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On the Choice of the Regularization Parameter for Iterated Tikhonov Regularization of Ill-Posed Problems*

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We propose a method for choosing the regularization parameter in iterated Tikhonov regularization of ill-posed linear equations that is based on quantities that arise during the calculations and leads to optimal convergence rates. © 1987 Academic Press, Inc.

1. INTRODUCTION

Let X, Y be Hilbert spaces, $T: X \to Y$ a bounded linear operator with non-closed range $R(T)$, and let $y \in D(T^\dagger) = R(T) + R(T)^\perp$, where $T^\dagger$ is the Moore–Penrose inverse T (cf. [9]).

The problem of determining the best approximate solution $T^\dagger y$ of

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

is ill-posed (cf. [11] for a general background on ill-posed problems). Throughout the paper, let $y_\delta \in Y$ satisfy

$$\| y - y_\delta \| \leqslant \delta. \tag{1.2}$$

Since $T^\dagger$ is unbounded, $T^\dagger y_\delta$ is not a reasonable approximation for $T^\dagger y$, even if $y_\delta \in D(T^\dagger)$. A standard method for approximating $T^\dagger y$ is Tikhonov regularization: For $\alpha > 0$, let $x_{\alpha,\delta}$ be the unique solution of

$$(T^*T + \alpha I)x = T^* y_\delta, \tag{1.3}$$

where T^* is the adjoint of T.

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A crucial problem is the choice of the "regularization parameter" α in dependence of the "noise level" δ (see [6] for a thorough discussion of this problem). An algorithm for a choice of α in dependence of the results of the calculations ("a posteriori choice") that leads to optimal convergence rates has been developed in [3]. However, this optimal convergence rate is at best

$$\|x_{\alpha,\delta} - T^\dagger y\| = O(\delta^{2/3}), \tag{1.4}$$

which can be achieved under the a priori smoothness condition

$$T^\dagger y \in R(T^* T). \tag{1.5}$$

A saturation result of C. Groetsch [5] says that a higher rate of convergence than in (1.4) cannot be expected even under higher smoothness assumptions.

However, higher rates of convergence can be obtained by "iterated Tikhonov regularization" (cf. [7]), which is defined as follows: Let $x^0_{\alpha,\delta} := 0$ and for all $j \in \mathbb{N}$, let $x^{j+1}_{\alpha,\delta}$ be the unique solution of

$$(T^* T + \alpha I)x = T^* y_\delta + \alpha x^j_{\alpha,\delta}. \tag{1.6}$$

Below, we will refer to $x^j_{\alpha,\delta}$ as the result of "iterated Tikhonov regularization of order j." It follows from the results in [7] (cf. [10] for corresponding superconvergence results) that (with suitable constants $D_1, D_2 > 0$),

$$\|x^j_{\alpha,\delta} - T^\dagger y\| \leqslant D_1 \frac{\delta}{\sqrt{\alpha}} + D_2 \alpha^\nu \tag{1.7}$$

under the smoothness condition

$$T^\dagger y \in R((T^* T)^\nu), \tag{1.8}$$

for $0 < \nu \leqslant j$. This implies that the best possible convergence rate under the condition (1.8) is

$$\|x^j_{\alpha,\delta} - T^\dagger y\| = O(\delta^{2\nu/(2\nu+1)}), \tag{1.9}$$

which can be arbitrarily close to the optimal rate $O(\delta)$ if the data are sufficiently smooth.

Note that iterated Tikhonov regularization is not much more expensive to compute than ordinary Tikhonov regularization, since the iteration (1.6) involves always the same operator, i.e., in its finite-dimensional version one Cholesky decomposition suffices. It is the aim of this paper to give an a posteriori method for choosing the regularization parameter for iterated Tikhonov regularization in such a way that the optimal rate (1.9) is achieved. This is done in the spirit of the "discrepancy principle" that is widely used for ordinary Tikhonov regularization (cf. [6, 8]) as modified in [3].

