| \leqslant \|(I - Q_k) Qy\| + \|T_k x(k, \alpha_k, y) - Q_k y\|,$$

where $\|(I - Q_k) Qy\| \to 0$, and (3.5), along with

$$Q_k y = Q_k Q y = Q_k T T^\dagger y = T_k T^\dagger y,$$

implies that

$$\begin{aligned} \|T_k x(k, \alpha_k, y) - Q_k y\|^2 &= \int_0^\infty (\lambda U(\alpha_k, \lambda) - 1)^2 \lambda d\|E_\lambda^k T^\dagger y\|^2 \\ &\to 0 \qquad \text{as} \quad k \to \infty. \end{aligned}$$

Hence, by (3.8) $Tu = Qy$ and $u = T^\dagger y$. Therefore,

$$x(m, \alpha_m, y) \rightharpoonup T^\dagger y \qquad \text{as} \quad m \to \infty. \tag{3.9}$$

By the weak lower semi-continuity of the norm in Hilbert spaces, we have

$$\|T^\dagger y\| \leqslant \liminf_{m \to \infty} \|x(m, \alpha_m, y)\|.$$

This together with (3.9) proves the assertion. ∎

Note that this theorem also holds for non-compact operators T. If we have noisy data y_δ with $\|Q_m(y - y_\delta)\| \leqslant \delta$, we get the following

COROLLARY 3.3. *Let Assumption* 3.1 *hold and let* δ_m *and* y_{δ_m} *be such that* $\delta_m \to 0$ *for* $m \to \infty$ *and* $\|Q_m(y - y_{\delta_m})\| \leqslant \delta_m$. *Moreover, assume that* $\alpha(m, \delta_m)$ *is a sequence such that* $\alpha(m, \delta_m) \to 0$ *for* $m \to \infty$ and $\delta_m^2 h(m, \alpha(m, \delta_m)) \to 0$ *for* $m \to \infty$, *where*

$$h(m, \alpha) := \sup\{\lambda U(\alpha, \lambda)^2 / \lambda \in \sigma(T_m T_m^*) \setminus \{0\}\}. \tag{3.10}$$

Then

$$\lim_{m \to \infty} x(m, \alpha(m, \delta_m), y_{\delta_m}) = T^\dagger y$$

holds.

Proof. It follows from the proof of Theorem 2.2 that $\|x(m, \alpha, y_\delta) - T^\dagger y\| \leqslant \|x(m, \alpha, y) - T^\dagger y\| + \delta h(m, \alpha)^{1/2}$. Now the assertion follows with Theorem 3.2 and the assumptions on $\alpha(m, \delta_m)$. ∎

Now let $\alpha(m, \delta_m)$ be some parameter choice. Then we define as in Section 2: The convergence rate for this strategy and y is *optimal*, if

$$\psi(m, y, \delta_m) = O(\tilde{\psi}(m, y, \delta_m)) \qquad \text{for} \quad m \to \infty \tag{3.11}$$

holds for every sequence $\delta_m \to 0$, where

$$\psi(m, y, \delta_m) := \sup\{\|x(m, \alpha(m, \delta_m), y_{\delta_m}) - T^\dagger y\| / \|Q_m(y_{\delta_m} - y)\| \leqslant \delta_m\} \tag{3.12}$$

and

$$\tilde{\psi}(m, y, \delta_m) := \sup\{\inf\{\|x(m, \alpha, y_{\delta_m}) - T^\dagger y\| / \alpha > 0\} / \|Q_m(y_{\delta_m} - y)\| \leqslant \delta_m\}. \tag{3.13}$$

The convergence rate is *quasi-optimal* if (3.11) holds for at least one sequence $\delta_m \to 0$. As in Section 2 we define

$$\bar{\psi}(m, y, \delta_m) = \inf\{\phi(m, \alpha, y)^2 + \delta_m^2 h(m, \alpha)^{1/2} / \alpha > 0\}, \tag{3.14}$$

where

$$\phi(m, \alpha, y) := \|x(m, \alpha, y) - T^\dagger y\|. \tag{3.15}$$

Analogously to Theorem 2.2 we now obtain

THEOREM 3.4. *Let $y \in D(T^\dagger)$ with $Qy \neq 0$ and let Assumption* 3.1 *be satisfied. Moreover, let us assume that $R(T)$ is non-closed. Then for every sequence δ_m with $\delta_m \to 0$ for $m \to \infty$*

$$\tfrac{1}{2}\bar{\psi}(m, y, \delta_m)^2 \leqslant \tilde{\psi}(m, y, \delta_m)^2 \leqslant 2\bar{\psi}(m, y, \delta_m)^2 \tag{3.16}$$

holds for m sufficiently large.

