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An Optimal Stopping Rule for the ν-Method for Solving Ill-Posed Problems, Using Christoffel Functions

MARTIN HANKE* AND HEINZ W. ENGL

Institut für Mathematik, Johannes-Kepler-Universität, A-4040 Linz, Austria

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We design an order-optimal stopping rule for the ν-method for solving ill-posed problems with noisy data. The construction of the ν-method is based on a sequence of Jacobi polynomials, and the stopping rule is based on a sequence of related Christoffel functions. The motivation for our stopping criterion arises from a careful comparison between the iterates of the ν-method and the approximations obtained from iterated Tikhonov regularization with (noninteger) order ν. The convergence results rely on asymptotic properties of the Christoffel functions.

1. INTRODUCTION

The concern of this paper is to introduce a new stopping rule for a family of iterative regularization methods for solving ill-posed linear equations with noisy data. This stopping rule is motivated by a parameter choice method for choosing the regularization parameter in iterated Tikhonov regularization, which is known to give (iterated) Tikhonov approximations of order-optimal accuracy for a maximum range of ill-posed problems. This method was developed by Gfrerer in [5] and has been generalized in [3] to a large class of regularization methods–iterative as well as noniterative ones. In Section 2 we will exemplify the resulting parameter choice strategy for iterated Tikhonov regularization, considered as an iterative method. Independently, Raus [17] suggested an order-optimal parameter choice strategy which coincides with the one from [5] in the case of iterated Tikhonov regularization.

Since its introduction by Brakhage [2] the so-called ν-method has been proven to be an attractive alternative to conventional regularization methods, cf., e.g. [7]. The ν-method is a two-step iterative method defined by a

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sequence of Jacobi polynomials; $\nu > 0$ is a parameter to be chosen in advance. It was shown in [2] that if the exact solution belongs to a certain set $\mathscr{X}_\nu$ to be specified below, then there exist stopping rules which yield approximations of order-optimal accuracy. Morozov's discrepancy principle [12] would be a natural choice for such a stopping rule: it monitors the size of the actual residual and terminates the iteration when the residual norm drops below the noise level in the data. However, it can be shown with an argument due to Groetsch [6, Theorem 3.3.6] that the discrepancy principle does not always lead to full accuracy; order-optimal accuracy of the corresponding approximations can only be guaranteed if the exact solution belongs to a proper subset $\mathscr{X}_{\nu-1/2} \subset \mathscr{X}_\nu$, cf. [7].

The parameter choice rules developed in [3] and in [17] do not work for the ν-method, as will be shown in Section 4. The reason is a more irregular behavior of the error in the ν-method compared to other regularization methods. However, via a surprising connection between the ν-method and iterated Tikhonov regularization we will still be able to construct an order-optimal stopping rule for the ν-method (Algorithm 4.2). One can think of our approach as a transformation of the irregular error curve into a smoothed one by using Christoffel functions associated to a related sequence of orthogonal polynomials; a similar idea has also been used in [8] where a heuristic stopping rule for the ν-method was developed for the case that even the data noise level is unknown. Our criterion will rely on an upper bound for the noise level; only for such criteria one can expect results about convergence (rates), cf. Bakushinskii [1].

2. Preliminaries

Throughout this paper we consider the linear equation

$$Kx = g, \tag{2.1}$$

where K is a bounded linear operator between two Hilbert spaces $\mathscr{X}_1$ and $\mathscr{X}_2$, and g is in $\mathscr{R}(K)$, the range of K. We denote by $\|\cdot\|$ the norms in the respective Hilbert spaces, and assume without loss of generality that $\|K\| = 1$. We are primarily interested in the case where $\mathscr{R}(K)$ is not closed. In this case the problem (2.1) is ill-posed because the Moore–Penrose generalized inverse $K^\dagger$ of K (the operator which assigns the *minimum norm solution* $x = K^\dagger g$ to g) is unbounded, cf. [6]. Thus, if we have noisy data g^ε with

$$\|g^\varepsilon - g\| \le \varepsilon, \tag{2.2}$$

then, even if $g^\varepsilon \in \mathscr{R}(K)$, $K^\dagger g^\varepsilon$ will in general be far from $K^\dagger g$. Hence, (2.1) must be *regularized*.

The construction of (linear) regularization methods can be based on spectral theory: if, for $\alpha > 0$, u_α: $[0, 1] \to \mathbb{R}$ is such that $u_\alpha(\lambda) \to 1/\lambda$ as $\alpha \to 0$, pointwise on $(0, 1]$, then one can define a *regularized solution* via

$$x_\alpha^\varepsilon := u_\alpha(K^*K)K^*g^\varepsilon \tag{2.3}$$

and

$$x_{\alpha(\varepsilon)}^\varepsilon \to K^\dagger g, \qquad \varepsilon \to 0,$$

if the *parameter choice strategy* $\alpha = \alpha(\varepsilon)$ *is suitably chosen*; for details and precise assumptions we refer to [6].

Iterative methods can be treated in a similar manner. The continuous regularization parameter α is replaced by the iteration index k, the regularized solutions are defined via

$$x_k^\varepsilon := u_k(K^*K)K^*g^\varepsilon, \tag{2.4}$$

where now u_k: $[0, 1] \to \mathbb{R}$ is such that $u_k(\lambda) \to 1/\lambda$ pointwise on $(0, 1]$ as $k \to \infty$.