2. Optimal Choice of the Regularization Parameter

For $j \in \mathbb{N}$, let $x^j_{\alpha,\delta}$ be the result of iterated Tikhonov regularization of order j as defined in Section 1, and let

$$\rho_j(\alpha) := \|T^*Tx^j_{\alpha,\delta} - T^*y_\delta\|^2. \tag{2.1}$$

Thus, $\rho_j(\alpha)$ is the square of the residual of the normal equation for (1.1) when $x^j_{\alpha,\delta}$ is used as the approximate solution.

Lemma 2.1. *ρ_j: $]0, +\infty[\to \mathbb{R}$ is continuous and strictly increasing. For all $j \geq 2$ and $\alpha > 0$, $\rho_j(\alpha) \leq \rho_{j-1}(\alpha)$. Furthermore, for all $j \in \mathbb{N}$, $\lim_{\alpha \to 0} \rho_j(\alpha) = 0$ and $\lim_{\alpha \to +\infty} \rho_j(\alpha) = \|T^*y_\delta\|^2$.*

Proof. Let $\{E_\lambda\}$ be the spectral family generated by T^*T. It follows by induction that for any $j \in \mathbb{N}$,

$$(\alpha I + T^*T)^j x^j_{\alpha,\delta} = \sum_{k=0}^{j-1} \binom{j}{k+1} \alpha^{j-k-1} (T^*T)^k T^*y_\delta, \tag{2.2}$$

so that $x^j_{\alpha,\delta} = (\int_0^\infty g_\alpha(\lambda)\, dE_\lambda)\, T^*y_\delta$, with

$$g_\alpha(\lambda) = (\alpha+\lambda)^{-j} \sum_{k=0}^{j-1} \binom{j}{k+1} \alpha^{j-k-1} \lambda^k = \frac{(\alpha+\lambda)^j - \alpha^j}{\lambda(\alpha+\lambda)^j}$$

(cf. [10]). Thus,

$$\rho_j(\alpha) = \int_0^\infty [\lambda g_\alpha(\lambda) - 1]^2\, d\,\|E_\lambda T^*y_\delta\|^2 = \int_0^\infty \left(\frac{\alpha}{\alpha+\lambda}\right)^{2j} d\,\|E_\lambda T^*y_\delta\|^2.$$

Since the integrand is continuous and strictly increasing in α, so is ρ_j. It also follows immediately that $\lim_{\alpha \to +\infty} \rho_j(\alpha) = \|T^*y_\delta\|^2$. It follows from the definition of iterated Tikhonov regularization that for all $j \in \mathbb{N}$,

$$T^*Tx^j_{\alpha,\delta} - T^*y_\delta = \alpha(x^{j-1}_{\alpha,\delta} - x^j_{\alpha,\delta}); \tag{2.3}$$

now,

$$\begin{aligned} x^{j-1}_{\alpha,\delta} - x^j_{\alpha,\delta} &= (T^*T + \alpha I)^{-1}[T^*Tx^{j-1}_{\alpha,\delta} + \alpha x^{j-1}_{\alpha,\delta} - T^*y_\delta - \alpha x^{j-1}_{\alpha,\delta}] \\ &= (T^*T + \alpha I)^{-1}[T^*Tx^{j-1}_{\alpha,\delta} - T^*y_\delta], \end{aligned}$$

so that

$$T^*Tx^j_{\alpha,\delta} - T^*y_\delta = \alpha(T^*T+\alpha I)^{-1}[T^*Tx^{j-1}_{\alpha,\delta} - T^*y_\delta] \tag{2.4}$$

holds for $j \geqslant 2$. Since $\|(T^*T+\alpha I)^{-1}\| \leqslant 1/\alpha$, this implies

$$\rho_j(\alpha) \leqslant \rho_{j-1}(\alpha). \tag{2.5}$$

Since $\lim_{\alpha\to 0} \rho_1(\alpha) = 0$ (cf. [4, Lemma 3.1]), this proves that $\lim_{\alpha\to 0} \rho_j(\alpha) = 0$. ∎

Note that (2.3) implies that

$$\rho_j(\alpha) = \alpha^2 \|x^{j-1}_{\alpha,\delta} - x^j_{\alpha,\delta}\|^2, \tag{2.6}$$

which can be computed without much effort during the calculations. From now on, we assume that

$$T^*y \neq 0, \qquad T^*y_\delta \neq 0; \tag{2.7}$$

otherwise either the exact or the approximate solution is 0.