Proof. Since $R(T)$ is non-closed and

$$\|T - T_m\| \to 0 \qquad \text{for} \quad m \to \infty \tag{3.17}$$

holds for compact operators T (cf., e.g., [7]), $\lambda_n^m \leqslant \bar{\lambda}$ for m sufficiently large, where λ_n^m is the smallest positive eigenvalue of $T_m T_m^*$. This means that Theorem 2.2 is applicable for T_m and m sufficiently large.

Following the proof of Theorem 2.2 it is not hard to check that due to Corollary 3.3, Assumption 3.1, and (3.17) δ_1, δ_2, and δ_3 (of the proof of Theorem 2.2) can be chosen independently of m, if m is sufficiently large. This means there is an $M \in N$ and a $\bar{\delta} > 0$ such that for all $m \geqslant M$ and $\delta \in (0, \bar{\delta}]$ the estimate

$$\begin{aligned}
&\tfrac{1}{2} \inf\{\|x(m, \alpha, y) - T_m^\dagger y\|^2 + \delta^2 h(m, \alpha)/\alpha > 0\} \\
&\quad \leqslant \sup\{\inf\{\|x(m, \alpha, y_\delta) - T_m^\dagger y\|^2/\alpha > 0\}/\|Q_m(y - y_\delta)\| \leqslant \delta\} \\
&\quad \leqslant 2 \inf\{\|x(m, \alpha, y) - T_m^\dagger y\|^2 + \delta^2 h(m, \alpha)/\alpha > 0\}
\end{aligned}$$

holds. This together with $\delta_m \to 0$ for $m \to \infty$ and $\|x - T^\dagger y\|^2 = \|x - T_m^\dagger y\|^2 + \|T_m^\dagger y - T^\dagger y\|^2$ for all $x \in V_m$ (cf. (3.1)) implies the assertion. ∎

In the next section we will discuss an a posteriori parameter selection method which at least always leads to quasi-optimal convergence rates and under a certain condition on $\bigcup_{m \in N} \sigma(T_m T_m^*)$ even optimal rates.

4. A Posteriori Parameter Selection Method

Theorem 3.4 and (3.1) imply that a choice of the regularization parameter α leading to an optimal convergence rate could be achieved by minimizing

$$\|x(m, \alpha, y) - T_m^\dagger y\|^2 + \delta^2 h(m, \alpha). \tag{4.1}$$

Of course, this is not possible in reality, since y is not known. But even if we replace y by y_δ in (4.1) there is, in general, no unique minimizer. Therefore, we replace $h(m, \alpha)$ by

$$\bar{h}(m, \alpha) := \sup\{\lambda U(\alpha, \lambda)^2/\lambda \geqslant \lambda_n^m\}. \tag{4.2}$$

It follows from (3.10) that $h(m, \alpha) \leqslant \bar{h}(m, \alpha)$. For a variety of regularization methods the minimization problem

$$\inf\{\|x(m, \alpha, y) - T_m^\dagger y\|^2 + \delta^2 \bar{h}(m, \alpha)/\alpha > 0\} \tag{4.3}$$

has a unique solution for every $y \in Y$ and the unique minimizer can be characterized in terms of the derivative of the functional in (4.3). The general assumptions on $U(\alpha, \lambda)$ to guarantee these properties are the following (compare [2, Assumption 2.1]).

ASSUMPTION 4.1. Let U: $R^+ \times R_0^+ \to R$ fulfill Assumption 3.1. Moreover, let U be continuously differentiable with respect to α and assume that

$$\alpha \to [U'(\alpha, \lambda)(1-\lambda U(\alpha, \lambda))] \bar{h}'(m, \alpha)^{-1} \tag{4.4}$$

is strictly increasing for all $m \in N$ and $\lambda \geqslant \lambda_n^m$, where $\bar{h}(m, a)$, defined by (4.2), is assumed to be continuously differentiable with $\bar{h}'(m, \alpha) < 0$ for all $\alpha > 0$ and $m \in N$. Furthermore, we assume that a constant K exists (independently of m) such that

$$|U'(\alpha, \lambda) \cdot \bar{h}(m, \alpha)^{-1}| \leqslant K \tag{4.5}$$

holds for all $m \in N$, $\alpha > 0$, and $\lambda \geqslant \lambda_n^m$ ($'$ denotes everywhere $\partial/\partial\alpha$).

