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A stopping criterion for iterative regularization methods

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ABSTRACT

We present a discrepancy-like stopping criterium for iterative regularization methods for the solution of linear discrete ill-posed problems. The presented criterium terminates the iterations of the iterative method when the residual norm of the computed solution becomes less or equal to the residual norm of a regularized Truncated Singular Value Decomposition (TSVD) solution. We present two algorithms for the automatic computation of the TSVD residual norm using the Discrete Picard Condition. The first algorithm uses the SVD coefficients while the second one uses the Fourier coefficients. In this work, we mainly focus on the Conjugate Gradient Least Squares method, but the proposed criterium can be used for terminating the iterations of any iterative regularization method. Many numerical tests on some selected one dimensional and image deblurring problems are presented and the results are compared with those obtained by state-of-the-art parameter selection rules. The numerical results show the efficiency and robustness of the proposed criterium.

1. Introduction

In this work we consider least squares problems

$$\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2, \quad \mathbf{A}\in\mathbb{R}^{m\times n}, \quad \mathbf{x}\in\mathbb{R}^n, \quad \mathbf{b}\in\mathbb{R}^m, \quad m\ge n \tag{1}$$

where the coefficient matrix $\mathbf{A}$ is ill-conditioned and derives from the discretization of a continuous ill-posed operator. The data $\mathbf{b}$ is assumed to be corrupted by measurement errors, which we will refer to as noise. In particular, we suppose that $\mathbf{b}=\mathbf{b}^{\text{exact}}+\mathbf{e}$, where $\mathbf{b}^{\text{exact}}$ is the unknown noise-free right-hand side vector and $\mathbf{e}$ is a zero-mean white noise vector. In (1) and in the sequel, $\|\cdot\|$ denotes the Euclidean norm.

Discrete ill-posed problems of the form (1) arise, for example, from the discretization of Fredholm integral equations of the first kind that are commonly used to model instrument distortions. They are often encountered in large-scale image deblurring applications, where $\mathbf{A}$ is typically the matrix representation of a convolution operator. Under periodic boundary conditions, $\mathbf{A}$ is block circulant with circulant blocks (BCCB) and matrix–vector products can be performed using FFTs [27]. This type of observation model may describe, for example, motion blur, atmospheric turbulence blur and out-of-focus blur.

Background Because of the ill-conditioning of $\mathbf{A}$, regularization techniques are necessary in order to reduce the sensitivity of the solution of (1) to the noise in $\mathbf{b}$. Iterative regularization methods are some methods of choice when the dimensions of problem (1) are large and $\mathbf{A}$ cannot be explicitly stored, but matrix–vector products involving $\mathbf{A}$ can be easily computed. Iterative methods have a semiconvergence behavior when applied to ill-posed problems and they can be used as regular-

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ization methods if suitably stopped before the noise enters the computed solution. The stopping iteration plays the role of the regularization parameter, providing a fair balance between data fidelity and solution smoothness.

For example, in image restoration problems, Krylov subspace methods are very important, as pointed out in [26] where an insightful analysis is performed. Popular iterative regularization methods are, for example, the Conjugate Gradient Least Squares (CGLS), the Preconditioned CGLS (PCGLS), the MINimal RESidual (MINRES), the Generalized Minimal Residual (GMRES) and the Range Restricted GMRES (RRGMRES) methods [16,18,31,43,10,35,32]. When nonnegativity constraints are added to the least squares problem (1), the Scaled Gradient Projection method (SGP), the Iterative Space Reconstruction Algorithm (ISRA), the Projected Landweber (PL) method or the Projected Newton (PN) method may be used as iterative regularization methods [4,11,13,5,38,39].

A wise choice of the regularization parameter is a vital issue in applying iterative regularization methods to practical applications, since the quality of the regularized solution crucially depends on this choice. The recent literature on ill-posed inverse problems shows that efficient regularization parameter selection techniques are under active research.

