THE MONOTONE ERROR RULE FOR PARAMETER CHOICE IN REGULARIZATION METHODS [1]

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Abstract. We consider ill-posed problems $Au = f$ with minimum-norm solution $u^\dagger$. We suppose that instead of f noisy data f_δ are available with $\|f - f_\delta\| \le \delta$ and that $A \in \mathcal{L}(H, F)$ is a linear bounded operator between Hilbert spaces H and F with non-closed range $R(A)$. Regularized solutions u_r are obtained by a general regularization scheme which includes Tikhonov regularization $u_r = (A^*A + r^{-1}I)^{-1}A^*f_\delta$, iterative regularization and others. We discuss a new *a posteriori* rule for choosing the regularization parameter $r = r(\delta)$ which we call *monotone error rule* (ME rule). In this rule we choose $r = r_{ME}$ as the largest r-value for which we are able to prove that the error $\|u_r - u^\dagger\|$ is monotonically decreasing for $r \in [0, r_{ME}]$. Our rule leads to order optimal error bounds. Numerical results are given.

1. Introduction

In this paper we consider linear ill-posed problems

$$Au = f \tag{1}$$

where $A \in \mathcal{L}(H, F)$ is a bounded operator with non-closed range $R(A)$ and H, F are infinite dimensional real Hilbert spaces with inner products $(\cdot, \cdot)$ and norms $\|\cdot\|$. We are interested in the minimum-norm solution $u^\dagger$ of problem (1) and assume that instead of *exact* data f there are given *noisy* data $f_\delta \in F$ with $\|f - f_\delta\| \le \delta$ and known noise level δ.

Ill-posed problems (1) arise in a wide variety of problems in applied sciences. For their stable numerical solution regularization methods are necessary, see [2, 5, 10]. A large class of regularization methods has the form

$$u_r = g_r(A^*A)A^*f_\delta\,. \tag{2}$$

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Here $g_r(\lambda) : [0,a] \to \mathbb{R}$ with $a = \|A^*A\|$ is a family of piecewise continuous functions depending on a positive regularization parameter $r > 0$, and the operator function g_r is defined according to $g_r(A^*A) = \int_0^a g_r(\lambda)\,\mathrm{d}E_\lambda$ where $A^*A = \int_0^a \lambda\,\mathrm{d}E_\lambda$ is the spectral decomposition of A^*A. For the function g_r which characterizes the special regularization method we suppose:

Assumption (A1). There exist positive constants γ_*, γ_p and p_0 such that the function $g_r(\lambda) : (0,a] \to \mathbb{R}$ with $\|A^*A\| \le a$ satisfies the estimates

$$\text{(i)} \qquad \sup_{0\le\lambda\le a} \sqrt{\lambda}\,|g_r(\lambda)| \le \gamma_* \sqrt{r}\,,$$

$$\text{(ii)} \qquad \sup_{0\le\lambda\le a} \lambda^p\,|1-\lambda g_r(\lambda)| \le \gamma_p r^{-p} \quad \text{for all} \quad p \in (0,p_0]\,,$$

$$\text{(iii)} \qquad |1-\lambda g_{r_1}(\lambda)| \le |1-\lambda g_{r_2}(\lambda)| \quad \text{for} \quad 0\le\lambda\le a \quad \text{and} \quad 0 \le r_2 \le r_1\,.$$

The (maximal) number p_0 in Assumption (A1) is called *qualification [10]* of the regularization method (2).

One of the main problems in applying regularization methods is the proper choice of the regularization parameter $r = r(\delta)$. Due to (ii) and (iii), in the case of *exact* data we have monotone convergence $\|u_r - u^\dagger\| \to 0$ for $r \to \infty$. In the case of *noisy* data the monotone decrease of the error $\|u_r - u^\dagger\|$ can only be guaranteed for small r. Typically $\|u_r - u^\dagger\|$ diverges for $r \to \infty$. Therefore a rule for the proper choice of r is necessary. In this paper we study a new rule in which $r = r_{ME}(\delta)$ is chosen as the largest r-value for which we are able to prove (under the assumption $\|f - f_\delta\| \le \delta$) that the error $\|u_r - u^\dagger\|$ is monotonically decreasing for $r \in [0, r_{ME}]$. We call this rule the *monotone error rule* (ME rule).