A method that can be considered both as a continuous and as an iterative regularization method is *iterated Tikhonov regularization*, where, for $\alpha > 0$ and $k \in \mathbb{N}$, the regularized solutions are defined via

$$\begin{aligned} x_{\alpha,0}^\varepsilon &= 0, \\ (K^*K + \alpha I)x_{\alpha,k}^\varepsilon &= K^*g^\varepsilon + \alpha x_{\alpha,k-1}^\varepsilon, \end{aligned} \tag{2.5}$$

which can also be written as

$$x_{\alpha,k}^\varepsilon = u_{\alpha,k}(K^*K)K^*g^\varepsilon \tag{2.6}$$

with

$$u_{\alpha,k}(\lambda) = \frac{(\lambda + \alpha)^k - \alpha^k}{\lambda(\lambda + \alpha)^k}. \tag{2.7}$$

If we keep k fixed and let $\alpha \to 0$ then we obtain iterated Tikhonov regularization of order k as studied, e.g., by King and Chillingworth [9]. But we can also keep $\alpha > 0$ fixed and consider (2.5) as an iterative method, cf., e.g., Kryanev [10]. In all regularization methods, an essential question is the choice of the regularization parameter α or, analogously, the choice of the stopping index k, the *stopping rule*. If the problem (2.1) is ill-posed then the convergence can be arbitrarily slow, cf., e.g., Schock [19]. Convergence rates can only be obtained under additional smoothness

assumptions, namely *source conditions* of the type

$$x := K^{\dagger} g \in \mathscr{X}_{\mu} := \mathscr{R}\big((K^{*}K)^{\mu}\big) \tag{2.8}$$

for some $\mu > 0$; (2.8) may be interpreted as an abstract smoothness assumption.

In practice μ is rarely known so that a priori parameter choice or stopping rules that depend on the knowledge of μ are not practical. This shortcoming can be overcome by using a posteriori parameter choice rules. For a wide class of regularization methods, a posteriori rules with optimal convergence rates were developed in [17, 5, 3]. We sketch the underlying principle for the case of iterated Tikhonov regularization following the approach in [5, 3]. The total error can be estimated in this case by

$$\frac{1}{2}\|x - x_{\alpha,k}^{\varepsilon}\|^2 \le \|x - x_{\alpha,k}^{0}\|^2 + \varepsilon^2 \frac{k^2}{\alpha^2}. \tag{2.9}$$

The basic idea (for (2.5) considered as a continuous regularization method with parameter α) is now to differentiate the right-hand side of (2.9) with respect to α and equate the result to zero. This equation would certainly determine an "optimal" regularization parameter because the (sharp) estimate (2.9) is minimized, but cannot be implemented as it involves the unknown exact right-hand side g. It turns out, however, that one may replace g by g^{ε} and the resulting nonlinear equation determines a regularization parameter $\alpha(\varepsilon)$ which is now *optimal* in the sense that for given g and ε, there is a positive constant C such that

$$\sup_{\|g-g^{\varepsilon}\| \le \varepsilon} \|x - x_{\alpha(\varepsilon),k}^{\varepsilon}\| \le C \sup_{\|g-g^{\varepsilon}\| \le \varepsilon} \inf_{\alpha > 0} \|x - x_{\alpha,k}^{\varepsilon}\|, \tag{2.10}$$

under quite reasonable conditions (cf. [3] for the precise statement). In particular (2.10) shows that the actual error obtained from this stopping rule has the same order of magnitude as the optimal error (minimized over α) for worst case data perturbations. Equation (2.10) heavily relies on a certain monotonicity assumption which implies that for exact data the error decreases monotonically.

We mention, cf. [9], that for $x = (K^{*}K)^{\mu} f \in \mathscr{X}_{\mu}$ with $0 < \mu \le k$ the optimality property (2.10) implies that

$$\|x - x_{\alpha(\varepsilon),k}^{\varepsilon}\| \le C\|f\|^{1/(2\mu+1)} \varepsilon^{2\mu/(2\mu+1)}, \tag{2.11}$$

where C depends on μ only. It is known (cf., e.g., Louis [11]), that the order of the exponent of ε on the right-hand side of (2.11) cannot be improved (uniformly in $\mathscr{X}_{\mu}$) by any other regularization method. A param-

eter choice rule (or a stopping rule) for which the corresponding error can be estimated as in (2.11) will be called *order-optimal for* $x \in \mathscr{X}_\mu$. Note that this notion is a bit weaker that the notion of optimality that we have introduced before. We will come back to this in Section 6.

Next, we consider (2.5) as an iterative regularization method, i.e., we keep $\alpha > 0$ fixed and let $k \to \infty$. A similar argument can now be used to derive a stopping rule $k = k(\varepsilon)$, if we replace differentiation (with respect to α) by a difference operator (with respect to k). The corresponding results from [3] yield the following stopping rule: take $k(\varepsilon)$ to be the smallest integer for which

$$\left(g^\varepsilon, \alpha^{2k+1}(KK^* + \alpha I)^{-2k-2}(KK^* + 2\alpha I)g^\varepsilon\right) \le \tau\varepsilon^2 \tag{2.12}$$

holds (with $\tau > 2$ fixed). The iteration may be rearranged so that the left-hand side of (2.12) can easily be evaluated: if we compute

$$\begin{aligned} z^\varepsilon_{\alpha,0} &= 0, \\ (KK^* + \alpha I) z^\varepsilon_{\alpha,k} &= g^\varepsilon + \alpha z^\varepsilon_{\alpha,k-1}, \\ x^\varepsilon_{\alpha,k} &= K^* z^\varepsilon_{\alpha,k}, \end{aligned} \tag{2.13}$$

then (2.12) can be reformulated as

$$\alpha^2\left(z^\varepsilon_{\alpha,k+1} - z^\varepsilon_{\alpha,k-1}, z^\varepsilon_{\alpha,k+1} - z^\varepsilon_{\alpha,k}\right) \le \tau\varepsilon^2, \tag{2.14}$$

and the iteration is stopped with $k = k(\varepsilon)$ as soon as (2.14) is satisfied for the first time.