Let $p, q > 0$; we propose to choose the regularization parameter α for iterated Tikhonov regularization of order j with noisy data y_δ as in (1.2) as the unique root of the equation

$$\rho_j(\alpha) = \delta^p \cdot \alpha^{-q}, \tag{2.8}$$

which we will denote by $\alpha_j(\delta)$. The values of p and q will be fixed later. The unique solvability of (2.8) for any $\delta > 0$ follows from Lemma 2.1.

The following Lemmata give information about the asymptotic behaviour of $\alpha_j(\delta)$.

LEMMA 2.2. $\lim_{\delta\to 0} \alpha_j(\delta) = 0$.

Proof. Assume first that there is a sequence $(\delta_n) \to 0$ such that $(\alpha_n) := (\alpha_j(\delta_n)) \to +\infty$. It follows from the definition of $x^j_{\alpha,\delta}$ that for sufficiently large $n \in \mathbb{N}$ and for all $i \in \mathbb{N}$,

$$\|x^i_{\alpha_n,\delta_n}\| \leqslant \frac{\|T^*y_{\delta_n}\| + \alpha_n \|x^{i-1}_{\alpha_n,\delta_n}\|}{\alpha_n - \|T^*T\|}, \tag{2.9}$$

which implies that $\lim_{n\to\infty} x^j_{\alpha_n,\delta_n} = 0$. Hence $0 = \lim_{n\to\infty}(\delta_n^p \alpha_n^{-q}) = \lim_{n\to\infty} \rho_j(\alpha_n) = \|T^*y_\delta\|^2$, which contradicts (2.7). Thus, $\limsup_{\delta\to 0} \alpha_j(\delta) < +\infty$. Now, assume that there is a sequence $(\delta_n) \to 0$ with

$$(\alpha_n) := (\alpha_j(\delta_n)) \to c > 0.$$

Since $(T^*T+\alpha_n I)^{-1}$ converges (in the operator norm) to $(T^*T+cI)^{-1}$, we have $\lim_{n\to\infty} x^1_{\alpha_n,\delta_n}=(T^*T+cI)^{-1}T^*y=: x_c$. Together with (2.8) and (2.4), this implies that

$$\begin{aligned} 0&=\lim_{n\to\infty}\rho_j(\alpha_n)=\lim_{n\to\infty}[\alpha_n^{2j-1}\,\|(T^*T+\alpha_n I)^{1-j}(T^*Tx^1_{\alpha_n,\delta_n}-T^*y_\delta)\|^2]\\ &=c^{2j-1}\,\|(T^*T+cI)^{1-j}(T^*Tx_c-T^*y)\|^2. \end{aligned}$$

Thus, $T^*Tx_c=T^*y$, hence $x_c=0$ by the definition of x_c, which contradicts (2.7). Thus, $\lim_{\delta\to 0}\alpha_j(\delta)=0$. ∎

LEMMA 2.3. *For all* $j\geqslant 2$ *and* $\delta>0$, $\alpha_j(\delta)\geqslant\alpha_{j-1}(\delta)$.

Proof. It follows from the definition of α_j and from Lemma 2.1 that $\alpha_{j-1}(\delta)^q\cdot\rho_j(\alpha_{j-1}(\delta))\leqslant\alpha_{j-1}(\delta)^q\rho_{j-1}(\alpha_{j-1}(\delta))=\delta^p$, which implies together with the monotonicity of $\alpha\to\alpha^q\cdot\rho_j(\alpha)$ that the assertion holds. ∎

LEMMA 2.4. *If* $0<p\leqslant 2q$, *then* $\lim_{\delta\to 0}\delta^2/(\alpha_j(\delta))=0$.