The famous *discrepancy principle* [41] is probably the most widely used parameter choice strategy in the context of regularization. It is an *a-posteriori* criterion choosing the regularization parameter as a function of the data and the noise norm which must be known. Unfortunately, this information may not be available in real-world applications and methods not requiring an estimate of the noise norm are actually desirable. The recent literature shows an increasing interest in *heuristic* (or *noise-level-free*) parameter choice strategies, even if the well-known Bakushinsky veto [1] states that, in Hilbert spaces, all heuristic parameter choice rules, which do not make use of the knowledge about the exact noise level, will never converge in the worst-case scenario analysis. Nevertheless, heuristic parameter selection techniques are used quite frequently in practical applications, often giving good results [46,3]. The L-curve method [40,23] and the Generalized Cross Validation method [14] are likely the most popular heuristic parameter selection strategies; they have been deeply investigated by several authors [9,34,17,53]. Some variants of the L-curve criterion have been described, e.g. the residual L-curve criterion [47,46] and the Reginska's method [45]. A number of other choice rules have been proposed in the literature, e.g. the Hanke–Raus rule [19] and the quasi-optimality criterion [52,51] which have recently received an increasing interest [2,37,36,42]. Other parameter choice techniques, called extrapolation methods [6,7], are based on suitable *a posteriori* estimates of the error norm in the solution of (1) while another method obtains estimates of the noise level from the Golub–Kahan iterative bidiagonalization [29] (this last method, referred to as quadrature method, is specific for LSQR). Several minimization rules for the selection of the regularization parameter for many iterative regularization methods as the Landweber method and the CGLS method are given in [15], both in case of known and unknown noise norm. A detailed and careful comparison of many parameter choice rules is performed in [3,46].

Other criteria for choosing the parameter of iterative regularization methods are based on the estimation of the residual norm of a regularized solution. A recent and innovative approach is illustrated in [50,49,48] where several diagnostic tools, which are statistically motivated, are presented to evaluate the suitability of a candidate regularization parameter for the Truncated Singular Value Decomposition (TSVD) and Tikhonov methods. In [50], an automatic procedure, based on the aforementioned diagnostic tools, is presented to select the regularization parameter so that the residual of the corresponding solution resembles white noise. In [25], the authors develop the so-called Normalized Cumulative Periodogram (NCP) method, an automatic procedure that chooses the regularization parameter making the residual as close as possible to white noise. The NCP method can be applied to direct regularization (TSVD and Tikhonov regularization) as well as iterative regularization and requires to calculate the NCP of the residual vector for each choice of the regularization parameter, starting from large values and stopping at the first parameter whose associated residual satisfies the Kolmogorov–Smirnov test. The methods developed in [50,49] and [25] use the Fourier coefficients to determine the regularization parameter since they all use the periodogram and the cumulative periodogram to judge if the residual resembles white noise.

Finally, even if the Singular Value Decomposition and the Discrete Picard Condition (DPC) [20,23] are well-known tools for the analysis of ill-posed inverse problems, to the best of the authors' knowledge, very little work has been done in the literature on the development of suitable parameter choice techniques using the DPC. Zama [54] has proposed a fast and efficient method based on the SVD coefficients for the computation of the regularization parameter of the TSVD and Tikhonov methods. Jones [33] has developed a method for automatically estimating the noise norm via the DPC and thus the regularization parameter for Tikhonov method.

Contribution In this work, we focus on iterative regularization methods such as, for example, Krylov subspace methods and other methods exhibiting a semiconvergence behavior [5,23]. In the sequel, therefore, the general term *iterative method* will refer to a method with the semiconvergence property.

The main purpose of this work is to propose a criterion for the selection of the stopping iteration of iterative methods. Our criterion is based on an estimate of the residual norm of a suitable regularized solution performed through the TSVD solution of (1). We present the criterion from an algorithmic point of view and we show that it is efficient on large size problems.

As pointed out in [25], almost all the parameter choice methods proposed in the literature involve some information about the norm of the residual vector of a regularized solution close to the exact one. For example, the famous discrepancy principle chooses the regularization parameter so that the residual norm is as close as possible to the noise norm, i.e. to the residual norm of the exact solution. In this work, we propose to choose the regularization parameter of iterative methods so that the residual norm of the corresponding solution is as close as possible to the residual norm of a suitable regularized