This stopping rule has the corresponding optimality property that

$$\sup_{\|g-g^\varepsilon\| \le \varepsilon} \|x - x^\varepsilon_{\alpha,k(\varepsilon)}\| \le C \sup_{\|g-g^\varepsilon\| \le \varepsilon} \inf_{k \in N_0} \|x - x^\varepsilon_{\alpha,k}\|, \tag{2.15}$$

cf. [3] for the precise conditions. Since the iteration (2.13) is known to reach order-optimal accuracy for *all* $\mathscr{X}_\mu$ with $\mu > 0$, cf., e.g., [17, 18], it follows from (2.15) that the parameter choice rule (2.14) is order-optimal for all $\mathscr{X}_\mu$, $\mu > 0$. Again, it is crucial for verifying (2.15) that for exact data the iteration error decreases monotonically. As we will see in Section 4, this property is lost for the ν-method, and therefore, the general rule from [3] is not applicable as a stopping rule for the ν-method.

The reason that we nevertheless include the above discussion stems from an intimate connection between the ν-method and iterated Tikhonov approximations of order ν that we will establish below.

3. The ν-Method

The ν-method was introduced by Brakhage [2], and studied subsequently in [7, 8]. The special case $\nu = \frac{1}{2}$ coincides with the Chebyshev method developed by Nemirovskii and Polyak [14]. To obtain order-optimal approximations, the positive parameter ν should be chosen such that $\nu \geq \mu$, where μ is as in (2.8). This requires some, but not very detailed prior knowledge about the exact solution x.

Given ν, the iterates x_k^ε of the ν-method are defined recursively for $k = 1, 2, \ldots$, by $x_0^\varepsilon = 0$, $z_0^\varepsilon = 0$, and

$$\begin{aligned} z_k^\varepsilon &= \mu_k z_{k-1}^\varepsilon + (1 - \mu_k) z_{k-2}^\varepsilon + \omega_k (g^\varepsilon - K x_{k-1}^\varepsilon), \\ x_k^\varepsilon &= K^* z_k^\varepsilon. \end{aligned} \tag{3.1}$$

The scalar parameters μ_k and ω_k are given explicitly,

$$\mu_1 = 1, \qquad \omega_1 = \frac{4\nu + 2}{4\nu + 1},$$

and, for $k > 1$,

$$\mu_k = 1 + \frac{(k-1)(2k-3)(2k+2\nu-1)}{(k+2\nu-1)(2k+4\nu-1)(2k+2\nu-3)},$$

$$\omega_k = 4\frac{(2k+2\nu-1)(k+\nu-1)}{(k+2\nu-1)(2k+4\nu-1)}.$$

For our analysis we will also require the "ideal" approximations z_k^0 and x_k^0 that would have been obtained in (3.1) if ε were zero, and which we denote by z_k and x_k from now on.

The ν-method fits into the general framework (2.4) with

$$u_k(\lambda) = \frac{1 - p_k(\lambda)}{\lambda},$$

and where p_k are rescaled shifted *Jacobi-polynomials*,

$$p_k(\lambda) = P_k^{(2\nu-1/2,\,-1/2)}(1 - 2\lambda)/P_k^{(2\nu-1/2,\,-1/2)}(1).$$

Note that u_k is a polynomial of degree $k - 1$. We refer to Szegö [20] for the many properties that are known about Jacobi polynomials.

For $x \in \mathscr{X}_\mu$ with $0 < \mu \leq \nu$, Brakhage [2] derived an order-optimal a priori stopping rule for the ν-method; it follows from the saturation results in [7] that no such rule can exist for $\mu > \nu$. As in Section 2, we now

want to find an implementable (a posteriori) stopping criterion which does not require knowledge of μ, but which nevertheless is order-optimal for the full range of $\mathscr{X}_\mu$, $0 < \mu \leq \nu$.

The stopping rule that we suggest below utilizes the fact that the polynomials

$$d_{k-1}(\lambda) = \frac{p_{k-1}(\lambda) - p_k(\lambda)}{\lambda}$$

are rescaled and shifted copies of the Jacobi-polynomials $P_{k-1}^{(2\nu+1/2,\,-1/2)}$. The d_{k-1} occur naturally during the iteration as

$$z_k^\varepsilon - z_{k-1}^\varepsilon = d_{k-1}(KK^*)g^\varepsilon, \tag{3.2}$$

and have therefore been termed *update polynomials* in [8]. As there, however, it is not the sequence $\{d_k\}$ of orthogonal polynomials that we will primarily use for our stopping rule, but rather their associated *Christoffel functions*: if we denote by $\check{d}_k$ the orthonormalized update polynomials, then the Christoffel functions associated with $\{d_k\}$ are defined as

$$\Lambda_n(\lambda) = \left(\sum_{k=0}^{n-1} \check{d}_k^2(\lambda) \right)^{-1}, \qquad 0 \leq \lambda \leq 1, \qquad n \in \mathbb{N}. \tag{3.3}$$

We will make essential use of the asymptotical properties of Λ_n that were obtained by Nevai [15] and subsequently refined by Erdélyi, Magnus, and Nevai [4] who provided explicit estimates for the associated constants. These results are reformulated in [8, Sect. 4] with special regard to our particular application. As in [8] we write $\alpha_k \sim \beta_k$ if there are positive constants c, C such that $c\alpha_k \leq \beta_k \leq C\alpha_k$, $k = 1, 2, \ldots$.

We conclude this section with an interesting connection between the ν-method and iterated Tikhonov regularization of *non-integer* order ν, defined via (2.6) and (2.7) if k is replaced by ν. Of course if $\nu \notin \mathbb{N}$ then (2.5) cannot be used for an implementation. This connection to iterated Tikhonov regularization is the basic motivation for our new stopping rule, but Theorem 3.1 might be interesting in itself:

THEOREM 3.1. *Let $\nu > 0$, and denote by $x_{\alpha,\nu}^\varepsilon$ (and $x_{\alpha,\nu}$, respectively) the approximations of iterated Tikhonov regularization of order ν. Then there is a constant C such that*

$$\|x - x_k\| \leq C\|x - x_{k^{-2},\nu}\|, \qquad k = 1, 2, \ldots, \tag{3.4}$$

while

$$\|x_k - x_k^\varepsilon\| \sim \|x_{k^{-2},\nu} - x_{k^{-2},\nu}^\varepsilon\|, \qquad k = 1, 2, \ldots. \tag{3.5}$$

