BIT
200x, Vol. xx, No. x, pp. 000–000
0006-3835/00/4004-0001 \$15.00

A NOTE ON TIKHONOV REGULARIZATION OF LARGE LINEAR PROBLEMS

MARTIN HANKE

Fachbereich Mathematik, Johannes Gutenberg-Universität, 55099 Mainz, Germany.
email: hanke@mathematik.uni-mainz.de

1 Introduction

In [1] Calvetti and Reichel consider an implementation of Tikhonov regularization for large linear problems

$$Ax = b, \qquad A \in \mathbb{R}^{m\times n}, \quad x \in \mathbb{R}^n, \quad b \in \mathbb{R}^m, \tag{1.1}$$

based on a partial Lanczos bidiagonalization of A. Their implementation, which takes up an idea of Golub and von Matt [3], computes on the fly upper and lower bounds for the Tikhonov residual, given a certain regularization parameter. Numerical examples suggest that the two bounds improve monotonically with the number of Lanczos steps, and in fact, Calvetti and Reichel prove the monotonicity of the lower bound.

In this note we complete their analysis and show that the upper bound is decreasing monotonically. The same technique can be used to give an alternative proof for the monotonicity of the lower bound.

2 The complete theorem

In Tikhonov regularization (cf. e.g., Groetsch [4]), an approximate solution of (1.1) is defined as

$$x_\alpha = (A^TA + \alpha I)^{-1}A^Tb,$$

where $\alpha > 0$ is the regularization parameter. It is often recommended to choose a regularization parameter for which the norm of the residual

$$b - Ax_\alpha = \alpha(AA^T + \alpha I)^{-1}b$$

is close to the noise level in the right-hand side b. Therefore it is of interest to have upper and lower bounds for

$$\phi(\alpha) = \|b - Ax_\alpha\|_2^2 = \alpha^2 b^T(AA^T + \alpha I)^{-2}b.$$

As in [1] we rewrite $\phi(\alpha)$ as a Stieltjes integral

$$\phi(\alpha) = \int_0^\infty \psi_\alpha(\lambda)\, d\omega(\lambda), \qquad \psi_\alpha(\lambda) = \alpha^2(\lambda + \alpha)^{-2}, \tag{2.1}$$

where ω is an appropriate piecewise constant function determined by the singular values of A and corresponding components of b.

The main idea from [3] and [1] consists in using Gauß and Gauß-Radau quadrature rules associated with the bilinear form

$$\langle f, g\rangle = \int_0^\infty f(\lambda)\, g(\lambda)\, d\omega(\lambda) \tag{2.2}$$

to estimate (2.1) from below and above. In fact, as shown in [3], the ℓ-point Gauß quadrature rule $\phi_\ell(\alpha)$ is a lower bound for $\phi(\alpha)$ whereas the corresponding Gauß-Radau rule $\overline{\phi}_\ell(\alpha)$ with prescribed node in the origin is an upper bound, i.e.

$$\phi_\ell(\alpha) < \phi(\alpha) < \overline{\phi}_\ell(\alpha). \tag{2.3}$$

The strict inequalites hold true for ℓ up to $r-1$, where r is the degree of the minimal polynomial for b with respect to AA^T (only in Π_{r-1}, i.e., the space of polynomials of degree strictly less than r, (2.2) is an inner product). For this reason we confine ourselves to the case $\ell < r$.