2. Continuous Regularization Methods

2.1. THE ME RULE

Three well known *a posteriori* rules for choosing the regularization parameter r in continuous regularization methods (2) are:

(i) *Morozov's discrepancy principle [2, 10].* In this principle (*D principle*) the parameter $r = r_D$ is chosen as the solution of the equation

$$d_D(r) := \|f_\delta - Au_r\| = C\delta \quad \text{with} \quad C \ge 1\,.$$

(ii) *Rule of Raus [7].* In this rule, which we call *R rule*, the regularization parameter $r = r_R$ is chosen as the solution of the equation

$$d_{RG}(r) := \left\| (I - g_r(AA^*)AA^*)^{1/(2p_0)}(f_\delta - Au_r) \right\| = C\delta \quad \text{with} \quad C \ge 1\,.$$

Here p_0 is the (largest) constant from Assumption (A1), (ii).

(iii) *Rule of Engl and Gfrerer [1].* In this rule, which we call *EG rule*, $r = r_{EG}$ is chosen as the solution of the equation

$$d_{EG}(r) := \gamma^{-1/2}\Big(f_\delta - Au_r, \frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big)^{1/2} = C\delta \quad \text{with} \quad C \geq 1\,.$$

Here γ is the (smallest) constant with $\sup\limits_{0\leq\lambda\leq a} |g_r(\lambda)| \leq \gamma r$.

For ordinary and iterated Tikhonov methods the $R-$ and EG rules coincide. We call the resulting rule Raus-Gfrerer rule (RG rule).

In our ME rule the aim consists in searching for the largest regularization parameter $r = r_{ME}$ for which we can guarantee that $\frac{\mathrm{d}}{\mathrm{d}r}\|u_r - u^\dagger\|^2 \leq 0$ for all $r \in (0, r_{ME}]$. From (2) and the identity $g_r(A^*A)A^* = A^*g_r(AA^*)$ we obtain

$$\begin{aligned} \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}r}\|u_r - u^\dagger\|^2 &= \Big((f_\delta - f) - (f_\delta - Au_r), \frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big) \\ &\leq \Big\|\frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big\| \left\{\delta - \frac{\Big(f_\delta - Au_r, \frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big)}{\Big\|\frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big\|}\right\}. \end{aligned}$$

This estimate leads us to following *a posteriori* rule of choosing the regularization parameter in continuous regularization methods (2):

ME rule. For regularization methods with monotonically decreasing functions $d_{ME}(r)$, choose $r = r_{ME}$ as the solution of the equation

$$d_{ME}(r) := \frac{\Big(f_\delta - Au_r, \frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big)}{\Big\|\frac{\mathrm{d}}{\mathrm{d}r}g_r(AA^*)f_\delta\Big\|} = \delta\,.$$

2.2. ORDINARY AND ITERATED TIKHONOV REGULARIZATION

In these methods we start with $u_{r,0} = 0$ and compute the regularized solution $u_r := u_{\alpha,m}$ recursively by solving the m operator equations

$$(A^*A + \alpha I)u_{\alpha,k} = A^*f_\delta + \alpha u_{\alpha,k-1}\,, \quad k = 1, 2, ..., m \tag{3}$$

where $r = 1/\alpha$. For $m = 1$ this method is the method of *ordinary* Tikhonov regularization. In these methods we have $g_r(\lambda) = [1 - (1 + r\lambda)^{-m}]/\lambda$ with some fixed positive integer $m \geq 1$. Assumption (A1) is satisfied with $p_0 = m$, $\gamma_p = (p/m)^p(1 - p/m)^{m-p} \leq 1$, $\gamma_* = 1/2$ for $m = 1$ and $\gamma_* = \sqrt{m}$ for $m \geq 2$. The functions for the $RG-$ and ME rules have the form

