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Global Golub–Kahan bidiagonalization applied to large discrete ill-posed problems

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ABSTRACT

We consider the solution of large linear systems of equations that arise from the discretization of ill-posed problems. The matrix has a Kronecker product structure and the right-hand side is contaminated by measurement error. Problems of this kind arise, for instance, from the discretization of Fredholm integral equations of the first kind in two space-dimensions with a separable kernel and in image restoration problems. Regularization methods, such as Tikhonov regularization, have to be employed to reduce the propagation of the error in the right-hand side into the computed solution. We investigate the use of the global Golub–Kahan bidiagonalization method to reduce the given large problem to a small one. The small problem is solved by employing Tikhonov regularization. A regularization parameter determines the amount of regularization. The connection between global Golub–Kahan bidiagonalization and Gauss-type quadrature rules is exploited to inexpensively compute bounds that are useful for determining the regularization parameter by the discrepancy principle.

1. Introduction

Linear ill-posed problems arise in essentially every branch of science and engineering, including in remote sensing, computerized tomography, and image restoration. Discretization of these problems gives rise to linear systems of equations,

$$Hx = b, \quad H \in \mathbb{R}^{N\times N},\ x, b \in \mathbb{R}^N, \tag{1.1}$$

with a matrix that has many singular values of different orders of magnitude close to the origin; in particular, H may be singular. This makes the solution x of (1.1), if it exists, very sensitive to perturbations in the right-hand side b. In applications of interest to us, the vector b represents available data and is contaminated by an error $e \in \mathbb{R}^N$ that may stem from measurement and discretization errors. Therefore, straightforward solution of (1.1), generally, does not yield a useful result.

Let $\widehat{b} \in \mathbb{R}^N$ denote the unknown error-free vector associated with b, i.e.,

$$b = \widehat{b} + e. \tag{1.2}$$

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We will assume the unavailable system of equations with error-free right-hand side,

$$Hx = \widehat{b}, \tag{1.3}$$

to be consistent and denote its solution of minimal Euclidean norm by $\widehat{x}$. It is our aim to determine an accurate approximation of $\widehat{x}$ by computing an approximate solution of the available linear system of Eq. (1.1). The first step in our solution process is to replace (1.1) by a nearby problem, whose solution is less sensitive to the error e in b. This replacement is commonly referred to as regularization. One of the most popular regularization methods is due to Tikhonov [1,2]. In its simplest form, Tikhonov regularization replaces the linear system (1.1) by the minimization problem

$$\min_{x\in\mathbb{R}^N}\{\|Hx-b\|_2^2+\mu^{-1}\|x\|_2^2\}. \tag{1.4}$$

Here $\mu > 0$ is a regularization parameter and $\|\cdot\|_2$ denotes the Euclidean vector norm. We will comment on the use of μ^{-1} instead of μ in (1.4). The minimization problem (1.4) has the unique solution

$$x_\mu := (H^TH+\mu^{-1}I_N)^{-1}H^Tb \tag{1.5}$$

for any fixed $\mu > 0$. Here and throughout this paper I_N denotes the identity matrix of order N. The choice of μ affects how sensitive x_μ is to the error e in b, and how accurately x_μ approximates $\widehat{x}$. Many techniques for choosing a suitable value of μ have been analyzed and illustrated in the literature; see, e.g., [3,1,4–6] and references therein. In this paper we will use the *discrepancy principle*. It requires that a bound ε for $\|e\|_2$ be available and prescribes that $\mu > 0$ be determined so that $\|b-Hx_\mu\|_2 = \eta\varepsilon$ for a user chosen constant $\eta \geq 1$ that is independent of ε; see [1,4,6] for discussions on this parameter choice method. In the present paper, we will determine a value $\mu > 0$ such that

$$\varepsilon \leq \|b-Hx_\mu\|_2 \leq \eta\varepsilon, \tag{1.6}$$

where the constant $\eta > 1$ is independent of ε.

The computation of a μ-value such that the associated solution x_μ of (1.4) satisfies (1.6) generally requires the use of a zero-finder, see below, and typically $\|b-Hx_\mu\|_2$ has to be evaluated for several μ-values. This can be expensive when the matrix H is large. A solution method based on first reducing H to a small bidiagonal matrix with the aid of Golub–Kahan bidiagonalization (GKB) and then applying the connection between GKB and Gauss-type quadrature rules to determine an approximation of x_μ that satisfies (1.6) is discussed in [7].

It is the purpose of this paper to describe an analogous method for the situation when H is the Kronecker product of two matrices, $H_1 = [h_{i,j}^{(1)}] \in \mathbb{R}^{n\times n}$ and $H_2 \in \mathbb{R}^{m\times m}$, i.e.,

$$H = H_1 \otimes H_2 = \begin{bmatrix} h_{1,1}^{(1)}H_2 & h_{1,2}^{(1)}H_2 & \cdots & h_{1,n}^{(1)}H_2 \\ h_{2,1}^{(1)}H_2 & h_{2,2}^{(1)}H_2 & \cdots & h_{2,n}^{(1)}H_2 \\ \vdots & \vdots & & \vdots \\ h_{n,1}^{(1)}H_2 & h_{n,2}^{(1)}H_2 & \cdots & h_{n,n}^{(1)}H_2 \end{bmatrix} \in \mathbb{R}^{N\times N} \tag{1.7}$$

with $N = mn$. Then the GKB method can be replaced by the global Golub–Kahan bidiagonalization (GGKB) method described by Toutounian and Karimi [8]. The latter method replaces matrix–vector product evaluations in the GKB method by matrix–matrix operations. It is well known that matrix–matrix operations execute efficiently on many modern computers; see, e.g., Dongarra et al. [9]. Iterative methods based on the GGKB method therefore can be expected to execute efficiently on many computers. We will exploit the relation between Gauss-type quadrature rules and the GGKB method to determine a value μ and an associated approximation of the vector x_μ that satisfies (1.6). We remark that matrices H with a tensor product structure (1.7) arise in a variety of applications including when solving Fredholm integral equations of the first kind in two space-dimensions with a separable kernel, and in imaging restoration problems where the matrix H models a blurring operator. It is well known that many blurring matrices have Kronecker structure (1.7) or can be approximated well by a matrix with this structure; see [10–12].

In applications of our solution method described in Section 5 both the matrices H_1 and H_2 are square. Then H is square. This simplifies the notation and, therefore, only this situation will be considered. However, only minor modifications of the method are necessary to handle the situation when one or both of the matrices H_1 and H_2 are rectangular.

This paper continues our exploration of the application of global Krylov subspace methods to the solution of large-scale problems (1.1) with a Kronecker structure that was begun in [13]. There a scheme for computing an approximation of $\widehat{x}$ of prescribed norm is described. It was convenient to base this scheme on the global Lanczos tridiagonalization method and use its connection to Gauss-type quadrature rules. The paper focuses on the more common situation that a bound for the norm of the error e in b is available or can be estimated. Then the regularization parameter $\mu > 0$ can be determined by the discrepancy principle, i.e., so that the computed solution satisfies (1.6); see [1,4]. The requirement (1.6) on the computed solution makes it natural to apply the GGKB method to develop an analogue of the approach in [7]. Timings and counts of arithmetic floating point operations (flops) show the structure-respecting method of the present paper to require less computing time and fewer flops than the structure-ignoring method described in [7], while giving an approximate solution