Proof. For $j=1$, this is proven in [3, Lemma 2.3]. The assertion follows now together with Lemma 2.3. ∎

PROPOSITION 2.5. *If* $0<p\leqslant 2q$, *then* $\lim_{\delta\to 0}x^j_{\alpha_j(\delta),\delta}=T^\dagger y$.

Proof. If (1.8) holds for some $\delta>0$, then the assertion follows from (1.7), Lemma 2.2, and Lemma 2.4. Otherwise, one has to use, e.g., [2, Theorem 3.2] with $U(\alpha,\lambda)=g_\alpha(\lambda)$, where g_α is as in Lemma 2.1. ∎

LEMMA 2.6. *Let* $j\geqslant 2$. *If* $0<p\leqslant(2q+4)/(2j-1)$ *and* $q\geqslant 1/(j-1)$, *then* $\lim_{\delta\to 0}(\delta^2\cdot\alpha_j(\delta)^{1-2j})=0$.

Proof. It follows as in Proposition 2.5 that $\lim_{\delta\to 0}x^{j-1}_{\alpha_j(\delta),\delta}=T^\dagger y$; note that under our assumptions, $p\leqslant 2q$ holds. Thus, $\lim_{\delta\to 0}\|x^j_{\alpha_j(\delta),\delta}-x^{j-1}_{\alpha_j(\delta),\delta}\|^2=0$, which implies together with (2.6) that

$$\lim_{\delta\to 0}(\rho_j(\alpha_j(\delta))\cdot\alpha_j(\delta)^{-2})=0. \tag{2.10}$$

Now, $(\delta^2\cdot\alpha_j(\delta)^{1-2j})^{p/2}=\delta^p\cdot\alpha_j(\delta)^{-q}\alpha_j(\delta)^{q+(p/2)-pj}=[\rho_j(\alpha_j(\delta))\cdot\alpha_j(\delta)^{-2}]\cdot\alpha_j(\delta)^{q+(p/2)-pj+2}\to 0$ as $\delta\to 0$ because of (2.10), Lemma 2.2, and the fact that for our choices of p and q, $q+(p/2)-pj+2\geqslant 0$. ∎

LEMMA 2.7. *Let* j, p, q *be as in Lemma* 2.6 *and assume that* (1.8) *holds with* $v=j-1$. *Then there are constants* $C_1, C_2>0$ *such that*

$$C_1\leqslant\delta^p\cdot\alpha_j(\delta)^{-q-2j}\leqslant C_2$$

holds.

Proof. Let $w \in X$ be such that $(T^*T)^{j-1}w = T^\dagger y$. Because of (2.7), $w \neq 0$. We may assume without loss of generality that $w \in N(T^*T)^\perp$. We first show that

$$\lim_{\delta \to 0} [\alpha_j(\delta)^{1-j}(x^j_{\alpha_j(\delta),\delta} - x^{j-1}_{\alpha_j(\delta),\delta})] = w. \tag{2.11}$$

Let z_j and z_{j-1} be defined as $x^j_{\alpha_j(\delta),\delta}$ and $x^{j-1}_{\alpha_j(\delta),\delta}$, respectively, but with y instead of y_δ (with the same values for $\alpha_j(\delta)$, however!). Then $\|(x^j_{\alpha_j(\delta),\delta} - x^{j-1}_{\alpha_j(\delta),\delta}) - (z_j - z_{j-1})\| \leqslant D \cdot \delta \cdot \alpha_j(\delta)^{-1/2}$ with suitable D (cf. [7, Theorem 4.1]). This shows together with Lemma 2.6 that it suffices to show that

$$\lim_{\delta \to 0} [\alpha_j(\delta)^{1-j}(z_j - z_{j-1})] = w \tag{2.12}$$

in order to prove (2.11). Let $\alpha := \alpha_j(\delta)$. It follows from (2.3) and (2.4) (both with z_j instead of $x^j_{\alpha,\delta}$) by induction that $z_j - z_{j-1} = \alpha^{j-1}(T^*T + \alpha I)^{-j}T^*y$. Since $T^*TT^\dagger y = T^*y$, this implies together with the definition of w that

$$z_j - z_{j-1} = \alpha^{j-1}(T^*T + \alpha I)^{-j}(T^*T)^j w. \tag{2.13}$$

Let $\{E_\lambda\}$ and g_α be as in the proof of Lemma 2.1; (2.13) implies then that $\|\alpha^{1-j}(z_j - z_{j-1}) - w\|^2 = \int_0^\infty ((\lambda^j/(\alpha+\lambda)^j) - 1)^2 d\,\|E_\lambda w\|^2$.