$$d_{RG}(\alpha) = (r_{\alpha,m}, r_{\alpha,m+1})^{1/2} \quad \text{and} \quad d_{ME}(\alpha) = \frac{(r_{\alpha,m}, r_{\alpha,m+1})}{\|r_{\alpha,m+1}\|}$$

with $r_{\alpha,m} = f_\delta - Au_{\alpha,m}$. The function d_{ME} possesses following properties (see Tautenhahn [8] for $m = 1$ and the papers [4, 9] for $m \geq 1$):

Theorem 1 *Let P denote the orthoprojection of F onto $N(A^*) = \overline{R(A)}^\perp$ and let $A^* f_\delta \neq 0$. Then:*

(i) *$d_{ME}(\alpha)$ is strictly monotonically increasing and obeys $d_{ME}(0) = \|Pf_\delta\|$ and $\lim_{\alpha\to\infty} d_{ME}(\alpha) = \|f_\delta\|$. The equation $d_{ME}(\alpha) = \delta$ has a unique solution α_{ME} provided $\|Pf_\delta\| < \delta < \|f_\delta\|$.*

(ii) *For all $\alpha \in (\alpha_{ME}, \infty)$ there holds $\frac{\mathrm{d}}{\mathrm{d}\alpha}\|u_{\alpha,m} - u^\dagger\|^2 > 0$.*

(iii) *There holds $d_{RG}(\alpha) < d_{ME}(\alpha) < d_D(\alpha)$. If $C = 1$ in the D principle and in the RG rule, then $\alpha_D < \alpha_{ME} < \alpha_{RG}$.*

From (ii) and (iii) there follows

$$\|u_{\alpha_{ME}} - u^\dagger\| < \|u_{\alpha_{RG}} - u^\dagger\| \,. \tag{4}$$

Hence, the ME rule provides always a smaller error than the RG rule. Exploiting the monotonicity property (ii) we obtain for the parameter choice $\alpha = \alpha_{ME}$ order optimal error bounds [9]:

Theorem 2 *Assume $u^\dagger = (A^*A)^{p/2} v$ with $\|v\| \leq E$. Then*

$$\|u_{\alpha_{ME}} - u^\dagger\| \leq \left\{ 2^{\frac{p}{p+1}} + 2^{\frac{-1}{p+1}} \gamma_*(\gamma_{p/2})^{\frac{1}{p}} \right\} E^{\frac{1}{p+1}}\, \delta^{\frac{p}{p+1}} \quad \textit{for} \quad p \in (0, 2m]\,.$$

2.3. ASYMPTOTICAL REGULARIZATION

In this regularization method the regularized solution is given by $u_r = u(r)$ where $u(r)$ is the solution of the initial value problem

$$\dot{u}(t) + A^*Au(t) = A^* f_\delta \quad \text{for} \quad 0 < t \leq r\,, \quad u(0) = 0\,.$$

This method has the form (2) with $g_r(\lambda) = (1 - e^{-r\lambda})/\lambda$ and Assumption (A1) is satisfied with $\gamma_p = (p/e)^p$, $p_0 = \infty$ and $\gamma_* = 0.6382$. For this method there holds $d_R(r) = d_{EG}(r) = d_{ME}(r) = d_D(r)$. Consequently, all the results known for the D principle [10, 2] are also true for the R rule, EG rule and ME rule, respectively. Exploiting the monotonicity property of our ME rule we obtain that Theorem 2 is valid for the range $p \in (0, \infty)$ and that in the D principle the best constant for C is $C = 1$:

Theorem 3 *Let $A^* f_\delta \neq 0$ and let r_D the regularization parameter of the D principle with $C = 1$. Then $\|u_{r_D} - u^\dagger\| < \|u_r - u^\dagger\|$ for all $r < r_D$.*

3. Iterative Regularization Methods

3.1. THE ME RULE

Iterative methods for approximately solving ill-posed problems are especially attractive for *large-scale* problems (cf., e.g., Hanke *et al.*[5]). Such problems arise e.g. in the field of parameter identification in differential equations.