For $m \in N$, $\alpha \geqslant 0$, and $w \in Y$ we define

$$f(m, \alpha, w) := \bar{h}'(m, \alpha)^{-1}(U'(\alpha, T_m T_m^*)[I - T_m T_m^* U(\alpha, T_m T_m^*)] Q_m w, Q_m w). \tag{4.6}$$

$f(m, \alpha, w)$ is defined as $f(\alpha, w)$ in [2] with T and $2g'(\alpha)^{-1}$ replaced by T_m and $\bar{h}'(m, \alpha)^{-1}$, respectively. Following the proofs in [2] we, therefore, get the following results.

PROPOSITION 4.2. (a) *For any $m \in N$, $\delta > 0$, and $y_\delta \in Y$ with $Q_m y_\delta \neq 0$, there is a unique $\alpha(m, \delta)$ such that*

$$f(m, \alpha(m, \delta), y_\delta) = \gamma\delta^2 \tag{4.7}$$

holds, provided that

$$0 < \gamma < R(m, y_\delta) \cdot \delta^{-2}, \tag{4.8}$$

where

$$0 < R(m, y_\delta) := \lim_{\alpha \to \infty} f(m, \alpha, y_\delta) < L_m \|Q_m y_\delta\|^2 \tag{4.9}$$

and

$$L_m := \sup\{|[U'(\alpha, \lambda)(1 - \lambda U(\alpha, \lambda))]\bar{h}'(m, \alpha)^{-1}| / \alpha \geqslant 0 \textit{ and } \lambda \geqslant \lambda_n^m\} \leqslant K(1 + C). \tag{4.10}$$

(b) *If $\gamma > L := \sup\{L_m / m \in N\}$, $Qy \neq 0$, and y_δ is such that $\|Q_m(y - y_\delta)\| \leqslant \delta$, then $Q_m y_\delta \neq 0$ and (4.8) holds for all $m \geqslant M$ and $0 < \delta \leqslant \bar{\delta}$, where $\bar{\delta}$ is independent of m.*

Proof. The proof follows with Proposition 2.4 and Lemma 2.5a) in [2] with T and $g(\alpha)$ replaced by T_m and $\bar{h}(m, \alpha)$, respectively. ▮

THEOREM 4.3. *Let U satisfy Assumption 4.1; let $y \in D(T^\dagger)$ with $Qy \neq 0$ be arbitrary, $\gamma > L$ (L as in Proposition 4.2(b)), and for $m \in N$ and $\delta > 0$, let $y_\delta \in Y$ with $Q_m y_\delta$ be such that $\|Q_m(y - y_\delta)\| \leqslant \delta$ and (4.8) holds. Then the following holds:*

If $\alpha(m, \delta)$ is chosen as the unique solution of (4.7), then

$$\|x(m, \alpha(m, \delta), y_\delta) - T^\dagger y\|^2 \leqslant \mu \cdot \inf\{\phi(m, \alpha, y)^2 + \delta^2 \bar{h}(m, \alpha) \mid \alpha > 0\} \tag{4.11}$$

holds, where μ is a constant independent of y, δ, y_δ, and m.

Proof. The proof follows with Theorem 2.7 in [2] with T and $g(\alpha)$ replaced by T_m and $\bar{h}(m, \alpha)$, respectively. ▮

We are now able to prove the following results about convergence rates, if the following assumption about U is fulfilled.

ASSUMPTION 4.4. Let Assumption 4.1 be satisfied. Moreover, assume that there are $\hat{\lambda} > 0$ and $\hat{\alpha} > 0$ such that for all $\alpha \in (0, \hat{\alpha}]$, $U(\alpha, \cdot)$ is decreasing on $[0, \hat{\lambda}]$. Furthermore, assume that for all $\alpha \in (0, \hat{\alpha}]$ there is a $\lambda(\alpha) < \hat{\lambda}$ such that $\lambda U(\alpha, \lambda)^2$ is strictly increasing on $[0, \lambda(\alpha)]$ and strictly decreasing on $[\lambda(\alpha), \hat{\lambda}]$ with respect to λ.