Proof. For the kth iterate x_k of the ν-method we obtain from (2.4) the iteration error

$$x - x_k = p_k(K^*K)x, \tag{3.6}$$

while for iterated Tikhonov regularization of order ν we have analogously

$$x - x_{\alpha,\nu} = r_{\alpha,\nu}(K^*K)x \tag{3.7}$$

with

$$r_{\alpha,\nu}(\lambda) = \left(\frac{\alpha}{\lambda + \alpha}\right)^{\nu}.$$

We first recall (cf., e.g., [2, 8]) that there is a constant C_* (depending on ν only) such that

$$|p_k(\lambda)| \leq C_*(k^2\lambda)^{-\nu}, \qquad 0 < \lambda \leq 1, \qquad k = 1, 2, \ldots . \tag{3.8}$$

Thus, for $\alpha = k^{-2} \leq \lambda \leq 1$ we conclude

$$r_{\alpha,\nu}(\lambda) \geq \left(\frac{\alpha}{2\lambda}\right)^{\nu} = 2^{-\nu}(k^2\lambda)^{-\nu} \geq \frac{1}{C_* 2^{\nu}}|p_k(\lambda)|.$$

On the other hand, for $0 \leq \lambda \leq k^{-2} = \alpha$ we have

$$|p_k(\lambda)| \leq 1 \leq 2^{\nu} r_{\alpha,\nu}(\lambda).$$

The spectral theorem, (3.6) and (3.7) now imply assertion (3.4) for the iteration error.

Next we turn our attention to the perturbation error. Inserting g and g^{ϵ} in (2.4), respectively, we have

$$\begin{aligned} x_k - x_k^{\epsilon} &= u_k(K^*K)K^*(g - g^{\epsilon}), \\ x_{\alpha,\nu} - x_{\alpha,\nu}^{\epsilon} &= u_{\alpha,\nu}(K^*K)K^*(g - g^{\epsilon}). \end{aligned} \tag{3.9}$$

For $0 \leq \lambda \leq k^{-2} = \alpha$ we apply the mean value theorem and Markov's inequality, cf. [7, Eq. (7.2)], to obtain

$$u_k(\lambda) = |p_k'(\tilde{\lambda})| \leq 2k^2,$$

and similarly,

$$u_{\alpha,\nu}(\lambda) = |r_{\alpha,\nu}'(\tilde{\lambda})| \geq |r_{\alpha,\nu}'(k^{-2})| = \frac{\nu}{2^{\nu+1}}k^2.$$

Hence,

$$0 \le u_k(\lambda) \le \frac{2^{\nu+2}}{\nu} u_{\alpha,\nu}(\lambda) \tag{3.10}$$

for $\lambda \in [0, k^{-2}]$. In the remaining interval $[k^{-2}, 1]$ we have

$$1 - r_{\alpha,\nu}(\lambda) \ge 1 - r_{\alpha,\nu}(k^{-2}) = 1 - 2^{-\nu} \ge 2^{-\nu}\nu \log 2,$$

while $|1 - p_k(\lambda)| \le 2$; dividing by λ we obtain (3.10) for $k^{-2} \le \lambda \le 1$ as well. Thus, the spectral theorem yields

$$\|x_k - x_k^\varepsilon\| \le C\|x_{\alpha,\nu} - x_{\alpha,\nu}^\varepsilon\| \tag{3.11}$$

for some positive C, $\alpha = k^{-2}$, and $k \in \mathbb{N}$.

To prove the converse of (3.11) we need to find a positive number C such that the inequality

$$u_{\alpha,\nu}(\lambda) \le C u_k(\lambda), \qquad 0 \le \lambda \le 1, \tag{3.12}$$

holds true for all $k \in \mathbb{N}$ and $\alpha = k^{-2}$. For $k = 1$ and $k = 2$ such a C obviously exists because $u_k/u_{\alpha,\nu}$ can be extended to a continuous, strictly positive function on $[0, 1]$. Therefore, we can assume $k > 2$ in the following. Let λ_k denote the smallest zero of p_k; it is well known, cf., e.g., [20, Theorem 8.9.1], that $\lambda_k \le ck^{-2}$ for some $c > 0$. Using the convexity of p_k in $[0, \lambda_k]$ we conclude

$$u_k(\lambda) \ge \lambda_k^{-1} \ge c^{-1}k^2, \qquad 0 \le \lambda \le \lambda_k. \tag{3.13}$$

On the other hand, the mean value theorem implies

$$u_{\alpha,\nu}(\lambda) = |r'_{\alpha,\nu}(\tilde{\lambda})| \le |r'_{\alpha,\nu}(0)| = \nu k^2, \qquad 0 \le \lambda \le \lambda_k. \tag{3.14}$$

To estimate p_k in $I \setminus [0, \lambda_k]$ we apply Sonin's theorem, cf. [20, Sects. 7.31 and 7.32] and we show that the maximum M_k of p_k in $[\lambda_k, 1]$ is less than some $1 - \delta$ for all $k > 2$; here, $\delta > 0$ is independent of k. Szegö [20, p. 169] has shown that M_k is attained at $\lambda = \lambda_k^*$, i.e., at the first relative maximum of the graph of p_k to the right of $\lambda = \lambda_k$. Moreover, from [20, Eq. (7.32.4)] we have

$$1 - M_k^2 = \frac{4\nu}{k(k + 2\nu)} \int_0^{\lambda_k^*} (1 - \lambda)(p'_k(\lambda))^2 d\lambda.$$

By means of [20, Theorem 7.32.4] we can now choose $c_* > 0$ so small that

$$|p'_k(\lambda)| \ge c_* k^2, \qquad 0 \le \lambda \le c_* k^{-2} \le \lambda_k^*;$$

consequently,

$$1 - M_k^2 \geq \frac{4\nu}{k(k+2\nu)} \int_0^{c_* k^{-2}} (1 - c_* k^{-2}) c_*^2 k^4 d\lambda$$
$$= 4\nu c_*^3 + o(1), \qquad k \to \infty.$$