We consider iterative methods of the general form

$$u_n = u_{n-1} + g(A^*A)A^*[f_\delta - Au_{n-1}]\,, \quad n = 1, 2, ..., r, \quad u_0 = 0 \qquad (5)$$

with continuous functions $g : [0, a] \to \mathbb{R}$ for which we assume that

$$0 < g(\lambda) < 2/\lambda \quad \text{for} \quad 0 \leq \lambda \leq a\,. \qquad (6)$$

Note that (5) has the form (2) with $g_r(\lambda) = [1 - (1 - \lambda g(\lambda))^r]/\lambda$. Two well-known *a posteriori* rules of choosing $r = r(\delta)$ are:

(i) *Morozov's discrepancy pinciple* [2, 10]. In this principle (*D principle*) the iteration number $r = r_D$ is chosen as the first index n satisfying

$$d_D(n) := \|r_n\| \leq C\delta \quad \text{with} \quad r_n = f_\delta - Au_n \quad \text{and} \quad C \geq 1\,.$$

(ii) *Rule of Engl and Gfrerer* [1]. In this rule, which we call *EG rule*, the iteration number $r = r_{EG}$ is chosen as the first index n satisfying

$$d_{EG}(n) := \frac{(r_n + r_{n+1}, g(AA^*)r_n)^{1/2}}{(2\kappa)^{1/2}} \leq C\delta \quad \text{with} \quad C \geq 1\,.$$

Here κ is a constant with $\kappa = \sup\{g(\lambda) \,|\, 0 \leq \lambda \leq a\}$.

In our ME rule we search for the *largest* iteration number $r = r_{ME}$ for which we can guarantee that

$$\|u_n - u^\dagger\| < \|u_{n-1} - u^\dagger\| \quad \text{for all} \quad n = 1, 2, ..., r_{ME}\,. \qquad (7)$$

We use (5) as well as the relations $r_n = [I - AA^*g(AA^*)]r_{n-1}$ and $g(A^*A)A^* = A^*g(AA^*)$ with $r_n = f_\delta - Au_n$ and obtain

$$\begin{aligned} \|u_n - u^\dagger\|^2 \quad - \quad \|u_{n-1} - u^\dagger\|^2 &= \Big(2(f_\delta - f) - (r_{n-1} + r_n), g(AA^*)r_{n-1}\Big) \\ &\leq \quad 2\|g(AA^*)r_{n-1}\| \left\{\delta - \frac{(r_{n-1} + r_n, g(AA^*)r_{n-1})}{2\|g(AA^*)r_{n-1}\|}\right\}. \qquad (8) \end{aligned}$$

This estimate leads us to the following *a posteriori* rule of choosing the iteration number $r = r_{ME}$ in method (5), which we call *monotone error rule*:

ME rule. Choose $r = r_{ME}$ as the first index n satisfying

$$d_{ME}(n) := \frac{(r_n + r_{n+1}, g(AA^*)r_n)}{2\|g(AA^*)r_n\|} \leq \delta\,.$$

Note that due to (8) the property (7) is satisfied. Some further general properties of this rule are studied in the paper of Hämarik [3].