By the Dominated Convergence Theorem, it follows that

$$\lim_{\delta \to 0} \|\alpha_j(\delta)^{1-j}(z_j - z_{j-1}) - w\|^2 = \int_0^\infty f(\lambda)\,d\,\|E_\lambda w\|^2,$$

with $f(0) = 1$ and $f(\lambda) = 0$ for $\lambda > 0$. But since $\int_0^\infty f(\lambda)d\,\|E_\lambda w\|^2$ is the projection of w onto $N(T^*T)$, this expression vanishes. This proves (2.12) and hence (2.11).

Because of (2.6), (2.11) implies that

$$\lim_{\delta \to 0} (\delta^p \cdot \alpha_j(\delta)^{-q-2j}) = \lim_{\delta \to 0} (\rho_j(\alpha_j(\delta)) \cdot \alpha_j(\delta)^{-2j}) = \|w\|^2 > 0.$$

From this, the assertion follows immediately. ∎

We have seen in Proposition 2.5 that for $0 < p \leqslant 2q$, the parameter choice according to (2.8) always leads to convergence. The estimates we derived enable us to give values of p and q that lead to the optimal convergence rates.

THEOREM 2.8. *For each $\delta > 0$ and $y_\delta \in Y$ fulfilling* (1.2), *let $x^j_{\alpha_j(\delta),\delta}$ be the result of iterated Tikhonov regularization of order $j \geqslant 2$ as described by* (1.6), *where $\alpha_j(\delta)$ is the unique solution of* (2.8); *assume that* (2.7) *holds, that*

$$\frac{p}{2}(1 + 2j) - 2j = q \geqslant 2j^2 - 3j - 1 \tag{2.14}$$

and that (1.8) *holds with* $v = j$. *Then*

$$\|x^j_{\alpha_j(\delta),\delta} - T^\dagger y\| = O(\delta^{2j/(2j+1)}) \tag{2.15}$$

holds.

Proof. An easy calculation shows that (2.14) implies that the assumptions of Lemma 2.7 are fulfilled. Let C_1, C_2 be as in Lemma 2.7, D_1, D_2 be as in (1.7); we conclude from (1.7) and Lemma 2.7 that

$$\begin{aligned}\|x^j_{\alpha_j(\delta),\delta} - T^\dagger y\| &\leqslant D_1\, \delta \cdot \alpha_j(\delta)^{-1/2} + D_2 \alpha_j(\delta)^j \\ &\leqslant D_1 \cdot C_2^{1/(2(q+2j))} \cdot \delta^{1-p/(2(q+2j))} \\ &\quad + D_2 \cdot C_1^{-j/(q+2j)} \cdot \delta^{jp/(q+2j)} = O(\delta^{2j/(2j+1)})\end{aligned}$$

because of (2.14). ∎

Remark 2.9. This result shows that if $T^\dagger y \in R((T^*T)^j)$ and if one chooses $\alpha_j(\delta)$ according to our method with p, q as in (2.14), then iterated Tikhonov regularization of order j converges with the optimal rate, as a comparison of (2.15) and (1.9) indicates. We will not try to derive similar results under weaker smoothness assumptions, since then one will probably use a correspondingly lower order of iterated Tikhonov regularization anyway.

For $j = 2$, (2.14) reduces to $5p/2 - 4 = q \geqslant 1$, so that $p = 2$ and $q = 1$ are feasible choices, which is (as for ordinary Tikhonov regularization, cf. [3, Remark 2.2]) a variant of Arcangeli's method [1].