Since the right-hand side is always positive, we can find $\delta > 0$ as desired, i.e.,

$$1 - p_k(\lambda) \geq \delta \geq \delta(1 - r_{\alpha,\nu}(\lambda)), \qquad \lambda_k \leq \lambda \leq 1.$$

Together with (3.13) and (3.14) we have verified (3.12) for all $\lambda \in [0, 1]$ and $k > 2$, and hence,

$$\|x_{\alpha,\nu} - x_{\alpha,\nu}^\varepsilon\| \leq C\|x_k - x_k^\varepsilon\|; \tag{3.15}$$

(3.11) and (3.15) finally imply (3.5). ∎

Note that no analog of (3.5) is valid for the approximation error (3.4): this will be exemplified in Example 6.1 where the left-hand side of (3.4) vanishes for some $k \in \mathbb{N}$ and $x \neq 0$; the right-hand side of (3.4) can only vanish for $x = 0$.

Roughly speaking, Theorem 3.1 states that the ν-method provides an accuracy comparable to iterated Tikhonov regularization of order ν. One may even go somewhat further and consider the ν-method as an (almost) equivalent implementation of Tikhonov regularization (of order ν) in which the update of the regularization parameter is much less cumbersome than in standard implementations of Tikhonov's method.

We further note that in conventional iterative regularization methods the iteration index k is usually connected with $1/\alpha$ in (2.3); here we have $k \sim 1/\sqrt{\alpha}$, which reflects the faster convergence of the ν-method.

4. The New Stopping Rule

In this section we derive a new stopping rule for the ν-methods. We restrict our attention to stopping criteria which are determined by a sequence of real functions $\{\rho_k\}$ in the following way, compare (2.12): stop iterating with $k = k(\varepsilon)$, when for the first time

$$|(g^\varepsilon, \rho_k(KK^*)g^\varepsilon)| \leq \tau\varepsilon^2, \tag{4.1}$$

where τ is such that

$$\tau > \|\rho_k(\lambda)\|_{[0,1]}, \qquad k = 0, 1, 2, \ldots . \tag{4.2}$$

As usual, $\|\cdot\|_{[0,1]}$ denotes the maximum norm on $[0, 1]$. Note that if ρ_k is a polynomial of degree $2k + 1$, then the left-hand side of (4.1) can be evaluated with little extra effort during the $(k + 1)$st step of the iteration.

We first consider the stopping rule developed in [3]; it fits into the above framework with

$$\tilde{\rho}_k(\lambda) = \frac{1}{d_k(0)} \frac{p_k^2(\lambda) - p_{k+1}^2(\lambda)}{\lambda} \tag{4.3}$$

and $\tau > 2$. However, it turns out that, as opposed to iterated Tikhonov regularization, the monotonicity requirements on the error mentioned in Section 2 are not fulfilled for the ν-method. Technically, these requirements [3, Assumption 3.1] would boil down to requiring that the sequences $\{\tilde{\rho}_k(\lambda)\}_k$, $0 < \lambda \leq 1$, are decreasing in k, which is not the case as computations using, e.g., MAPLE, immediately show.[1] These oscillations in the error curve have already been noted in [8].

It is for this reason that not only the optimality results from [3] cannot be applied, but the stopping rule (4.1) with $\tilde{\rho}_k$ from (4.3) does not even lead to a convergent regularization method, as the following example shows:

EXAMPLE 4.1. Let ξ_1 and ξ_2 denote the smallest zeros of p_1 and p_2, respectively, and consider the function $\tilde{\rho}_1$ (a polynomial of degree 3): because of the interlacing properties of the zeros of orthogonal polynomials we have $\xi_2 < \xi_1$ and $\tilde{\rho}_1$ changes sign between ξ_2 and ξ_1; in fact, it is not difficult to see that $\tilde{\rho}_1$ has a unique zero λ_*^2 in the open interval (ξ_2, ξ_1). Now we consider a compact selfadjoint operator K with infinite dimensional range and eigenvalue λ_*; let the exact solution x of (2.1) be an associated eigenvector with unit norm. Then, by construction and by (4.2),

$$|(g^\epsilon, \tilde{\rho}_1(KK^*)g^\epsilon)| \leq \|\tilde{\rho}_1\|_{[0,1]}\|g^\epsilon - g\|^2 < \tau\epsilon^2.$$

According to the stopping rule (4.1), the iteration will therefore be

[1] We kindly thank F. Peherstorfer for providing us with a theoretical analysis concerning this question of monotonicity.

terminated either with

$$x_0^\varepsilon = 0 \qquad \text{or with} \qquad x_1^\varepsilon = \frac{4\nu + 2}{4\nu + 1} K^* g^\varepsilon.$$

In both cases, we conclude from the decomposition (3.6), (3.9), for the error of the $k(\varepsilon)$th iterate that

$$\|x - x_{k(\varepsilon)}^\varepsilon\| \geq p_1(\lambda_*^2) - O(\varepsilon),$$

and therefore, $x_{k(\varepsilon)}^\varepsilon$ does not approach the solution x as $\varepsilon \to 0$.