THEOREM 4.5. *If Assumption 4.4 holds and $R(T)$ is non-closed, then the parameter choice strategy (4.7) (which is well-defined for sufficiently small $\delta > 0$ if $\gamma > L$) is of quasi-optimal order for all $y \in D(T^\dagger)$ with $Qy \neq 0$. If in addition,*

$$\limsup_{m \to \infty} C_m < \infty, \tag{4.12}$$

holds, where $C_m := \sup\{(\lambda_k^m / \lambda_{k+1}^m) / 1 \leqslant k \leqslant n\}$ and $\lambda_1^m > \lambda_2^m > \cdots > \lambda_n^m > 0$ are the positive eigenvalues of $T_m T_m^*$, then the strategy is of optimal order for all $y \in D(T^\dagger)$ with $Qy \neq 0$.

Proof. Let $\{\delta_m\}$ be a sequence such that $\delta_m \to 0$ for $m \to \infty$. Proposition 4.2 implies that (4.7) has a unique solution $\alpha(m, \delta)$ for m sufficiently large. Now Theorem 4.3 and Theorem 3.4 imply that (3.11) holds if and only if

$$\inf\{\phi(m, \alpha, y)^2 + \delta_m^2 \bar{h}(m, \alpha) / \alpha > 0\} \leqslant \tilde{C} \cdot \inf\{\phi(m, \alpha, y)^2 + \delta_m^2 h(m, \alpha) / \alpha > 0\} \tag{4.13}$$

is satisfied for some constant $\tilde{C}$. To prove quasi-optimality we have to show that (4.13) holds at least for one sequence $\delta_m \to 0$.

Assumption 4.4 and the non-closedness of $R(T)$ imply that for m sufficiently large there is an $\alpha_m > 0$ such that $\bar{h}(m, \alpha) = h(m, \alpha) = \lambda_n^m U(\alpha, \lambda_n^m)^2$ for all $\alpha \in (0, \alpha_m]$. Now let $\alpha_m(\delta)$ be the largest global minimizer of $\bar{\psi}(m, y, \delta)$ (see (3.14)). Then, by Corollary 3.3, there is a $\bar{\delta}_m > 0$ such that for all $\delta \in (0, \bar{\delta}_m]$ $\alpha_m(\delta) \leqslant \alpha_m$. Now choose a sequence δ_m such that $\delta_m \to 0$ for $m \to \infty$ and $\delta_m \leqslant \bar{\delta}_m$ for m sufficiently large. Then we have $\bar{h}(m, \alpha_m(\delta)) = h(m, \alpha_m(\delta))$ for m sufficiently large. Hence, (4.13) holds with $\tilde{C} = 1$. This proves quasi-optimality of our selection method.

Now suppose that (4.12) is satisfied and let $\delta_m \to 0$ be an arbitrary, but fixed sequence. Again, let $\alpha_m(\delta_m)$ be the largest global minimizer of $\bar{\psi}(m, y, \delta_m)$. Then

$$\bar{h}(m, \alpha_m(\delta_m)) = \lambda U(\alpha_m(\delta_m), \lambda)^2,$$

where $\lambda = \lambda(m, \alpha_m(\delta_m)) \in [\lambda_{k+1}^m, \lambda_k^m]$ for some $1 \leqslant k < n$ or $\lambda < \lambda_n^m$. If $\lambda < \lambda_n^m$, then $\tilde{C} = 1$ as above. If $\lambda \in [\lambda_{k+1}^m, \lambda_k^m]$, then

$$\begin{aligned} \bar{h}(m, \alpha_m(\delta_m)) &= \lambda U(\alpha_m(\delta_m), \lambda)^2 \\ &\leqslant \lambda_{k+1}^m U(\alpha_m(\delta_m), \lambda_{k+1}^m)^2 \cdot \lambda/\lambda_{k+1}^m \\ &\leqslant \lambda_{k+1}^m U(\alpha_m(\delta_m), \lambda_{k+1}^m)^2 \cdot \lambda_k^m/\lambda_{k+1}^m \\ &\leqslant h(m, \alpha_m(\delta_m)) \cdot C_m. \end{aligned}$$