THEOREM . *For $1 \le m < \ell < r$ there holds*

$$\phi_m(\alpha) < \phi_\ell(\alpha) < \phi(\alpha) < \overline{\phi}_\ell(\alpha) < \overline{\phi}_m(\alpha). \tag{2.4}$$

Proof. Let $R_\ell[f]$ and $R_m[f]$ denote the ℓ-point and m-point Gauß-Radau quadrature rules, with prescribed nodes in the origin, for approximating the integral

$$\int_0^\infty f(\lambda)\, d\omega(\lambda).$$

We shall make use of the fact that these quadrature rules are uniquely determined by the fact that they integrate exactly all polynomials up to degree $2\ell-2$, resp. $2m-2$, cf. Chihara [2, p. 64/65] or Krylov [5]. Following [2],

$$R_\ell[f] = w_1 f(0) + \sum_{i=2}^{\ell} w_i f(\lambda_i)$$

is a positive definite functional on $\Pi_{\ell-1}$ because the nodes λ_i, $i = 1, \ldots, \ell$, with $\lambda_1 = 0$, are all mutually different and the weights w_i, $i = 1, \ldots, \ell$, are positive. In particular, R_ℓ can be rewritten as a Stieltjes integral

$$R_\ell[f] = \int_{0-}^\infty f(\lambda)\, d\omega_\ell(\lambda), \tag{2.5}$$

where ω_ℓ is a step function with jumps of height w_i at $\lambda = \lambda_i$, $i = 1, \ldots, \ell$. Now, since

$$R_m[p] = \int_0^\infty p(\lambda)\, d\omega(\lambda) = R_\ell[p] = \int_{0-}^\infty p(\lambda)\, d\omega_\ell(\lambda)$$

for all $p \in \Pi_{2m-2}$, it follows that R_m is at the same time the m-point Gauß-Radau rule associated with the integral (2.5). Therefore, the same argument used for (2.3) establishes the inequality

$$\overline{\phi}_\ell(\alpha) = R_\ell[\psi_\alpha] < R_m[\psi_\alpha] = \overline{\phi}_m(\alpha).$$

To prove the first inequality in (2.4) we use the fact that the ℓ-point and m-point Gauß quadrature rules $G_\ell[p]$ and $G_m[p]$ yield the same values for all $p \in \Pi_{2m-1}$, hence G_m is also the m-point Gauß quadrature rule associated with the positive definite functional G_ℓ on $\Pi_{\ell-1}$. Therefore, the argument for (2.3) can also be used to show that

$$\phi_m(\alpha) = G_m[\psi_\alpha] < G_\ell[\psi_\alpha] = \phi_\ell(\alpha).$$

This completes the proof. □

It should be pointed out that the theorem and its proof immediately extend to ill-posed linear problems, where A is an operator between two Hilbert spaces X and Y. In this case, however, ω in (2.1) is not piecewise constant but a bounded nondecreasing function.

3 Concluding remarks

We mention that the first inequality in (2.4) has been proved by Calvetti and Reichel using matrix theoretic arguments; the assumption $\varrho_\ell \sigma_{\ell+1} > 0$ which has been employed in [1, Theorem 2.5] is equivalent to our restriction that ℓ be less than r.

We also remark that the numbers $\phi_\ell(\alpha)$ and $\overline{\phi}_\ell(\alpha)$ for $\ell = 1, 2, \ldots,$ can efficiently be computed if the Lanczos process is used to bidiagonalize A and to approximate x_α from certain expanding Krylov subspaces, see [3] or [1] for the details.

The two implementations from [1, 3] only differ in the respective stopping rules for the termination of the Lanczos process. The numerical results in [1] impressively demonstrate the potential of these algorithms for large problems.

REFERENCES

1. D. Calvetti and L. Reichel, Tikhonov regularization of large linear problems, BIT, 2003, to appear.
2. T. S. Chihara, An Introduction to Orthogonal Polynomials, Gordon and Breach, New York, 1978.
3. G. H. Golub and U. von Matt, Tikhonov regularization for large scale problems, in: “Workshop on Scientific Computing”, eds. G. H. Golub, S. H. Lui, F. Luk, R. J. Plemmons, Springer, New York, 1997, pp. 3-26.
4. C. W. Groetsch, The Theory of Tikhonov Regularization for Fredholm Equations of the First Kind, Pitman, Boston, 1984.
5. V. I. Krylov, Approximate Calculation of Integrals, MacMillan, New York, 1962.