We will now utilize Theorem 3.1 to construct an order-optimal stopping rule. To this end, we will always assume ν to be fixed and refer to the iterated Tikhonov regularization method of order ν briefly as the "iterated Tikhonov method." One conclusion that we may draw from Theorem 3.1 is, that a strategy for choosing the regularization parameter α which works well for iterated Tikhonov regularization should yield similar results for the ν-method, when replacing α by k^{-2}. Note that the strategy (2.12) has the form (4.1) with

$$\hat{\rho}_\alpha(\lambda) = \left(\frac{\alpha}{\lambda + \alpha}\right)^{2\nu+1}.$$

However, this choice of ρ would require inversion of $KK^* + \alpha I$, which is a price that we do not want to pay. Therefore, we will instead use polynomials of degree $2k + 1$ to approximate $\hat{\rho}_\alpha$. Keeping in mind that $\alpha = k^{-2}$ we thus have to approximate

$$\hat{\rho}_\alpha(\lambda) = \frac{1}{(1 + k^2\lambda)^{2\nu+1}} \sim \begin{cases} 1, & 0 \leq \lambda \leq k^{-2}, \\ (k^2\lambda)^{-2\nu-1}, & k^{-2} \leq \lambda \leq 1. \end{cases} \tag{4.4}$$

This can be achieved with the Christoffel functions Λ_k of (3.3) after suitable normalization: we take

$$\rho_k(\lambda) = \Lambda_{k+1}(0)/\Lambda_{k+1}(\lambda), \tag{4.5}$$

and obtain from [8, Eq. (4.8)] and (4.4)

$$\rho_k(\lambda) \sim \hat{\rho}_\alpha(\lambda) \qquad \text{if } \alpha = k^{-2}, k \in \mathbb{N}, \tag{4.6}$$

uniformly for $\lambda \in [0, 1]$.

At this point we mention that the general scheme by Raus [17] would suggest the choice

$$\check{\rho}_k(\lambda) = |p_k(\lambda)|^{(2\nu+1)/\nu}; \tag{4.7}$$

although the conditions required in [17] are not satisfied here, and there is no realistic way of implementing (4.1) with $\check{\rho}_k$, it is nevertheless interesting to remark that $\check{\rho}_k$ has a majorant with the same asymptotics as our ρ_k, cf. (3.8).

Note that ρ_k of (4.5) is a polynomial of degree $2k$, and—because the maximum of Λ_{k+1}^{-1} is attained at $\lambda = 0$—we have

$$\|\rho_k\|_{[0,1]} = 1, \qquad k = 0, 1, 2, \ldots .$$

For our stopping rule, we insert ρ_k of (4.5) into (4.1); then the left hand side of (4.1) can be evaluated during the iteration with the following algorithm (see Lemma 4.3 below).

ALGORITHM 4.2. Let $\eta_0 = \|g^\varepsilon\|^2$, and select $\tau > 1$. Within the $k+1$st iterative step, $k = 1, 2, \ldots,$ compute

$$\eta_k = (1 - \alpha_k)\eta_{k-1} + \beta_k \|z_{k+1}^\varepsilon - z_k^\varepsilon\|^2, \tag{4.8}$$

where the parameters α_k and β_k are determined recursively by $\alpha_0 = 1$ and

$$\alpha_k^{-1} = 1 + \frac{k(2k-1)(2k+2\nu-1)}{(k+2\nu)(2k+4\nu+1)(2k+2\nu+1)}\alpha_{k-1}^{-1},$$

$$\beta_k = \frac{\left(2\nu + \frac{1}{2}\right)^2}{(2k+2\nu+1)^2}\alpha_k, \qquad k = 1, 2, \ldots . \tag{4.9}$$

Then, as stopping index $k = k(\varepsilon)$, choose the smallest integer $k > 0$ such that

$$\eta_k \le \tau\varepsilon^2.$$

LEMMA 4.3. *The numbers η_k computed by Algorithm 4.2 satisfy*

$$\eta_k = (g^\varepsilon, \rho_k(KK^*)g^\varepsilon), \qquad k = 0, 1, 2, \ldots,$$

with ρ_k as in (4.5).

Proof. We show first that the α_k as defined by (4.9) satisfy

$$\alpha_k = \check{d}_k^2(0)\Lambda_{k+1}(0), \qquad k = 0, 1, 2, \ldots . \tag{4.10}$$

For $k = 0$ this is clearly true by the definition (3.3) of Λ_k. The numbers

$\check{d}_k(0)$ are explicitly known (cf. [20] or [8]), so that (4.9) can be rewritten as

$$\alpha_k^{-1} = 1 + \frac{\check{d}_{k-1}^2 0}{\check{d}_k^2(0)} \alpha_{k-1}^{-1}, \qquad k = 1, 2, \ldots .$$

Now the assertion (4.10) follows easily by induction. Note that (4.10) implies

$$1 - \alpha_k = \Lambda_{k+1}(0)/\Lambda_k(0), \qquad k = 1, 2, \ldots . \tag{4.11}$$

Second, from the definition of β_k and from [8, Eq. (2.17)] we have

$$\beta_k = \alpha_k / d_k^2(0).$$

According to (3.2), the second term on the right-hand side of (4.8) therefore equals

$$\begin{aligned} \beta_k \| z_{k+1}^\varepsilon - z_k^\varepsilon \|^2 &= \frac{\alpha_k}{\check{d}_k^2(0)} \left(g^\varepsilon, \check{d}_k^2(KK^*) g^\varepsilon \right) \\ &= \Lambda_{k+1}(0) \left(g^\varepsilon, \check{d}_k^2(KK^*) g^\varepsilon \right). \end{aligned} \tag{4.12}$$

We finally observe that we have $\rho_0 \equiv 1$ so that the assertion of the lemma holds for $k = 0$. The general claim follows from (4.11) and (4.12) by induction. ∎

5. Order-Optimality of Algorithm 4.2

We now derive the convergence properties of our stopping rule. We begin by showing that the iteration will always terminate:

Proposition 5.1. *If $g \in \mathcal{R}(K)$ then Algorithm 4.2 determines a finite stopping index.*

Proof. This is a standard argument, see, e.g., [3, Lemma 2.3]. According to (4.4) and (4.6), ρ_k converges pointwise to zero for $\lambda \in (0, 1]$; furthermore, ρ_k is uniformly bounded. From the dominated convergence theorem we conclude that

$$\left(g^\varepsilon, \rho_k(KK^*) g^\varepsilon \right) \to \| (I - P) g^\varepsilon \|^2, \qquad k \to \infty,$$

where P is the orthogonal projector onto the closure of $\mathcal{R}(K)$. Since $g \in \mathcal{R}(K)$, the right-hand side does not exceed ε^2 and the claim follows. ∎