Inequality (4.12) implies that $1 \leqslant C_m \leqslant \tilde{C} < \infty$ and hence (4.13) holds with this constant $\tilde{C}$ for every sequence $\delta_m \to 0$. This proves the optimality of our selection method under condition (4.12). ∎

Remark 4.6. We have shown in the proof of Theorem 4.5 that (3.11) holds without condition (4.12) if δ_m converges to 0 sufficiently fast. Of course, (3.11) holds for every sequence δ_m where $h(m, \alpha_m(\delta_m)) = \bar{h}(m, \alpha_m(\delta_m))$, or equivalently $\bar{h}(m, \alpha_m(\delta_m)) = \lambda U(\alpha_m(\delta_m), \lambda)^2$ for some $\lambda \in \sigma(T_m T_m^*) \setminus \{0\}$.

Note that (4.12) is a sufficient condition for optimality of our strategy. Since $\phi(m, \alpha, y)$ can converge arbitrarily slowly towards 0 for $m \to \infty$ and $\alpha \to 0$, if y fulfills no smoothness conditions, it can happen that $\phi(m, \alpha, y)^2$ is the dominant term in $\phi(m, \alpha, y)^2 + \delta^2 h(m, \alpha)$. In this situation one would get even optimal convergence without condition (4.12).

It follows from results in [3] that if $\lim_{m \to \infty} \sup \operatorname{gap}(W_m, \psi_m) < 1$, where ψ_m is the span of the first $n(m)$ eigenvectors of TT^* and the gap is defined by $\operatorname{gap}(W_m, \psi_m) := \| Q_m - \tilde{Q}_m \|$, where $\tilde{Q}_m$ is the orthogonal projector onto ψ_m, then condition (4.12) is equivalent to

$$\lim \sup\{\lambda_k \lambda_{k+1}^{-1} / k \in N\} < \infty,$$

where $\lambda_1 > \lambda_2 > \cdots > 0$ are the eigenvalues of TT^*. This is the same condition as in [2], which is also needed there to obtain optimal convergence rates. This means, if W_m is not "too far away" from ψ_m (cf. [3, Remark 2.7]) and the eigenvalues of TT^* do not decay faster than exponentially, then condition (4.12) is always fulfilled and hence our strategy is then optimal.

Remark 4.7. For iterative regularization methods $U(\alpha, \cdot)$ is replaced by $U(n, \cdot)$, where $1/n$ plays the role of α. Therefore, one cannot define a derivative with respect to α (see Assumption 4.1). But, nevertheless, all results we have shown so far can also be proved for iterative regularization methods, if one replaces α by $1/n$ in our assumptions and (4.4), $\bar{h}'(m, \alpha) < 0$, and (4.5) by

$$n \to \frac{\Delta U(n, \lambda)}{\Delta \bar{h}(m, n)} [2 - \lambda(U(n, \lambda) + U(n+1, \lambda))], \tag{4.14}$$

$$\Delta \bar{h}(m, n) > 0, \qquad \text{for all} \quad m, n \in N$$

and

$$|\Delta U(n, \lambda) / \Delta \bar{h}(m, n)| \leqslant K, \tag{4.15}$$

respectively. $\bar{h}(m, n)$ is defined by (4.2) with α replaced by n and $\Delta v(n) := v(n+1) - v(n)$. The parameter selection method (4.7) has to be replaced by the stopping rule

$$f(m, n(\delta), y_\delta) \leqslant \gamma \delta^2, \tag{4.16}$$

where $n(\delta)$ is the minimal $n \in N_0$ such that (4.16) holds and

$$\begin{aligned} f(m, n, w) := {} & [\Delta \bar{h}(m, n)]^{-1}([\Delta U(n, T_m T_m^*)] \\ & \times [2I - T_m T_m^*(U(n, T_m T_m^*) + U(n+1, T_m T_m^*))] \, Q_m w, Q_m w). \end{aligned} \tag{4.17}$$

For changes in the proofs of Proposition 4.2 and Theorem 4.3 caused by these replacements see [2].