The question of how to solve (2.8) numerically remains. As we will see, this can be done by Newton's method, which converges globally here. Let

$$f(\alpha) := \alpha^q \cdot \rho_j(\alpha) - \delta^p, \tag{2.16}$$

and for $\alpha_0 > 0$, let

$$\alpha_n = \alpha_{n-1} - \frac{f(\alpha_{n-1})}{f'(\alpha_{n-1})} \qquad (n \in \mathbb{N}). \tag{2.17}$$

We will see that this algorithm can be performed (see (2.18) for a formula for f') and converges to $\alpha_j(\delta)$:

PROPOSITION 2.10. *Let* $q \geqslant 1$. *For any* $\alpha_0 > 0$, *the sequence* (α_n) *defined by* (2.17) *converges to* $\alpha_j(\delta)$, *the unique solution of* (2.8). *The convergence is monotonically decreasing and locally quadratic.*

Proof. As has been noted (for $i = 2$) in [4], an easy calculation shows that for any $i \geqslant 2$ and $\alpha > 0$,

$$\alpha \frac{dx^{i-1}_\alpha}{d\alpha} = x^{i-1}_\alpha - x^i_\alpha \tag{2.18}$$

holds, where we write x_α^j for $x_{\alpha,\delta}^j$ throughout this proof. This implies together with (2.6) that

$$f'(\alpha)=(q+2)\,\alpha^{q+1}\,\|x_\alpha^{j-1}-x_\alpha^j\|^2 + 2\alpha^{q+2}\left\langle x_\alpha^{j-1}-x_\alpha^j,\frac{d}{d\alpha}(x_\alpha^{j-1}-x_\alpha^j)\right\rangle$$
$$=(q+2)\,\alpha^{q+1}\,\|x_\alpha^{j-1}-x_\alpha^j\|^2 + 2\alpha^{q+2}\left\langle x_\alpha^{j-1}-x_\alpha^j,\frac{dx_\alpha^{j-1}}{d\alpha}+\frac{x_\alpha^{j+1}-x_\alpha^j}{\alpha}\right\rangle$$

and hence

$$f'(\alpha)=(q+4)\,\alpha^{q+1}\,\|x_\alpha^{j-1}-x_\alpha^j\|^2+2\alpha^{q+1}\langle x_\alpha^{j-1}-x_\alpha^j, x_\alpha^{j+1}-x_\alpha^j\rangle. \tag{2.19}$$

Together with (2.5) and (2.6), (2.19) implies that $f'(\alpha)\geqslant (q+2)\,\alpha^{q+1}\,\|x_\alpha^{j-1}-x_\alpha^j\|^2$ and hence $f(\alpha)/f'(\alpha)\leqslant \alpha/(q+2)$. Thus, for $n\in\mathbb{N}$, $\alpha_{n+1}\geqslant\alpha_n-\alpha_n/(q+2)=(q+1)/(q+2)\,\alpha_n>0$, so that (2.17) can actually be performed. The same methods that were used for estimating $f'(\alpha)$ yield after some calculation that $f''(\alpha)\geqslant 0$.

Hence, it follows by Taylor expansion around $\alpha_j(\delta)$ that $0=f(\alpha_j(\delta))\geqslant f(\alpha)+f'(\alpha)\cdot(\alpha_j(\delta)-\alpha)$ holds for all $\alpha>0$. Since $f'>0$, this implies $\alpha-(f(\alpha))/(f'(\alpha))\geqslant\alpha_j(\delta)$, for all $\alpha>0$, and hence

$$\alpha_n\geqslant\alpha_j(\delta)\qquad\text{for all } n\in\mathbb{N}. \tag{2.20}$$

Now, let $\alpha_n>\alpha_j(\delta)$; because of the monotonicity of f (cf. Lemma 2.1), this implies $f(\alpha_n)>0$ and hence $\alpha_{n+1}<\alpha_n$. Thus, (α_n) is monotonically decreasing and hence (cf. (2.20)) convergent. It follows by continuity that the limit point is a zero of f and hence equals $\alpha_j(\delta)$. Since $f'(\alpha_j(\delta))>0$, the convergence is locally quadratic. ▮

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