3.2. LANDWEBER'S METHOD

This method is characterized by (5) with $g(\lambda) = \beta$ and $\beta \in (0, 2/a)$. For this method Assumption (A1) holds with $\gamma_p = [p/(\beta e)]^p$, $p_0 = \infty$ and $\gamma_* = \sqrt{\beta}$. The EG– and ME rules are characterized by

$$d_{EG}(n) = \frac{(r_n + r_{n+1}, r_n)^{1/2}}{\sqrt{2}} \quad \text{and} \quad d_{ME}(n) = \frac{(r_n + r_{n+1}, r_n)}{2\|r_n\|}\,.$$

From the identity $r_{n+1} = [I - g(AA^*)AA^*]r_n$ we obtain in case $A^*f_\delta \neq 0$ that

$$\|r_{n+1}\|^2 < (r_n, r_{n+1}) < \|r_n\|^2 \quad \text{for all} \quad n \geq 0 \tag{9}$$

holds true for arbitrary iteration methods (5) that fulfill (6). Consequently,

$$d_D(n+1) < d_{ME}(n) < d_{EG}(n) < d_D(n) \quad \text{for all} \quad n \geq 0\,. \tag{10}$$

From (10) and the fact that $d_D(n)$ is strictly monotonically decreasing with $\lim_{n\to\infty} d_D(n) = \|Pf_\delta\|$ we conclude:

Theorem 4 *Let $A^*f_\delta \neq 0$. Then:*

(i) *The functions $d_{ME}(n)$ and $d_{EG}(n)$ are strictly monotonically decreasing and obey $\lim_{n\to\infty} d_{ME}(n) = \lim_{n\to\infty} d_{EG}(n) = \|Pf_\delta\|$.*

(ii) *Let $\|Pf_\delta\| < C\delta$, then the regularization parameters r_D, r_{ME} and r_{EG} are well defined and in case $C = 1$ we have $r_D - 1 \leq r_{ME} \leq r_{EG} \leq r_D$.*

From Theorem 4 and property (7) we obtain that the iteration should not be stopped as long as $\|Au_{n+1} - f_\delta\| \geq \delta$ holds:

Theorem 5 *Let $A^*f_\delta \neq 0$. If $\|Au_{n+1} - f_\delta\| \geq \delta$, then $\|u_n - u^\dagger\| < \|u_{n-1} - u^\dagger\|$.*

3.3. IMPLICIT ITERATION SCHEME

This method is characterized by (5) with $g(\lambda) = (\lambda + \rho)^{-1}$ and $\rho > 0$. Assumption (A1) holds with $\gamma_p = (p/\rho)^p$, $p_0 = \infty$ and $\gamma_* = 0.6382/\sqrt{\rho}$. Since $g(AA^*)r_n = \rho^{-1}r_{n+1}$, for the EG– and ME rules we obtain

$$d_{EG}(n) = \frac{(r_n + r_{n+1}, r_{n+1})^{1/2}}{\sqrt{2}} \quad \text{and} \quad d_{ME}(n) = \frac{(r_n + r_{n+1}, r_{n+1})}{2\|r_{n+1}\|}\,.$$

Exploiting (9) we find

$$d_D(n+1) < d_{EG}(n) < d_{ME}(n) < d_D(n) \quad \text{for all} \quad n \geq 0\,. \tag{11}$$

From (11) and the fact that $d_D(n)$ is strictly monotonically decreasing we conclude that analogous properties as in Theorems 4 and 5 hold true.

4. Numerical Experiments

In this section we summarize some of our numerical experiments for integral equations of the first kind

$$(Au)(s) = \int_0^1 K(s,t)u(t)\,\mathrm{d}t = f(s)\,, \quad 0 \leq s \leq 1 \tag{12}$$

in a L^2-space setting with $H = F = L^2(0,1)$. The discretization is done by $n = 1200$ piecewise constant spline basis functions.

In our numerical experiments Tikhonov's method (3) with $m = 1$ has been used. The regularization parameter α has been chosen by the ME rule, the RG rule and the D principle, respectively. For C we have used $C = 1$.