5. Applications to Specific Regularization Methods

5.1. (*Iterated*) *Tikhonov Regularization*

Iterated Tikhonov regularization of order n is defined in the following way. Let $x_{\alpha,0}^{m,\delta} := 0$ and for all $j \in N$, let $x_{\alpha,j+1}^{m,\delta}$ be the unique solution of

$$(T_m^* T_m + \alpha I) x = T_m^* y_\delta + \alpha x_{\alpha,j}^{m,\delta}. \tag{5.1}$$

As a regularized solution one takes $x_{\alpha,n}^{m,\delta}$. $x_{\alpha,n}^{m,\delta}$ can be written in the form of (3.4) with

$$U(\alpha, \lambda) = \frac{(\alpha+\lambda)^n - \alpha^n}{\lambda(\alpha+\lambda)^n} \tag{5.2}$$

(cf., e.g., [2]). One can show that U satisfies Assumption 4.4 with $C=1$, $K=L=L_m=n/b$, $R(m, w)=K\|Q_m w\|^2$, and no restrictions on $\bar{\alpha}, \bar{\lambda}, \hat{\alpha}, \hat{\lambda}$; $b=4n^2a^{2n+1}(1+a)^{-2(n+1)}$ and a is the unique positive solution of

$$(2n+1)\,a^n + a^{n+1} - (1+a)^{n+1} = na^n - \sum_{k=0}^{n-1} \binom{n+1}{k} a^k = 0. \tag{5.3}$$

For the actual values of a, b, and K for $n=1, 2, 3, 4$ see Table I. The function $\bar{h}(m, \alpha)$ is given by

$$\bar{h}(m, \alpha) = \begin{cases} b/\alpha & \text{if } \alpha \geqslant a\lambda_n^m \\ \lambda_n^m U(\alpha, \lambda_n^m)^2 & \text{if } \alpha < a\lambda_n^m. \end{cases}$$

(The index n of λ_n^m has nothing to do with the order n of iteration.) Let $e(m, \alpha) = K$ if $\alpha \geqslant a\lambda_n^m$ and $e(m, \alpha) = (\alpha+\lambda_n^m)^{2n+1}[\alpha^{n+1}(\alpha+\lambda_n^m)^n - \alpha^{2n+1}]^{-1}/2$, otherwise. Then the parameter choice (4.7) reads

$$e(m, \alpha)\,\alpha^{2n+1}((T_m T_m^* + \alpha I)^{-(2n+1)} Q_m y_\delta, Q_m y_\delta) = \gamma\delta^2. \tag{5.4}$$

In [7] numerical aspects of this method have been discussed for the case $n=1$. Equation (5.4) can be solved using Newton's method. In our numerical examples it turned out that one needs about 7 to 12 iterations to find the solution of (5.4) with reasonable accuracy. After a special transformation of the system matrices, which needs $O(n(m)^3)$ operations, each iteration step can be performed in $O(n(m))$ operations. $n(m)$ is the dimension of W_m. For actual calculations and results about the optimal choice of γ see [7].

TABLE I

n	a	b	K
1	1	0.25	4
2	1.7808	0.6197	3.2274
3	2.5694	1.0101	2.97
4	3.3611	1.4078	2.8413

5.2. *Showalter's Method*

Here the regularized solution is defined by

$$x(m, \alpha, y_\delta) := \int_0^{\alpha^{-1}} \exp(-tT_m T_m^*)\, T_m^* \mu_\delta \, dt \tag{5.5}$$

which can be written in the form (3.4) with

$$U(\alpha, \lambda) = \begin{cases} \lambda^{-1}[1-\exp(-\lambda\alpha^{-1})] & \text{if } \lambda > 0 \\ \alpha^{-1} & \text{if } \lambda = 0. \end{cases} \tag{5.6}$$

Again U satisfies Assumption 4.4 with $C=1$, $K=L=L_m=1/b=2.455$, $b=4a\exp(-2a)\approx 0.4073$, where $a\approx 1.2564$ is the unique positive solution of $2a\exp(-a)+\exp(-a)-1=0$; there are no restrictions on $\bar{\alpha}, \bar{\lambda}, \hat{\alpha}, \hat{\lambda}$; $R(m, w) = K\|Q_m w\|^2$. The function $\bar{h}(m, \alpha)$ is given by

$$\bar{h}(m, \alpha) = \begin{cases} b/\alpha & \text{if } \alpha \geqslant \lambda_n^m/a \\ \lambda_n^m U(\alpha, \lambda_n^m) & \text{if } \alpha < \lambda_n^m/a. \end{cases} \tag{5.7}$$