We now show that the ν-method with the stopping rule proposed in Algorithm 4.2 is order-optimal in all sets $\mathscr{X}_\mu$ with $0 < \mu \leq \nu$, i.e., in the full range where this is possible:

THEOREM 5.2. *Assume that $g = Kx$, x being the solution of minimal norm. Then, Algorithm 4.2 is order-optimal for $x \in \mathscr{X}_\mu$, $0 < \mu \leq \nu$.*

Proof. In view of (3.8) and (4.6) we can find a constant C such that

$$|p_k(\lambda)| \leq C\rho_k(\lambda)^{\nu/(2\nu+1)}, \qquad k = 1, 2, \ldots . \tag{5.1}$$

Moreover, it can easily be seen that for $0 < \mu \leq \nu$ there exist constants C_μ such that

$$\lambda^{2\mu+1}\rho_k(\lambda) \leq C_\mu k^{-4\mu-2}. \tag{5.2}$$

Now, fix $0 \leq \mu \leq \nu$ and assume that

$$x = (K^*K)^\mu f.$$

As mentioned previously, the iterates of the ν-method when g^ε in (3.1) is replaced by g are denoted by x_k. Also, from now on, let k be the termination index obtained from Algorithm 4.2 (equivalently, from (4.1) with ρ as in (4.5)). With this choice of k we finally introduce the operator

$$R = \left(\rho_k(K^*K)\right)^{1/(2\nu+1)},$$

and observe that $\|R\| \leq 1$.

Since ρ_k is bounded by 1, the triangle inequality yields

$$(g, \rho_k(KK^*)g) \leq 2(g^\varepsilon, \rho_k(KK^*)g^\varepsilon) + 2\varepsilon^2 \leq 2(\tau+1)\varepsilon^2. \tag{5.3}$$

Using (5.1) and applying the interpolation inequality to RK^*K we obtain the following estimate for the iteration error at the stopping index,

$$\begin{aligned}\|x - x_k\| &= \|p_k(K^*K)(K^*K)^\mu f\| \leq C\|(RK^*K)^\mu R^{\nu-\mu} f\| \\ &\leq C\|R^{\nu-\mu} f\|^{1/(2\mu+1)}\|(K^*K)^{1/2} R^{\nu+1/2}(K^*K)^\mu f\|^{2\mu/(2\mu+1)} \\ &\leq C\|f\|^{1/(2\mu+1)}(g, \rho_k(KK^*)g)^{\mu/(2\mu+1)}.\end{aligned}$$

Inserting (5.3) we deduce the order-optimality of the iteration error,

$$\|x - x_k\| \leq C\|f\|^{1/(2\mu+1)}\varepsilon^{2\mu/(2\mu+1)}. \tag{5.4}$$

If $k = 0$ then we have no additional error due to the noise and we are done. For the remaining cases we will first show that, for some constant C,

$$k \le C\left(\frac{\|f\|}{\varepsilon}\right)^{1/(2\mu+1)}. \tag{5.5}$$

In fact, if $k = 1$ then we have

$$\tau\varepsilon^2 < \eta_0 = \|g^\varepsilon\|^2 = \|K(K^*K)^\mu f + g^\varepsilon - g\|^2 \le (\|f\| + \varepsilon)^2.$$

From this we conclude that (5.5) holds with $C = (\sqrt{\tau} - 1)^{-1/(2\mu+1)}$. For $k > 1$ we use the inverse triangle inequality to obtain the following analog of (5.3),

$$(\sqrt{\tau} - 1)^2\varepsilon^2 \le (g, \rho_{k-1}(KK^*)g),$$

and then apply (5.2) to estimate the right-hand side,

$$\begin{aligned}(g, \rho_{k-1}(KK^*)g) &= \left(f, (K^*K)^{2\mu+1}\rho_{k-1}(K^*K)f\right) \\ &\le C_\mu(k-1)^{-4\mu-2}\|f\|^2.\end{aligned}$$

Since $k - 1 \ge k/2$ in this final case, there is a constant C such that (5.5) always holds. In view of (5.5), [7, Lemma 8.2] yields

$$\|x_k^\varepsilon - x_k\| \le C\|f\|^{1/(2\mu+1)}\varepsilon^{2\mu/(2\mu+1)}. \tag{5.6}$$

Combining (5.4) and (5.6) the assertion follows. ∎

We mention that Theorem 5.2 in particular implies, cf. Plato [16], that our stopping rule is a convergent regularization method, i.e., if $g \in \mathscr{R}(K)$ then $x_{k(\varepsilon)}^\varepsilon \to K^\dagger g$ as $\varepsilon \to 0$. Estimates for the constants in (5.4) and (5.6) may be deduced from [4], but this is beyond the scope of our paper.

6. Comparison of the Actual Error and the Optimal Error

In the previous section we have seen that our stopping rule is order-optimal for $x \in \mathscr{X}_\mu$, $0 < \mu \le \nu$, i.e., the resulting approximations satisfy (2.11). In this section we deal with the question whether our stopping index is also optimal in the sense of (2.15). To simplify the notation, we call $\|x - x_{k(\varepsilon)}^\varepsilon\|$ the *actual error* $e(g, g^\varepsilon)$ of Algorithm 4.2, if $k(\varepsilon)$ is the corresponding stopping index. Obviously, the actual error depends on

g, g^ε, and on τ. We compare the actual error $e(g, g^\varepsilon)$ with the *optimal error* $e_{\text{opt}}(g, \varepsilon)$ which is the error of the best iterate in a worst-case situation,

$$e_{\text{opt}}(g, \varepsilon) := \sup_{\|g - g^\varepsilon\| \le \varepsilon} \inf_{k \in N_0} \|x - x_k^\varepsilon\|.$$

Clearly, if we could find some $C > 0$ such that $e(g, g^\varepsilon) \le C e_{\text{opt}}(g, \varepsilon)$ for all perturbed right-hand sides g^ε satisfying (2.2), then our stopping rule would be optimal.