Our test problem is taken from [6]. It is an equation (12) with kernel

$$K(s,t) = \begin{cases} s(1-t)(2t-t^2-s^2)/6 & \text{for} \quad 0 \leq s \leq t \leq 1 \\ t(1-s)(2s-s^2-t^2)/6 & \text{for} \quad 0 \leq t \leq s \leq 1\,. \end{cases}$$

The right-hand side f, the solution $u^\dagger$ and the maximal smoothness parameter p_* for which $u^\dagger = (A^*A)^{p/2}v$ with $\|v\| \leq E$ for all $p \in (0, p_*)$ are:

$$f(s) = \sin \pi s/\pi^4\,, \quad u(t) = \sin \pi t\,, \quad p_* = \infty\,. \tag{13}$$

In our computations we used instead of f randomly perturbed noisy data f_δ with $\|f - f_\delta\| = \delta$. Actually f has randomly perturbed 20 times. For every f_δ the regularized solution has been computed and the errors in Table 1 represent mean values. Following abbreviations have been used:

$$e_D = \|u_{\alpha_D} - u^\dagger\|\,, \quad e_{RG} = \|u_{\alpha_{RG}} - u^\dagger\|\,, \quad e_{ME} = \|u_{\alpha_{ME}} - u^\dagger\|\,.$$

Let us discuss the numerical results. Since $u^\dagger = (A^*A)^{p/2}v$ with $p \geq 2$ we conclude from Theorem 2 that we should obtain the convergence rate $O(\delta^{2/3})$ for the parameter choice $\alpha = \alpha_{ME}$, which also holds for $\alpha = \alpha_{RG}$. For $\alpha = \alpha_D$ we have to expect the convergence rate $O(\delta^{1/2})$. Table 1 verifies these results and shows that the ME– and RG rules provide more accurate regularized solutions than the D principle for δ sufficiently small.

Table 1. Errors for example (13)

δ	e_D	e_{RG}	e_{ME}	$e_D/\delta^{1/2}$	$e_{RG}/\delta^{2/3}$	$e_{ME}/\delta^{2/3}$
10^{-1}	.24581	.28266	.25211	.777	1.31	1.17
10^{-2}	.06768	.09226	.07889	.677	1.99	1.70
10^{-3}	.02039	.02073	.01721	.645	2.07	1.72
10^{-4}	.00624	.00493	.00415	.624	2.29	1.93
10^{-5}	.00212	.00117	.00098	.670	2.51	2.12

Finally we note that in all examples we observed that $e_{ME} < e_{RG}$ and that $\alpha_D < \alpha_{ME} < \alpha_{RG}$ which is in agreement with (4) and Theorem 1, (iii).

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References

1. H.W. Engl and H. Gfrerer, *Appl. Numer. Math.* **4**, 395–417 (1988).
2. H.W. Engl, M. Hanke and A. Neubauer, *Regularization of Inverse Problems* (Kluwer, Dordrecht, 1996).
3. U. Hämarik, in *Differential and Integral Equations: Theory and Numerical Analysis*, ed. A. Pedas (Estonian Math. Society, Tartu, 1999).
4. U. Hämarik and T. Raus, *Proc. Estonian Acad. Sci. Phys. Math.* **48**, 133–145 (1999).
5. M. Hanke and P.C. Hansen, *Surv. Math. Ind.* **4**, 253–315 (1993).
6. A. Neubauer, *SIAM J. Numer. Anal.* **25**, 1313–1326 (1988).
7. T. Raus, *Acta et Comment. Univ. Tartuensis* **715**, 12–20 (1985).
8. U. Tautenhahn, in *Proc. of the HERCMA'98 Conf. Sept. 24–26 1998, Athens*, ed. E.A. Lipitakis (Lea Publishers, 1999) (to appear).
9. U. Tautenhahn and U. Hämarik, *Inverse Problems*, accepted (1999).
10. G.M. Vainikko and A.Y. Veretennikov, *Iteration Procedures in Ill-Posed Problems* (Nauka, Moscow, 1986) (in Russian).