Let $e(m, \alpha) = K$ if $\alpha \geqslant \lambda_n^m/a$ and $e(m, \alpha) = [2(1-\exp(-\lambda_n^m/\alpha))\exp(-\lambda_n^m/\alpha)]^{-1}$ otherwise. Then the parameter choice (4.7) reads

$$e(m, \alpha)(\exp(-2T_m T_m^*/\alpha)\, Q_m y_\delta, Q_m y_\delta) = \gamma\delta^2. \tag{5.8}$$

5.3. *Landweber–Fridman Iteration*

Let $\beta \in (0, \|T\|^{-2})$. The method is defined by

$$x_0^m(y_\delta) := \beta T_m^* y_\delta, \qquad x_{n+1}^m(y_\delta) = (I - \beta T_m^* T_m)\, x_n^m(y_\delta) + \beta T_m^* y_\delta \tag{5.9}$$

and can be written in the form (3.4) with

$$U(n, \lambda) = \lambda^{-1}[1-(1-\beta\lambda)^{n+1}]. \tag{5.10}$$

This function satisfies Assumption 4.4 on $(0, \|T\|^2)$ with $C=1$, $K=2$, $L_m = 2(2-\beta\lambda_n^m)(1-\beta\lambda_n^m)^4$, $L=4$, and no restrictions on $\bar{\lambda}, \hat{\lambda}, \bar{n}, \hat{n}$ (compare $\bar{\alpha}, \hat{\alpha}$), and hence on an interval containing $\sigma(T_m T_m^*)$ for each $m \in N$. We replace $\bar{h}(m, n)$ by

$$\tilde{h}(m, n) = \begin{cases} \beta(n+1)/2 & \text{if } n \leqslant n_0 + 1, \\ (\lambda_n^m)^{-1}[1 - b(1-\beta\lambda_n^m)^{n+1} & \text{if } n > n_0 + 1, \end{cases} \tag{5.11}$$

where $n_0 + 1 = [(\beta\lambda_n^m)^{-1}]$ and $b = b(n_0) = [2-\beta\lambda_n^m(n_0+2)](1-\beta\lambda_n^m)^{-(n_0+2)} \to \exp(1)$ as $n_0 \to \infty$. $\tilde{h}$ is easier to calculate than $\bar{h}$. Since one can show that there exist $0 < C_1 < C_2$ such that $C_1\tilde{h} \leqslant \bar{h} \leqslant C_2\tilde{h}$ for all $m, n \in N$, all results which have been proven above also hold with $\tilde{h}$ replaced by $\bar{h}$. Let

$e(m,n)=2$ if $n \leqslant n_0$ and $e(m,n)=b^{-1}(1-\beta\lambda_n^m)^{-(n+1)}$ if $n>n_0$ (again the index n of λ_n^m has nothing to do with the nth iteration). Then the stopping rule reads: Take $n=n(\delta)$ as the smallest integer which satisfies

$$e(m,n)((I-\beta T_m T_m^*)^{2(n+1)}(2I-\beta T_m T_m^*)\, Q_m y_\delta, Q_m y_\delta) \leqslant \gamma\delta^2. \quad (5.12)$$

One can rearrange iteration (5.9) in such a way that (5.12) can be checked at no extra cost. For $n \in N$ let

$$u_0^m(y_\delta)=Q_m y_\delta, \qquad u_{n+1}^m(y_\delta)=(I-\beta T_m T_m^*)\, u_n^m(y_\delta)+Q_m y_\delta; \quad (5.13)$$

then

$$x_n^m(y_\delta)=\beta T_m^* u_n^m(y_\delta) \quad (5.14)$$

and (5.12) is equivalent to

$$e(m,n)(u_{n+2}^m(y_\delta)-u_n^m(y_\delta), u_{n+1}^m(y_\delta)-u_n^m(y_\delta)) \leqslant \gamma\delta^2. \quad (5.15)$$

Once $u_{n+2}^m(y_\delta)$ has been calculated, (5.15) can be checked in $O(n(m))$ operations.

For some other iteration procedures, e.g., Lardy's method and Schulz' method, see [2].

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