As it turns out, however, our stopping rule is not optimal in this stronger sense:

EXAMPLE 6.1. Let λ_*^2 be a zero of the k_*th Jacobi polynomial p_{k_*}, where $k_* \in \mathbb{N}$ is arbitrary but fixed. We consider a compact selfadjoint operator K with spectrum $\{\lambda_*, \lambda_1, \lambda_2, \ldots\}$, where $\lambda_1 > \lambda_2 > \ldots$ are infinitely many eigenvalues of K (different from λ_*) converging to zero. We assume that the exact solution x of our problem (2.1) is a unit eigenvector of K for λ_*. Then, by construction and by (3.6),

$$\|x - x_{k_*}^\varepsilon\| \le \|u_{k_*}(K^*K)K^*\|\varepsilon \le 2k_*\varepsilon,$$

cf. [7, Lemma 8.2]. Note that the right-hand side depends on ε only. Consequently, we have

$$e_{\text{opt}}(g, \varepsilon) = O(\varepsilon), \qquad \varepsilon \to 0. \tag{6.1}$$

Now let k be the stopping index determined from Algorithm 4.2. From (5.3) we then have

$$p_k(\lambda_*^2) \le 2\frac{\tau + 1}{\lambda_*^2}\varepsilon^2,$$

hence, using the asymptotics (4.4) and (4.6) for the Christoffel functions, we can find a (possibly) small but positive number c depending on λ_* and ν only, such that

$$k \ge c\varepsilon^{-1/(2\nu+1)}. \tag{6.2}$$

Now, we choose perturbed data $g^{\varepsilon_j}, j = 1, 2, \ldots$, in such a way that

$$g^{\varepsilon_j} - g = \varepsilon_j v_j, \qquad \varepsilon_j = \theta\lambda_j^{2\nu+1}, \qquad j = 1, 2, \ldots,$$

where θ is a positive constant to be determined later, and v_j is a unit eigenvector of K for λ_j. We denote by k_j the corresponding stopping index of Algorithm 4.2. From (3.6) and (3.9) we conclude that the actual

error is

$$\|x - x_{k_j}^{\varepsilon_j}\| \geq u_{k_j}(\lambda_j^2)\lambda_j\varepsilon_j = \theta\lambda_j^{2\nu}\left(1 - p_{k_j}(\lambda_j^2)\right). \tag{6.3}$$

Now, set

$$\theta = c^{2\nu+1}(2C_*)^{-(2\nu+1)/2\nu},$$

with c as in (6.2) and C_* as in (3.8); then it follows from (3.8) and (6.2) that

$$\begin{aligned} 1 - p_{k_j}(\lambda_j^2) &\geq 1 - C_*(k_j\lambda_j)^{-2\nu} \geq 1 - c^{-2\nu}C_*\lambda_j^{-2\nu}\varepsilon^{2\nu/(2\nu+1)} \\ &= 1 - c^{-2\nu}C_*\theta^{2\nu/(2\nu+1)} = \tfrac{1}{2} \end{aligned}$$

for all $j \in \mathbb{N}$. Thus we conclude from (6.3) that

$$e(g, g^{\varepsilon_j}) \geq \tfrac{1}{2}\theta^{1/(2\nu+1)}\varepsilon_j^{2\nu/(2\nu+1)}, \qquad j = 1, 2, \ldots .$$

Clearly, for $j \to \infty$, i.e., for $\varepsilon_j \to 0$, this rate of convergence is worse than the convergence rate of the optimal error $e_{\text{opt}}(g, \varepsilon_j)$ as determined in (6.1).

We may conclude from the above example that our stopping rule is based on a certain estimate of the actual error which does not recover the fluctuations of the error norm as k increases. As we have indicated previously, our error estimate is based on a smoothed copy of the actual error curve, and this reflects the role of the Christoffel functions. We also observe from the construction in Example 6.1 that, to obtain an order-optimal stopping rule, it is necessary that the functions ρ_k in (4.1) have the same zeros as the polynomials p_k. Note that this would be satisfied by the functions $\check{p}_k$ of (4.7).

We finally mention that we have implemented Algorithm 4.2, and compared it with the discrepancy principle for a "model ill-posed problem," a first kind integral equation with a Green's function as kernel function,

$$Kx(s) = \int_0^1 k(s,t)x(t) = g(s), \qquad 0 \leq s \leq 1,$$

with

$$k(s,t) = \begin{cases} \pi^2 s(1-t), & 0 \leq s \leq t \leq 1, \\ \pi^2 t(1-s), & 0 \leq t < s \leq 1. \end{cases}$$

This is a standard test example; in [7] it was reported that the discrepancy principle terminates the iteration too late, when applied to the Chebyshev

TABLE 1

	Performance of the $\frac{1}{2}$-method			
	Optimal	Algorithm 4.2	Discrepancy	
1% noise	19	18	25	iterations
	0.0293	0.0301	0.0415	relative error
0.1% noise	30	52	92	iterations
	0.0087	0.0158	0.0222	relative error

method of [14] (i.e., the $\frac{1}{2}$-method). Note that $\nu = \frac{1}{2}$ is of special interest as with this choice of ν the discrepancy principle fails to be order-optimal for *any* set $\mathscr{X}_\mu$ with $\mu > 0$.

Using the discretization and the second choice for x from [7, Sect. 11] (the details are provided there) we obtain a significantly better performance of our new stopping rule. We have run the Chebyshev method on this example with 1% noise and with 0.1% noise in the data; the iteration count of the optimal iterate, the stopping index obtained from the discrepancy principle and from Algorithm 4.2, together with the corresponding actual (relative) errors are collected in Table I. These numbers correspond to a choice of $\tau = 1.2$.

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